2019

INVESTIGATION OF ATMOSPHERIC EFFECTS ON VAPOR INTRUSION PROCESSES USING MODELLING APPROACHES

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Digital Object Identifier: https://doi.org/10.13023/etd.2019.331

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INVESTIGATION OF ATMOSPHERIC EFFECTS ON VAPOR INTRUSION PROCESSES USING MODELLING APPROACHES

DISSERTATION

A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the College of Engineering at the University of Kentucky

By
Elham Shirazi
Lexington, Kentucky

Director: Dr. Kelly G. Pennell, Associate Professor of Civil Engineering
Lexington, Kentucky
2019
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ABSTRACT

INVESTIGATION OF ATMOSPHERIC EFFECTS ON VAPOR INTRUSION PROCESSES USING MODELLING APPROACHES

Most people in the United States (US) spend considerable amount of time indoors—about 90% of their time as compared to outdoors, which makes the US population vulnerable to adverse health effects of indoor air contaminants. Volatile organic compound (VOC) concentrations are well-known to be higher in indoor air than outdoor air. One source of VOC concentrations in indoor air that has gained considerable attention in public health and environmental regulatory communities is vapor intrusion. Vapor intrusion is the process by which subsurface vapors enter indoor spaces from contaminated soil and groundwater. It has been documented to cause indoor air contamination within hundreds of thousands of communities across the US. Vapor intrusion is well-known to be difficult to characterize because indoor air concentrations exhibit considerable temporal and spatial variability in homes throughout impacted communities. Unexplained variations in field data have not been systematically investigated using theoretical fate and transport processes. This study incorporates the use of numerical models to better understand processes that influence spatial and temporal variability in field data. The overall research hypothesis is that variability in indoor air VOC concentrations can be (partially) explained by variations in building air exchange rate (AER) and pressure differentials between indoor spaces and outdoor spaces. Neither AER nor pressure differentials are currently calculated by existing vapor intrusion numerical models. To date, most vapor intrusion models have focused on subsurface fate and transport processes; however, there is a need to understand the role of aboveground processes in the context of vapor intrusion exposure risks, which are commonly measured as indoor air VOC concentrations. Recent field studies identify these parameters as potentially important and their important role within the broader field of indoor air quality sciences has been well-documented, but more research is needed to investigate these parameters within the specific context of vapor intrusion. To test the overall hypothesis, the dissertation research developed a new vapor intrusion modeling technique that combines subsurface fate and transport modeling with building science approaches for modeling driving forces, such as wind and stack effects. The modeling results are compared with field data measurements from actual vapor intrusion sites and confirms that the research is relevant to not only academic researchers, but also policy decision makers.

KEYWORDS: Vapor Intrusion, Wind and Stack Effects, Indoor Air Contamination, Air Exchange Rate, Indoor-outdoor Pressure Difference

Elham Shirazi

7/15/2019
INVESTIGATION OF ATMOSPHERIC EFFECTS ON VAPOR INTRUSION PROCESSES USING MODELLING APPROACHES

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7/15/2019
Date
To my Mom and Mother in-law

In loving memory of my Father and Father in-law
ACKNOWLEDGMENTS

First and foremost, I would like to express my deepest thanks to my advisor, Dr. Kelly Pennell, who has always been supportive, helpful, and motivating to me. I have received really great assistance from her on all aspects of this dissertation and my PhD studies. Without her guidance this dissertation and my completion of the program would have not been possible.

Next, I am grateful to the members of my PhD committee, Dr. Lindell Ormsbee, Dr. Yi-Tin Wang and Dr. Donald Colliver, for their great advice and guidance on my research during these years. I need to thank Dr. Aaron Cramer for accepting to serve as the outside examiner on my PhD dissertation. I am also thankful for the technical assistance of Dr. Paul Dahlen at Arizona State University for access to and background information related to the study house in Layton, UT.

I would like to thank my colleagues and friends, Rivka Reichman, Amir Roghani, Evan Willett and Sweta Ojha, who helped me a lot during these years. I have had a wonderful group of friends inside and outside of the university that have reminded me to have fun, have cheered me on, and made our move to the United Sates much sweeter. I specially want to thank my friends in the department, Atena Amirsoleimani and Erika Hernandez, who have been there for me continually over these years.

I am truly grateful to my mom, my lovely sister, Mitra, my mother in-law who are thousands of miles away and have sacrificed so very much during these years for me and my husband. Their love and encouragement has been helping me go through all situations and successfully complete my doctoral study. I would like to thank my brother, Reza, and
sisters, Maryam and Sara, here in the United States for their immeasurable love, care, and support, and for keeping me motivated throughout this dissertation. Last but not least, I am truly grateful to my husband, Iman, who thinks I can do anything, who keeps me sane, makes me laugh, and loves me dearly.

This study is supported by a CAREER Award from the National Science Foundation (Award #1452800) and by Grant Number P42ES007380 (University of Kentucky Superfund Research Program) from the National Institute of Environmental Health Sciences. The content is solely the responsibility of the author and does not necessarily represent the official views of the National Institute of Environmental Health Sciences, the National Institutes of Health or the National Science Foundation.
# TABLE OF CONTENTS

## Contents

ACKNOWLEDGMENTS ........................................................................................................ iii

LIST OF TABLES ............................................................................................................ ix

LIST OF FIGURES .......................................................................................................... x

CHAPTER 1: INTRODUCTION ....................................................................................... 1

1.1. Research objectives ............................................................................................. 2

1.2. Dissertation organization .................................................................................... 5

CHAPTER 2: BACKGROUND ......................................................................................... 7

2.1. Overview of the Vapor Intrusion Process ........................................................... 7

2.2. Stack effect ........................................................................................................ 15

2.3. Wind effect ........................................................................................................ 17

CHAPTER 3: AER VALUES USED BY VI REGULATORS AND PRACTITIONERS IN VI STUDIES COMPARED TO AER VALUES REPORTED BY BUILDING SCIENCE (Published Article) ............................................................................................................ 19

3.1. Abstract ............................................................................................................. 19

3.2. Introduction ....................................................................................................... 20

3.3. Background ....................................................................................................... 22

3.3.1. VI Conceptual Model ................................................................................... 22

3.3.2. Current VI Site-specific Exposure Risk Assessment Approach .............. 22
5.1. Abstract ............................................................................................................. 75

5.2. Introduction ....................................................................................................... 76

5.3. Theory and Methods ......................................................................................... 79

5.3.1. Background ................................................................................................... 80

5.3.2. Model Methods ........................................................................................... 82

5.3.3. COMSOL Multiphysics ........................................................................... 91

5.3.4. CONTAM coupled with CFD0 ............................................................... 92

5.4. Results and Discussion ..................................................................................... 96

5.4.1. Indoor air pressure and AER................................................................. 96

5.4.2. Pressure and concentration profiles ..................................................... 99

5.4.3. Indoor air concentration ................................................................. 101

5.5. Special considerations and limitations ............................................................ 105

5.5.1. Comparison with Previous Modeling Studies................................. 105

5.5.2. Wind Effects and Paved Ground Surface ............................................. 107

5.5.3. Comparison with Field Data ............................................................. 108

5.5.4. Steady State Limitations of the Current Study ................................. 109

5.6. Conclusions ..................................................................................................... 110

5.7. Supplement Information: Qualitative Model Comparison with Field Data .. 111
LIST OF TABLES

Table 3-1: Typical Residential AER values reported in VI studies. ................................. 27
Table 3-2: Summary of database sources for AER distribution. ................................. 38
Table 3-3: Typical Residential AER distribution studies. ................................. 39
Table 4-1: Advantages and disadvantages of models used in vapor intrusion and building
science............................................................................................................................... 70
Table 4-2: Values calculated in previous vapor intrusion models compared to values
calculated in vapor intrusion model linked to CFD0-CONTAM programs .............. 73
Table 5-1: Effective air leakage areas used in this study (best estimate values in (ASHRAE
2001) ................................................................................................................................. 94
Table 5-2: Summary of Model Results ....................................................................... 102
Table 5-3: Comparison of Model Results for Select Cases ................................. 105
Table 6-1: List of inputs related to study house used in CONTAM ....................... 122
Table 6-2: Information related to zones....................................................................... 123
Table 6-3: Information related to openings (Continue next page)......................... 124
Table 6-4: Effective leakage area corresponding to openings in study house (best estimate
values suggested in ASHRAE Handbook of Fundamentals, 2001)...................... 127
Table 6-5: Mass entry rate (g/d) values used as input in models......................... 129
LIST OF FIGURES

Figure 2-1: Conceptual model of vapor intrusion process .................................................. 8

Figure 2-2: Air Exchange Rate Description ...................................................................... 10

Figure 3-1: Distribution of inside and outside pressures (green arrows) over height of a building, and airflow directions (blue arrows) for; (A) Stack effect only for case where inside air is warmer than outside air (winter) and NPL is at the mid-height, (B) Wind effect only, and (C) Wind and stack effects combined. For simplicity of illustration pressure differences due to the wind and stack effect have the same magnitude, which is rare in reality. Adapted from ASHRAE Handbook – Fundamentals (ASHRAE 2013) .............. 32

Figure 3-2: Characteristic examples of residential AER distribution curves. ............... 40

Figure 3-3: AER effect on $C_{\text{indoor}}/C_{\text{source}}$ distribution curves for Detroit test case. ........ 44

Figure 3-4: Combined effect of AER distribution and geology on $C_{\text{indoor}}/C_{\text{source}}$ in comparison to USEPA VI database range (shaded area). Error bar present maximum and minimum values ............................................................................................................... 46

Figure 3-5: AER distribution that considers important building features within four geographic areas. The error bar show maximum and minimum values. ......................... 47

Figure 3-6: USEPA VI database groundwater attenuation factor ($C_{\text{indoor}}/C_{\text{source}}$) distribution (5th to 95th percentile) for a filter of groundwater VOCs 1000 times greater than background VOCs ................................................................................................................................. 47

Figure 3-7: A comparison of AER distribution curves measured with the PFT method (Isaacs et al. 2013) and the air leakage method (Chan et al. 2005). ....................... 53

Figure 4-1: Advantages (pros) and disadvantages (cons) of various building simulation tools .................................................................................................................................. 67
Figure 4-2: Combination of vapor intrusion models, CFD and multizone indoor air quality programs to predict indoor air quality impacted by vapor intrusion sites. ...................... 71

Figure 5-1: Overview of modeling process ................................................................................................................................. 85

Figure 5-2: a) 1st floor plan view and wind directions blew on building b) elevation of the modeled building ................................................................................................................ 93

Figure 5-3: Average daily wind speed in Lexington, KY (1 Jan-31 Dec, 2014). Weather Underground (Accessed June 2019) .......................................................................................................... 95

Figure 5-4: Wind and Stack Effect on Building AER (a) and Basement Pressure (b) ..... 98

Figure 5-5: a) Pressure profile in air and soil domains, with 10 m/s wind flow (a-1) and without wind flow (a-2), b) Normalized concentration profile in air and soil, without wind flow (b-1) and with 10 m/s wind flow (b-2) ........................................................................... 100

Figure 5-6: a) The mass entry rate of contaminant through the crack vs. basement pressure, b) Normalized contaminant concentration in first floor vs. AER and c) Normalized contaminant concentration in basement vs. AER ........................................................................ 104

Figure 5-7: (a) Wind rose and (b) time-averaged subslab soil-gas pressure relative to indoor air (ΔP_{soil-indoor}) (Luo et al. 2009) ...................................................................................................................... 112

Figure 5-8: Pressure difference in present study for a 5 m/s wind speed in soil 0.6 m underground surface (indoor pressure equals to -3.2 Pa) ......................................................... 113

Figure 5-9: O₂ and TPH soil gas distribution at 1.2 m below ground surface (Luo et al. 2009) .................................................................................................................................................. 114

Figure 5-10: Normalized TCE concentration 2m below and around building foundation when 10m/s wind is blowing on west side of the building.............................................. 115

Figure 6-1: Front yard (a) and backyard (b) of study house. ........................................... 119
Figure 6-2: Floor plan of study house showing first and second floor. ......................... 120
Figure 6-3: Modeling process by coupled CFD0 and CONTAM for the study house ... 121
Figure 6-4: Zones and opening numbers related to Table 6-2 and Table 6-3 (openings
shown in figures but not numbered are the openings considered for external walls)..... 126
Figure 6-5: Pressure profile view from west side, 10 m/s is blowing from north side... 129
Figure 6-6: Pressure coefficient (Cp) estimated by CFD0 for opening number 11 in Figure
6-4 (each opening has a specific Cp profile, opening 11 is chosen as an example)....... 130
Figure 6-7: Modeled air exchange rates under different wind speeds, wind directions and
outdoor air temperatures ................................................................................................................................. 131
Figure 6-8: AER vs time (a) and (b) AER vs seasons: Modeled (Box and Whisker) and
Measured (Shaded) ................................................................................................................................. 133
Figure 6-9: Indoor Air TCE Concentrations versus time (a) and versus seasons (b): .... 134
Figure 6-10: Indoor pressure variation caused by different weather conditions in study
house ......................................................................................................................................................... 135
CHAPTER 1: INTRODUCTION

Volatile organic compound (VOCs) concentrations in indoor environments can exist at higher concentrations than in outdoor environments (Adgate et al. 2004, Dodson et al. 2009). The presence of higher VOC concentrations in indoor areas compared to outdoor areas is due to two reasons: 1) indoor sources of VOCs are present in consumer products, such as solvents, paints, household cleaners, oils, air fresheners, fuels, etc.; and 2) can enter indoor space due to vapor intrusion (VI), which is the migration of VOCs from either contaminated soil or groundwater through soil into overlying buildings (USEPA 2015).

VI is a potential health risk at thousands of contaminated sites. Most people in the United States (US) spend considerable amounts of their time indoors. Children and the elderly spend even more time indoors and are most vulnerable to the effects of indoor air contaminants (Klepeis et al. 2001). The US Environmental Protection Agency (USEPA) lists 107 compounds whose toxicity and volatility produce a potentially unacceptable inhalation risk to receptors (USEPA 2002). VOCs are often divided into two wide classifications: chlorinated VOCs (CVOCs) and petroleum hydrocarbon VOCs. CVOCs can persist for decades in the environment and are among the most frequently detected contaminants and their remediation is difficult (Tillman and Weaver 2005), while petroleum hydrocarbon VOCs are known to readily degrade in aerobic environments (USEPA 2015).

Tetrachloroethene (PCE) and trichloroethene (TCE) are two well-known CVOCs and have both short-term and long-term impacts on human health. Short-term exposure to CVOCs has been linked to irritations such as nausea, vomiting, and chest pain; long-term
exposure may cause cancer, asthma, kidney and liver disease and reproductive problems, such as pregnancy loss, fetal growth restrictions, abnormalities and low birth weights (Doyle et al. 1997, Beliles 2002, Aschengrau et al. 2009, Makris et al. 2016). Due to the potential for VI to result in human exposure at buildings located above or near VOC-contaminated groundwater or soil, many research studies have been conducted since 1990s (e.g. Moseley and Meyer 1992, McDonald and Wertz 2007, McHugh et al. 2007, Holton et al. 2013, Erdogan and Hsieh 2014, Johnston and Gibson 2014, Holton et al. 2015).

Considering human health effects of VOCs, it is important to understand the physical, chemical, and biological processes that affect vapors to move through the soil from a subsurface source to a building foundation, and then through foundation cracks into the indoor air. The transport is complex and depends on several factors, such as presence and concentration of the pollutants, distance to the contamination source, direction of groundwater flow, spatial variations in geology and soil type, depth to groundwater below foundation, type of foundation, pressure difference between indoor and outdoor and occupant behavior. Some studies suggest using models to estimate contaminant concentration in soil and indoor air. Existing models that incorporate these factors still lack enough accuracy in predicting the contaminant transport and indoor air concentrations observed at contaminated sites (Hers et al. 2002, Hers et al. 2003, Johnson 2005, Tillman and Weaver 2006, Bozkurt et al. 2009). One significant challenge has been the temporal and spatial variability of indoor air VOC concentrations observed at VI sites.

1.1. Research objectives

The overall research hypothesis was that variability in indoor air VOC concentrations can be (partially) explained by variations in building air exchange rate (AER) and pressure
differentials between indoor spaces and outdoor spaces. To test the overall hypothesis, the dissertation research developed a new vapor intrusion modeling technique that combines subsurface fate and transport modeling with building science approaches for modeling driving forces, such as wind and stack effects. Three research objectives were completed.

Research Objective 1 establishes connections between the disparate fields of subsurface vapor intrusion and building (and/or indoor air quality) science. The main goal of this objective is to show a body of literature and tools exist within the building science field that has not been incorporated into VI science. For instance, AERs commonly referenced by the VI community are not representative of the wider range of AER values reported within the indoor air quality literature. A tutorial review in a peer-reviewed journal (*Environmental Science Processes and Impacts*) by Reichman, Shirazi et al., 2017 discusses previously omitted connections between VI fate and transport processes and indoor air quality research. A mini-review “in press” in a peer-reviewed journal (*Reviews on Environmental Health*) by Shirazi et al. 2019 discusses available building science modeling tools to investigate wind and stack effects on indoor air VOC concentrations.

Research Objective 2 develops a new model to combine three different domains: the atmospheric domain (outdoor aboveground), indoor domain, and subsurface domain. This new model incorporates three software packages: COMSOL Multiphysics computational fluid dynamics (CFD) model, CONTAM multi-zone model, and CFD0. It models subsurface vapor VOC transport, as well as wind flow above and around a building, and stack effects. The results show: 1) the distribution of VOCs in the subsurface are not significantly impacted by wind and stack effects (under most relevant conditions); and 2)
indoor air pressures influence the indoor air VOC concentration by altering AERs. The AERs are influenced by building characteristics, wind directions/speeds and stack effects. This is the first vapor intrusion modeling approach that fully-resolves all three domains (atmosphere-subsurface-indoor). Shirazi and Pennell (2017) published a peer-reviewed article in a journal (Environmental Science Processes and Impacts) that describes the modeling approach.

Research Objective 3 verifies the new modeling approach using field data that were previously collected by others. The results indicate that AER and indoor air VOC concentrations calculated by the model and measured in the field agree well. In addition, the outcome of this objective provides implications for improving VI exposure risk assessments using this new modeling approach as a tool. Shirazi and Pennell (2019) are preparing a new manuscript for submission to a peer-reviewed journal that summarizes the model verification and implications of wind and stack effects on indoor air VOC concentration variability (see Chapter 6).

Overall contribution: Indoor air contamination caused by VI is difficult to characterize because indoor air concentrations of VOCs vary temporally and spatially in homes throughout impacted communities. There are many explanations for indoor air concentration variability, one of them that has gained a recent interest is AER. The driving force of AER is pressure differential between indoor and outdoor which is the driving force for convective transport of contaminant into the building through foundation cracks, as well. In this study, research objective 1 develops contextual framing to emphasize the potential importance of AERs when evaluating VI exposure risks. The modeling approach developed in research objective 2 tests the hypothesis in this research and helps decision
makers to better understand the effect of weather condition and building characteristics in VOC concentration variability. Research objective 3 compares the measured data of VOC indoor air concentration and AER in a house with modeling results of these values. The agreement observed between the field data and model results suggests that the modeling approach presented here may be a useful tool for decision makers as they continue to assess complex and variable processes that influence exposure risks at hundreds of thousands of vapor intrusion sites across the United States, and countless more worldwide.

1.2. Dissertation organization

Chapter 1: This chapter provides a brief overview of the dissertation.

Chapter 2: This chapter provides general information about the effect of different factors (such as soil properties, source depth, foundation type and surrounding caps) on VOC VI. This chapter also provides information related to estimation of AER and two lesser studied factors; wind and stack effects.

Chapter 3: This chapter addresses Research Objective 1 by reviewing building science (and indoor air science) concepts that are relevant for vapor intrusion studies. It includes an article that is published in the Environmental Science Processes & Impacts journal (R. Reichman, E. Shirazi, D. G. Colliver and K. G. Pennell, 2017). “US residential building air exchange rates: new perspectives to improve decision making at vapor intrusion sites.” DOI: 10.1039/c6em00504g)

Chapter 4: This chapter also addresses Research Objective 1. It summarizes multizone indoor air quality models and recommends their use as tools in VI risk assessment. Most of this chapter is an “in press” article and accepted in Reviews on Environmental Health

**Chapter 5:** This chapter addresses Research Objective 2 by describing the details of a new VI modeling approach. This chapter includes an article that is published in the Environmental Science Processes & Impacts journal (E. Shirazi and K. G. Pennell, 2017). “Three-dimensional vapor intrusion modeling approach that combines wind and stack effects on indoor, atmospheric, and subsurface domains.”

**Chapter 6:** This chapter addresses Research Objective 3. Modeling approaches introduced in chapter 4 and developed in chapter 5 are used to predict AERs and indoor air VOC concentrations. The modeled data are compared with existing field data from VI sites to verify the modeling approaches. Most of the chapter includes a manuscript that is “in-preparation” for submission to a peer-reviewed journal.

**Chapter 7:** This chapter summarizes the main findings of this study and describes limitations for this research and offers suggestions for future studies to improve vapor intrusion risk assessment.
CHAPTER 2: BACKGROUND

This chapter summarizes existing literature to provide context for the scientific contributions of this research, which build from previously published research to include lesser studied factors that affect vapor intrusion (VI). These factors include atmospheric effects, such as outdoor temperature, wind; and building specific features that influence building air exchange rate (AER). Atmospheric conditions and building characteristics play an important role in changing AER and pressure difference between indoor and outdoor which are important explanations of indoor air concentration variability in vapor intrusion process.

2.1. Overview of the Vapor Intrusion Process

Groundwater plumes or soils contaminated by volatile organic compounds (VOCs) under or near buildings may be a source of indoor air contamination. In the VI process, VOCs volatilize and can be transported through the subsurface into overlying buildings. Figure 2.1 shows a simplified conceptual model of VI process.
If the vapor source is groundwater, the contaminant partitions from groundwater to soils gas. Vapor partitioning depends on the chemical, its Henry constant, and the groundwater temperature. The the layer of saturated soil directly above groundwater table is the capillary zone than this layer can play an important role in attenuating VOCs concentration by decreasing vapor diffusion due to high moisture content in this area. The vadose zone can have a variable moisture content and extends from the top of the capillary zone to ground surface.

Molecular diffusion and con- (ad-)vection are two important mechanisms of VI into the buildings. Diffusion in the subsurface occurs due to the concentration gradient that
exists between contamination source and ground surface, which causes contaminants to move from locations where higher concentrations of VOCs exist to locations where lower VOC concentrations exist. Convection is caused by pressure differentials between result in soil gas movement. Mechanical ventilation, temperature gradients and wind flow can create pressure differentials between the indoor air and the subslab.

The transport of VOCs vapors near the groundwater table to indoor air spaces can be complex and depends on several factors such as the distance to the contamination source, direction of groundwater flow, spatial variations in geology and soil type, depth to groundwater below foundation, type of foundation, pressure difference between indoor and outdoor and occupant behavior. In the subsurface, the dominant process for mass transport into the building is typically diffusion, but near the building foundation (<2m per (Bozkurt et al. 2009), both diffusion and advection processes may be important (Johnson 2002, Johnson 2005). The pressure gradient creates a soil gas flow which transports the contaminant inside the building through the foundation cracks (Olson and Corsi 2001). Once inside, the contaminant can be diluted due to mechanical ventilation, infiltration and other building processes that affect the AER. Ultimately, the indoor air concentration ($C_{\text{indoor}}$, mg/m$^3$) is a function of the mass entry rate of contaminant into the building and the AER (hr$^{-1}$) (see Equation 2.1). Importantly, the pressure difference between the indoor and outdoor air (which is a focus of this dissertation research) impacts both the numerator and the denominator of Equation 2.1.

$$C_{\text{indoor}} = \frac{M_{\text{ER}}}{AER \times V_B}$$ (2.1)
Where $M_{ER}$ (mg/hr) is the mass entry rate of contaminant into the building and $V_B$ (m$^3$) is the volume of the building. AER is the rate at which the whole house volume air exchanges with the outdoor air. When the time unit is hours, AER is referred to as air changes per hour (ACH, hr$^{-1}$). AER is the combination of two processes: infiltration/exfiltration and ventilation (Figure 2.2).

![Image: Air Exchange Rate Description](image)

**Figure 2-2: Air Exchange Rate Description**

Infiltration and exfiltration refer to uncontrolled outdoor air flow through unintentional openings in the building envelope, that is, leaks. These leaks include the cracks and penetrations that exist in all buildings, including those that are of importance for VI. In residential buildings, many common leak locations have been established as major sources of infiltration, including: the main envelope area; wall, roof and floor junctions; doors and windows; penetrations through the envelope, including electrical components, as well as chimneys, wood burning stoves, etc (ASHRAE 2013). Ventilation includes natural ventilation and mechanical ventilation; and can be highly variable.
depending on a range of factors (ASHRAE 2013) including occupant behavior in buildings. Natural ventilation is outdoor airflow through intentional openings such as open windows, and is driven by weather condition. Mechanical ventilation is airflow induced by powered equipment. A detailed description of AER and driving forces that induce AER is provided in Chapter 3.

Existing research suggest that the relationship between contaminant concentration in indoor air and groundwater depends on source concentration, soil type, contaminant source depth and lateral distance, foundation type, meteorological conditions, and household characteristics (USEPA 2012). Previous studies showed that single factors are not adequate substitutes for accessing VI exposure potential. For instance, spatial and temporal variability in soil, and building characteristics can lead to a higher concentration of vapor contaminant concentration in indoors above low-concentration sources than homes above higher concentration sources (Fitzpatrick and Fitzgerald 2002, McHugh et al. 2003, Folkes et al. 2009, Johnston and Gibson 2014).

The soil matrix properties (e.g., porosity, layers, permeability and moisture content) influences vapor transport from a contaminant source to overlying building (Hers et al. 2002, Tillman and Weaver 2006, Pennell et al. 2009, Bekele et al. 2014). Tillman and Weaver (2006) indicated that for different source depth (20m, 9m and 4.75m below grade), moisture content for the clay and sandy loam soil plays an important role in vapor intrusion. They also showed that the moisture content is more important in soils with smaller grain size and lower porosity. As the moisture content increases, the subsurface concentration decreases. Depth to contamination source affects cancer risk in their study, which means by increasing the contamination source the cancer risk decreases (Tillman and Weaver
Bekele et al. (2014) reported that assessment for VI is greatly influenced by subsurface soil properties such as temperature and moisture that fluctuate with the seasons of the year. The study showed the lowest subsurface concentration of VOC in wet seasons (winter) in which moisture content is high and the soil pore space outside the footprint of the building will be occupied by infiltrating soil-water. They claimed this phenomena can cause soil-gas vapor to result in higher concentrations near the foundation slab and lead to higher concentrations of VOCs in indoor area due to stack effect in winter (Bekele et al. 2014).

Pennell et al. (2016) compared VI model results with field data in a community in a Metro-Boston neighborhood to investigate the importance of subsurface features on VOC vapor intrusion. Indoor air concentrations in three different buildings were lower than the expected concentration based on groundwater concentrations. Comparing model results and field data, they highlighted that the presence of a soil layer with high moisture content can be the reason of steep gradient between groundwater concentration and soil gas concentration above the groundwater table. Bozkurt et al. (2009) indicated that soil layers with lower permeability and diffusivity limit VI rates into the building. Furthermore, increasing the moisture content in the subsurface creates a soil-water interface that decreases vapor transport rates (Bozkurt et al. 2009). Soil grain size, which influence on porosity and permeability of soil, controls the contaminant vapor distribution profile which consequently affect vapor concentration in indoors. Very coarse-grained soil is associated with an increase in the vapor concentration in indoors comparing to fine-grained soils (Johnston and Gibson 2013).
Previous studies have shown that in sites with homogeneous soil, as the distance (lateral or vertical) between the building and the contaminant source increases, the soil gas and indoor air concentrations of VOCs decreases (Lowell and Eklund 2004, Abreu and Johnson 2005, Tillman and Weaver 2006, Yao et al. 2011, Johnston and Gibson 2013, Yao et al. 2013). Tillman and Weaver (2006) indicated that the concentration of VOCs in subsurface and health risk decrease when the depth of contaminant source increase (Tillman and Weaver 2006). Lowell and Eklund (2004) showed that soil-gas concentration and emission flux are both a decreasing exponential function of the lateral distance from the edge of the contaminant plume. Their results showed the emission flux and the soil-gas concentration are insignificant within a relatively short lateral distance from the source (e.g., 30 m) and suggested to ignore the risk health from breathing contaminated indoor air for buildings with long lateral distance to the contaminant plume (Lowell and Eklund 2004).

Johnston and Gibson (2013) found a negative nonlinear relationship between attenuation in subsurface and the distance between the structure and the source which was statistically significant. They showed changes in source depth may contribute up to 1 order of magnitude difference in attenuation. They used a multiple regression analysis approach and showed that the relationship between groundwater depth and the attenuation factor is mediated by soil type, which means the interaction between soil type and groundwater depth is significant. For example, shallow groundwater (less than 3m below ground level) coupled with coarse or very coarse soil type puts a site at risk for higher-than-expected attenuation factors (Johnston and Gibson 2013). Abreu and Johnson (2005) reported that VOCs concentration in indoors decrease with increasing vapor source-building lateral
separation. They also showed that the decrease in indoor air concentration with increasing lateral separation is greater for shallower source depths. For example, changes in source depth (from 8m to 3m) may contribute up to 3 order of magnitude decrease in attenuation of vapors from soil to indoors for 20m of lateral distance (Abreu and Johnson 2005).

Foundation type and the surrounding soil surface caps are another potentially important factor that may affect vapor intrusion entry rates into buildings. Yao et al. (2011) investigated the influence of building/foundation and capping near foundation on soil gas contaminant concentration profiles around a building. The study showed that in the presence of paved surroundings, contaminant concentration at the crack is twice as high for a building with 2m deep foundation, and five times as high for a building with 0.1m deep foundation, as compared to a building without surrounding cap. Capping surrounding a structure has a more significant impact on contaminant entry rates for slab on grade than for cases with 2m deep foundation (Yao et al. 2011). Johnston and Gibson (2013) reported that homes with crawl space foundations were associated with more attenuation, while those with slab-on-grade foundations were associated with less attenuation when compared to homes with basements. They used a multiple regression analysis approach and indicated that slab foundation and very coarse soil type are associated with the highest attenuation factors; at shallow groundwater levels, homes with these characteristics are predicted to experience much more vapor intrusion than the current generic attenuation factor in EPA (0.001) (Johnston and Gibson 2013).

The factors mentioned above focus on subsurface features and are frequently studied in the VI community. The following sections discuss some lesser studied factors such as stack and wind effects.
2.2. Stack effect

Temperature differences between indoor spaces and outdoor environments create pressure differences that drive airflows across the airflow paths of the building envelope. When the indoor air is warmer and less dense in a building, air starts raising toward the upper floors and eventually leaks out via the roof; this draws air up from the basement, and in turn, the basement finds its replacement air from the soil gas through foundation cracks. In addition, temperature difference between indoors and outdoors cause air leakage through the airflow paths at different levels on building envelope which creates pressure differential between indoor and outdoor and also change the AER in buildings. This common phenomenon is called the stack effect which reduces the pressure in the lower parts of the building and causes gas to be pulled upwards, including soil gases, which enter into basements through cracks due to the pressure gradient (USEPA 2008).

Previous research has shown that seasonal temporal variability of VI exposure risks in southern climates may differ from those in northern climates. In studies in northern climates, in homes with basements, higher concentrations of CVOCs have been observed in winter compared with other seasons (Fitzpatrick and Fitzgerald 2002, Holton et al. 2012). While Johnston and Gibson (2014) observed an inverse relationship in the hot and arid San Antonio, TX climate, and justified it by the tighter sealing of homes during the summer months (to keep out the heat) (Johnston and Gibson 2014). Du et al. (2015) showed that AERs in residential buildings with basements had strong and opposite seasonal trends than a multistory building. For example, AERs were highest in the upper-level living spaces during the summer, and highest in basements during the winter. Airflows from
basements to occupied spaces also varied seasonally (Du et al. 2015). Dodson et al. (2007) indicated that airflows from basements to occupied zones significantly increased in winter (average of 174 m$^3$/h) compared with summer (67 m$^3$/h) (Dodson et al. 2007). Johnston and Gibson (2013) showed that seasonal effects depend on foundation type. For homes with basements, VI exposure risks in the winter was determined to be significantly higher than in summer. However, for crawl-space homes, the seasonal effect was opposite, with significantly higher intrusion attenuation factors in summer than in winter (Johnston and Gibson 2013). Some other studies indicated that in homes with basements in the northern United States have found higher concentrations of indoor CVOCs in the winter compared to other seasons (Fitzpatrick and Fitzgerald 2002, McHugh et al. 2007, Holton et al. 2012). In vapor intrusion studies, it is hypothesized that the differential pressure gradients across the foundation increases during the heating season, as a result of indoor-outdoor temperature differences, increasing the vapor flow rate into the home (Nazaroff et al. 1987). Stack effect is also important in changing AER value in buildings which is an important factor that affects contaminant indoor air concentration; therefore, understanding how pressures differentials and AER change by indoor-outdoor temperature difference is important.

These results include different types of studies with different levels of controls. It is difficult to draw conclusions across the studies, other than to note that temporal variability is widely acknowledged to exist in AERs. These studies note that importance of seasonal effect/outdoor temperature effect on VI exposure risks and warrants additional investigation.
2.3. Wind effect

Wind flow above and around a building can affect the pressure distribution in outdoor air, on the ground surface around the building, in subsurface under the building and on the building envelope. The outdoor air pressure in windward side is higher than air pressure on the leeward side. Song et al. (2013) suggest that these pressure differences cause air to leak in on the building’s windward side and leaks out on the leeward side.

A previous study of the intrusion of VOCs into a building in Australia indicated that decreases in barometric pressure caused a negative pressure differential between the building interior and subslab, increasing the rate of convective mass transfer of VOCs into the indoor air (Patterson and Davis 2009). Johnston and Gibson also showed that an ambient pressure drop may increase the mass of VOC leaking into the home (Johnston and Gibson 2014).

Changes in wind and temperature fluctuations all can influence indoor–outdoor pressure distribution profile and hence vapor flow into homes (Garbesi and Sextro 1989, Adomait and Fugler 1997, McHugh et al. 2012). When these processes lead to negative building pressure (i.e., outdoor pressure greater than indoor pressure), the rate of mass entry into building increases. However, the interrelationships among these factors are complex, and the net effects on VI exposure risks are difficult to predict (Nazaroff and Doyle 1985, Luo 2009), the AER can be highly variable between houses depending upon heating/cooling systems, opening of windows, and the energy efficiency of a building. A better understanding of the drivers of temporal and spatial variability in VI can inform decisions regarding monitoring and exposure assessment in affected communities. Screening level models are now commonly used to estimate VI for subsurface VOCs;
however these models do not incorporate atmospheric effects (e.g. (USEPA 2004, USEPA 2017)).
CHAPTER 3: AER VALUES USED BY VI REGULATORS AND PRACTITIONERS IN VI STUDIES COMPARED TO AER VALUES REPORTED BY BUILDING SCIENCE (Published Article)


(DOI: 10.1039/c6em00504g)

This article draws connections between the well-established yet disparate fields of subsurface vapor intrusion (VI) and building air exchange rate (AER) studies. The main purpose of this study is to increase awareness within the VI scientific community about the potential importance of AERs when evaluating VI exposure risks. We show that AERs commonly referenced by the VI community are not representative of the wider range of AER values reported within the indoor air science literature. The atmospheric effects discussed in Chapter 2 are widely acknowledged in the indoor air science literature; however these effects have not been routinely incorporated into decision making at VI sites. A summary of recent AER values from the indoor air science literature are summarized and implications for VI exposure risk assessment are discussed in this published article.

3.1. Abstract

Vapor intrusion (VI) is well-known to be difficult to characterize because indoor air concentrations exhibit considerable temporal and spatial variability in homes
throughout impacted communities. To overcome this and other limitations, most VI science has focused on subsurface processes; however there is a need to understand the role of aboveground processes, especially building operation, in the context of VI exposure risks. This tutorial review focuses on building air exchange rates (AERs) and provides a review of literature related building AERs to inform decision making at VI sites. Commonly referenced AER values used by VI regulators and practitioners do not account for the variability in AER values that have been published in indoor air quality studies. The information presented herein highlights that seasonal differences, short-term weather conditions, home age and air conditioning status, which are well known to influence AERs, are also likely to influence indoor air concentrations at VI sites. Results of a 3D VI model in combination with relevant AER values reveal that indoor air concentrations can vary more than one order of magnitude due to air conditioning status and one order of magnitude due to house age. Collectively, the data presented strongly support the need to consider AERs when making decisions at VI sites.

3.2. Introduction

Vapor intrusion (VI) involves indoor air contamination resulting from the migration of volatile organic compounds (VOCs) from contaminated groundwater and soil into overlying buildings, and can pose health risks to building occupants. Measuring indoor air concentrations to evaluate VI exposure risks is complicated by many factors, including temporal variations in VOC concentrations, multiple chemical sources (some of which are not related to VI), as well as changes in building operation, among others. One of the most challenging aspects of collecting indoor air data is related to spatial and temporal variability of VOC concentrations (Holton et al. 2013, Johnston and Gibson 2014, USEPA 2015), and
there is a lack of definitive guidance for indoor air sampling strategies that effectively
address this variability (Holton et al. 2013).

Amidst the variability in indoor air concentration, VI site investigations often focus
on the collection and analysis of subsurface samples along with indoor air data, and, in
some cases VI modeling, as part of a multiple lines of evidence approach to evaluate the
potential for VI exposure risks (e.g. Pennell et al. 2016). Recently, the importance of
building operation has gained recognition within the VI community (Mosley 2007, Luo
2015, Schumacher and Zimmerman 2015, Dawson 2016, Shen and Suuberg 2016,
Reichman et al. 2017). Newer approaches for characterizing VI exposure risks have begun
focusing on building operation (e.g. McHugh et al. 2012, Guo et al. 2015, Dawson 2016);
however, the United States (US) federal and state regulatory documents (e.g. USEPA 2015)
lack well-defined guidance about how to incorporate building operation into site-specific
investigations.

The goal of this tutorial review paper is to connect the field of VI characterization
with the established field of indoor air quality research related to building air exchange
rates (AERs). AERs are widely acknowledged throughout the indoor air literature as an
important parameter controlling indoor air quality (Koontz and Rector 1995, Murray and
Here, we provide information for the VI community about the importance of considering the
role of building AERs when evaluating VI exposure risks.
3.3. Background

3.3.1. VI Conceptual Model

VOC migration from contaminated groundwater and soil into overlying buildings includes three main processes: 1) vapor transport through soil from a chemical source; 2) VOC vapor entry into building; and, 3) dilution/dispersion within the building. Vapor transport through the soil is predominantly governed by vapor diffusion and is determined by the properties of contaminant and the soil. Vapor entry into the building occurs by combination of diffusion and convective transport mechanisms. The convective transport is driven by the pressure difference between the inside of the building and the outside of the building. This pressure difference, known as the driving force for vapor entry, is caused by a combination of the stack effect (which occurs due to air density gradient due to the temperature difference between the outside and inside of the building), wind effects, and building ventilation processes. Once soil vapors enter the building, it undergoes a mixing that is influenced by the AER. A detailed description of VI conceptual model is provided in 2015 USEPA VI guidance (USEPA 2015).

3.3.2. Current VI Site-specific Exposure Risk Assessment Approach

USEPA (USEPA 2015) recommends using multiple lines of evidence to make decisions at VI sites. This approach includes the collection of many types of data and may include modeling, with a strong interest in characterizing indoor air exposure risks. Field data have shown substantial spatial (house-to-house) and temporal variability in indoor air concentrations. For instance, Johnston and Gibson (Johnston and Gibson 2014) found a one-order-of-magnitude variability in tetrachloroethylene (PCE) concentrations in indoor air across both space and time among the residential study homes in San Antonio, Texas.
Holton et al. (2013) conducted extensive indoor air sampling for 2.5 years in a single house overlying a dilute chlorinated solvent plume (10 – 50 μg/L TCE). Indoor air concentrations varied by 3 orders of magnitude (>0.01 – 10 ppbv TCE). One source of indoor air variability has been linked to preferential pathways, in particular the unintentional entry of sewer gas entering indoor spaces (e.g. Pennell et al. 2013, Guo et al. 2015). However, experimental results have also shown that induced building-pressure variations influence the temporal and spatial variability of both radon and VOC concentrations in sub-slab and indoor air (Mosley 2007). Factors that may be responsible for variations in building pressures include, among others, changes in atmospheric conditions (e.g., temperature, wind and barometric pressure) and changes in building conditions (e.g., fluctuation in building AER due to resident behavior/heating, ventilation and air-conditioning (HAVC) system operation) (Luo 2009, McHugh et al. 2012, Song et al. 2013, Guo et al. 2015, Schumacher and Zimmerman 2015, Dawson 2016, Shen and Suuberg 2016, Reichman et al. 2017). Numerical results using 3D model and actual field barometric pressure and wind data as input have shown two to four orders of magnitude variability across the instantaneous indoor air concentrations and about an order of magnitude variability for 24 h averages for a month-long simulation and non-degrading chemical (Luo 2009).

The conceptual understanding of VI is predominately focused on subsurface transport and this perspective has been incorporated into many VI models (Johnson 2005, Pennell et al. 2009, USEPA 2012, Shen et al. 2013, Yao et al. 2013, Yao et al. 2013), with few exceptions (e.g. Luo 2009, Song et al. 2013). Virtually all VI models use Equation (3.1) to calculate indoor air concentration, which relies on two parameters that describe the
building characteristics; building AER and the indoor space volume (Yao et al. 2013). Many simulations will use a default value such as of 0.5 (USEPA 2004, Johnson 2005, Patterson and Davis 2009, Pennell et al. 2009, Picone et al. 2012, USEPA 2012, Shen et al. 2013, Yao et al. 2013) or 0.25 (USEPA 2004) for AER; however, as will be discussed later, these default values do not adequately account for the uncertainty and variability in AER.

\[
C_{\text{indoor}} = \frac{A_{\text{ck}} J_T}{A_{\text{ER}} V_b + Q_{\text{ck}}} \tag{3.1}
\]

Where,

\[
J_T – \text{Soil gas flux from the subsurface into the building (M/L}^2/t) \\
A_{\text{ER}} – \text{Air exchange rate (1/t)} \\
A_{\text{ck}} – \text{Area of the crack in the floor that permits soil gas entry (L}^2) \\
Q_{\text{ck}} – \text{Soil gas flow through crack into building (L}^3/t) \\
V_b – \text{Volume of the enclosed building space (L}^3)
\]

AER is a controlling factor for energy consumption and indoor air quality for all buildings, not only at VI sites. Air quality studies have shown variation in AER based on geographical differences in weather conditions, building characteristics, and occupant behavior (Koontz and Rector 1995, Murray and Burmaster 1995, Chan et al. 2005, Breen et al. 2010, USEPA 2011, ASHRAE 2013, Chan et al. 2013, Isaacs et al. 2013, Breen et al. 2014, Breen et al. 2014, Baxter et al. 2017). AER depends on many factors including meteorological conditions (e.g. indoor/outdoor temperature differences and wind speed) building characteristics (e.g. tightness of the building envelope, type of mechanical ventilation, surrounding terrain, and local wind sheltering) and occupant behavior (e.g.
opening windows and the mechanical ventilation operating manner). As will be discussed later these factors are related to the physical driving forces of the airflows.

Typical AER values reported in VI literature (presented in Table 3.1) show that most studies are restricted to the range of values recommended by USEPA (USEPA 2015) as part of the screening process to identify “at-risk” buildings for VI exposures. The range that USEPA recommends is at the lower end of typical AER distributions found in the air quality literature (presented in Table 3.3 and Figure 3.2). This lower range is reasonable for conservative risk assessment screening purposes but does not adequately reflect the AER values published literature (e.g. Isaacs et al. 2013).

USEPA’s conservative AER range (0.18-1.26 1/h) is not intended to be used as an assumption when interpreting indoor air concentration data or evaluating a range of possible exposure scenarios. However, this range has been commonly used during VI studies (Table 3.1). The assumption that a building has a low AER value (i.e. 0.18-1.26 1/h) when a building has a low measured indoor air VOC concentration may incorrectly suggest that a building has a low potential for VI exposure risks. As shown in Equation 3.1, a high AER may result in a low indoor air concentration. But, in this scenario, the potential for VI exposure risks could actually be quite high.

It is important to note that when AERs are altered, then the indoor air concentration could change. While the general trends can be expected to be inverse (e.g. as AER increases, indoor air concentration decrease and vice versa), exact relationships cannot be easily extracted because as discussed below, AERs are influenced by many factors; and, some of those factors also impact $J_T$ (Equation 3.1). But, by understanding that AERs can
span much broader ranges (Table 3.3 and Figure 3.2) than conservative risk screening values, the VI community can become better informed when making decisions at VI sites.

Further, the challenge of house-to-house variability has long been reported as a risk communication challenge during VI investigations. When engaging with VI communities and communicating exposure risks to homeowners and building occupants, regulators and practitioners could share broader perspectives about the well-established variability of AERs, and the role that AERs play in the variability of indoor air quality.
Table 3-1: Typical Residential AER values reported in VI studies.

<table>
<thead>
<tr>
<th>Study</th>
<th>values (h⁻¹)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>• Range used for developing various protocols (e.g. sampling of indoor air, soil gas, etc.): 0.25 - 1.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Values used to develop generic attenuation factors: 0.45 and 0.18.</td>
<td></td>
</tr>
<tr>
<td>(Schumacher and Zimmerman 2015)</td>
<td>• April/May 2011: 0.56 - 0.74</td>
<td>Measured in a specific house (Indianapolis, IN).</td>
</tr>
<tr>
<td></td>
<td>• September: 0.34 – 0.72</td>
<td></td>
</tr>
<tr>
<td>(USEPA 2012)</td>
<td>• One home: 0.5.</td>
<td>Table B-1.</td>
</tr>
<tr>
<td></td>
<td>• Multiple homes: 0.25 and 1.</td>
<td></td>
</tr>
<tr>
<td>(USEPA 2004)</td>
<td>• Range of values for VI models: 0.1 - 1.5.</td>
<td>Table 9.</td>
</tr>
<tr>
<td></td>
<td>• Default value: 0.25.</td>
<td></td>
</tr>
<tr>
<td>(Johnson 2005)</td>
<td>• Reasonable primary input values: 0.2-1.</td>
<td>Sensitivity analysis study.</td>
</tr>
<tr>
<td></td>
<td>• For various sensitivity analysis scenarios use values: 0.6 – 1.3.</td>
<td></td>
</tr>
<tr>
<td>(Picone et al. 2012)</td>
<td>• Values: 0.2 and 2.</td>
<td>Sensitivity analysis study.</td>
</tr>
<tr>
<td>(Moradi et al. 2015)</td>
<td>• Range: 0.18 - 1.26.</td>
<td>Sensitivity analysis study.</td>
</tr>
<tr>
<td>(Shen and Suuberg 2016)</td>
<td>• Fall: 0 - 0.6, [0.3 + 0.3 sin(2πt/12[h])].</td>
<td>Sensitivity analysis study.</td>
</tr>
<tr>
<td></td>
<td>• Summer: 0 – 2, [1 + sin(2πt/12[h])].</td>
<td></td>
</tr>
<tr>
<td>(Patterson and Davis 2009)</td>
<td>• Ambient building pressure, fully sealed: 0.66±0.04</td>
<td>Measured in a specific house (Perth, Western Australia).</td>
</tr>
<tr>
<td></td>
<td>• Ambient building pressure, partly sealed: 1.3±0.1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Reduced building pressure (-12Pa): 2.0±0.1</td>
<td></td>
</tr>
<tr>
<td>(Holton et al. 2013)</td>
<td>• Fall to spring months:</td>
<td>Measured in a specific house (Layton, UT).</td>
</tr>
<tr>
<td></td>
<td>− Typical daily averages: 0.6 - 1.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>− Instantaneous excursions: 0.4 - 1.5.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Summer:</td>
<td></td>
</tr>
<tr>
<td></td>
<td>− Typical daily averages: 0.2 - 0.4.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>− Instantaneous excursions: 0.2 - 0.5.</td>
<td></td>
</tr>
</tbody>
</table>
3.3.3. **Building Air Exchange Rates (AER)**

AER is the rate at which the whole house volume air exchanges with the outdoor air. When the time unit is hours, AER is referred to as air changes per hour (ACH, 1/h). Air exchange is the combination of two processes: infiltration and ventilation. As shown in Equation 3.1, the VI community often shows $Q_{ck}$ (second term in denominator) as separate from total air flow rate through the building envelope (first term in denominator); however $Q_{ck}$ is included in that as part of the formal definition of infiltration.

Infiltration refers to uncontrolled outdoor air flow through unintentional openings in the building envelope, that is, leaks. These leaks include the cracks and penetrations that exist in all buildings, including those that are of importance for VI (e.g. $Q_{ck}$). In residential buildings, many common leak locations have been established as major sources of infiltration, including: the main envelope area; wall, roof and floor junctions; doors and windows; penetrations through the envelope, including electrical components, as well as chimneys, wood burning stoves, etc (ASHRAE 2013, Bailly et al. 2015). An extensive study by (Bailly et al. 2015) conducted at over 35,000 French single family houses reported that leaks through windows and doors were responsible for the majority of total measured building leaks, followed closely by leaks through electrical components. Over the period of one year, this same study showed little fluctuation in infiltration rates (reported as airtightness) based on monthly measurements, suggesting that building tightness is not (typically) biased by measurement season.

Ventilation includes natural ventilation and mechanical ventilation; and can be highly variable depending on a range of factors. For purposes herein, natural ventilation is outdoor airflow through intentional openings such as open windows, and is driven by
weather condition. Mechanical ventilation is airflow induced by powered equipment. These definitions are fairly commonly accepted; however alternate definitions do exist. A detailed description of infiltration and ventilation is provided in the ASHRAE Handbook – Fundamentals (ASHRAE 2013).

In residential construction, energy-saving trends have resulted in homes being tighter and less prone to infiltration. As a result, ventilation systems are an important part of providing adequate AERs. ASHRAE standard 62.2 (ASHRAE 2010) establishes ventilation airflow and measurement requirements for residential buildings. The required whole house ventilation rate is based on the number of bedrooms in the house, and the number of occupants. There are a variety of ways to meet the airflow requirements set forth by this standard, either through mechanical systems or via natural forces. The exact nature of a residential ventilation system will play an important role in the overall AER; however, because of the complexity of residential ventilation systems, a thorough discussion is beyond the scope of this work. The reader is directed to (Russell et al. 2007) which provides a review of residential ventilation systems.

In 2012, Stratton et al. (2012) conducted a study in California to evaluate whole house ventilation rates, as well as air flow from various components (exhaust fans, hoods, etc.) and documented the accuracy of measurement techniques that comply with ASHRAE Standard 62.2 (ASHRAE 2010). Thirteen (13) of the fifteen (15) homes met the ASHRAE Standard 62.2 requirements. As an example, to be compliant with ASHRAE Standard 62.2, a 2000 ft² home with 3 bedrooms would require a whole building airflow of 50 ft³/min. In the 15 houses (3-4 bedroom homes) that were measured, the whole-building ventilation
rates ranged from 32 to 116 ft³/min, which demonstrates the variability in ventilation rates among housing stocks.

Another important aspect in ventilation variability is occupant behavior. Bathroom fans, kitchen hoods and other airflow devices can have relatively high flow rates (10s of ft³/min), as compared to whole-house ventilation rates. While these components may only be operated intermittently, their operation should be considered, especially if indoor air concentrations are being measured while they may be operating.

In terms of natural ventilation, opening windows and doors also can have an important impact on AERs. Howard-Reed et al. (2002) reported that opening windows were substantially more important than stack or wind effects in changing AERs in building. They also reported that the effect of opening windows was important for homes located in both the east and west geographical areas of the US; and quantified the effect based on the dimensions of the opened area. The effect of opening windows was more recently investigated by (Jeong et al. 2016) and highlighted the role of building occupants seeking to control their own environments. Opening windows is an effective way to control temperature when mechanical ventilation systems are ineffective, inefficient or too expensive. Within VI communities, building occupants also desire to control their indoor environments and VI practitioners should anticipate indoor air concentrations may be influenced by changes in AER due to building occupant behaviors.

3.3.4. Driving Forces for AER

AER is driven by pressure differences across the building envelope caused by: 1) air density differences due to temperature differences between indoor and outdoor air (stack effect); 2) wind; and, 3) the operation of mechanical equipment. A brief description
of these forces is given in the following subsections, further information can be found in ASHRAE Handbook – Fundamentals (ASHRAE 2013).

**Stack effect**

Temperature difference between indoor and outdoor causes density differences, and results in a pressure difference. During the heating season (winter), indoor air is warmer and therefore lighter than outdoor air, thereby creating a pressure difference across the building envelope. As a simple representation, the building acts like a chimney, exhausting warm air in the upper part of the building, and drawing in cool outdoor air in the lower part of the building (Figure 3.1A). During the cooling season (summer), the flow directions are reversed and generally lower, because the indoor-outdoor temperature differences are smaller. The height at which the interior and exterior pressures are equal is called the neutral pressure level (NPL). Above this point (during the heating season) the interior pressure is greater than the exterior, below this point, the greater exterior pressure causes airflow into the building (Figure 3.1A). The location of the NPL at zero wind speed is a structure dependent parameter. If the openings are uniformly distributed vertically, they have the same resistance to airflow, and there is no internal airflow resistance, the NPL is at the mid-height of the building (Figure 3.1A).

Pressure difference \( P_s, (M/L.t^2) \) caused by stack effect at height \( H \) is computed using Equation 3.2 based on ASHRAE Handbook – Fundamentals (ASHRAE 2013).

\[
P_s = \rho g (H_{NPL} - H) \left( \frac{T_{in} - T_{out}}{T_{in}} \right)
\]

(3.2)

Where \( \rho \) (M/L\(^3\)) is outdoor air density, \( g \) (L/t\(^2\)) is gravitational acceleration, \( H_{NPL} \) (L) is the location in the building envelope where there is no indoor-to-outdoor pressure
difference, and $T_{\text{in}}$ (absolute temperature) and $T_{\text{out}}$ (absolute temperature) are the indoor and outdoor temperatures, respectively.

Figure 3-1: Distribution of inside and outside pressures (green arrows) over height of a building, and airflow directions (blue arrows) for; (A) Stack effect only for case where inside air is warmer than outside air (winter) and NPL is at the mid-height, (B) Wind effect only, and (C) Wind and stack effects combined. For simplicity of illustration pressure differences due to the wind and stack effect have the same magnitude, which is rare in reality. Adapted from ASHRAE Handbook – Fundamentals (ASHRAE 2013)

Wind effect

As wind flows around a building, it generally produces a positive pressure (over-pressure) on the windward side of a building and negative pressure (under-pressure) on the leeward side. The pressure on the other sides can be either negative or positive, depending on wind angle, local terrain, and building shape. These pressure differences (as compared to the inside of the building) cause inflow (infiltration) on the windward side(s) and outflow (exfiltration) on the leeward side(s) (Figure 3.1B).

Pressure difference ($P_w$, $(\text{M/L.t}^2)$) caused by wind effect at height $H$ is calculated using Equation 3.3 based on ASHRAE Handbook - Fundamentals (ASHRAE 2013):

$$P_w = \frac{1}{2} \rho U_H^2 \left( C_{p,\text{out}} - C_{p,\text{in}} \right)$$

(3.3)
Where $C_{p,\text{out}}$ (dimensionless) is the wind pressure coefficient at a leakage point on the building, $C_{p,\text{in}}$ (dimensionless) is the interior wind pressure coefficient, $C_p$ values are a function of location of the paths on a building surface and wind direction. A detailed description about $C_p$ values is provided in ASHRAE Handbook – Fundamentals (ASHRAE 2013).

$U_H$ (L/t) is the wind velocity at the reference height $H$ (L) that can be calculated as follows:

$$U_H = U_{\text{met}} \left( \frac{\delta_{\text{met}}}{H_{\text{met}}} \right)^{\alpha_{\text{met}}} \left( \frac{H}{\delta} \right)^{\alpha}$$ \hspace{1cm} (3.4)

In which, $U_{\text{met}}$ (L/t) is the wind velocity at the height of $H_{\text{met}}$ (L), $H_{\text{met}}$ is the reference height at the meteorological station (Usually 10m above ground level); $\delta_{\text{met}}$ (L) and $\alpha_{\text{met}}$ (dimensionless) are the atmospheric boundary layer thickness and the exponent at meteorological station, respectively. $\delta$ (L) and $\alpha$ (dimensionless) are the corresponding values for the local building terrain which can be found in table 1, chapter 24 of ASHRAE Handbook – Fundamentals (ASHRAE 2013).

**Mechanical systems**

Mechanical systems can be “unbalanced” (e.g., exhaust fans that force air out, or supply fans that force it into the building) or “balanced” (e.g., systems that have both exhaust and supply fans). Excess exhaust airflow depressurizes the building by creating a net negative pressure and excess supply airflow pressurizes the building by creating a net positive pressure. If a perfect balanced ventilation system is installed (which is rare on-site), the internal pressure of the building does not change, but an unbalanced system changes the internal pressure and consequently affects infiltration rate through the leaks.
**Combining driving forces**

The flow rate through an opening in the building envelope is a subject to the total pressure differences at the location, which is the sum of all the driving forces. Figure 3.1C qualitatively shows the addition of stack (Figure 3.1A) and wind (Figure 3.1B) driving forces for a simplified case where the NPL is in the mid-height, there is no mechanical ventilation, the wind pressure coefficients are uniform on each side, and the magnitude of pressure differences caused by stack effect and wind are equal (which is rare in reality). Total airflow is similar to that with the wind acting alone, but significantly larger than the airflow due only to the stack effect. The total pressure difference through each opening due to stack and wind effects can be estimated by adding $P_s$ and $P_w$ as follows:

$$\Delta P = P_s + P_w$$  \hspace{1cm} (3.5)

The infiltration rate ($Q_f$ $(L^3/t)$) created by wind- and stack-induced pressure differential can be estimated using a power law relationship (Walker and Wilson 1998):

$$Q_f = \kappa \Delta P^n$$  \hspace{1cm} (3.6)

Where,

$\kappa$ – Leakage coefficient ($((L^3/t).(M/L.t^2))^n$)

$n$ – Power law flow exponent.

Accurate calculation of flow rates through a real building envelop based on the driving forces described above requires a considerable computational capability and excessive amount of input that makes it non-realistic for large scale usage. To overcome this difficulty simplified models were developed (e.g., see AER Estimation Models).

The relative importance of the wind and stack pressures in a building depends on building characteristics (e.g., height, shape, internal resistance to vertical airflow and...
location of openings), local terrain and the immediate shielding of the building. For any building, there will be ranges of wind speed and temperature difference for which the building’s infiltration is dominated by the stack effect, the wind or a regime in which the driving pressures of both must be considered.

The effect of mechanical ventilation on the total envelope pressure difference depends on the direction of the ventilation flow and differences in these ventilation flows among the zones of the building. Pressurizing or depressurizing all levels uniformly has little effect on the pressure differences across floors and vertical shaft enclosures, but pressurizing individual stories increases the pressure drop across these internal separations. In a balanced system, the total flow rate \( Q_t \) is the addition of flow created by balanced mechanical system and the infiltration.

\[
Q_t = Q_f + Q_{bm}
\]

(3.7)

In which, \( Q_f \) is the flowrate through the leaks in a building caused by wind and stack effects and \( Q_{bm} \) is the flow rate created by balanced mechanical systems.

An unbalanced system influences the indoor air pressure in a building which consequently interacts with flows induced by wind and stack effect (infiltration). There are several numerical approaches that attempt to combine infiltration and unbalanced mechanical ventilation rates (Table 1 in (Hurel et al. 2016)). These models exhibit a wide range of errors, which demonstrates the difficulty in capturing the complexity of various factors, including: building envelop leakage, weather conditions, leakage distributions and strengths of mechanical ventilation. Hurel et al. (2016) used a subadditivity function to calculate the total airflow caused by infiltration and unbalanced mechanical ventilation in single family detached buildings which reduced the long-term errors to 1% or less.
3.3.5. **Summary of Residential AERs**

**AER Distributions**

AER distributions are usually expressed using the lognormal distribution. Several key existing datasets for US residential AER distribution are summarized in Table 3.2. These datasets are a collection of various projects at different regions in the US that were collected on the course of two types of programs: human exposure programs and residential energy efficiency (e.g. BNL, DEAR, and RIOPA) and weatherization assistance programs (WAPs) (e.g. LBNL). In human exposure programs, AER is measured using the perfluorocarbon tracer method (PFT). WAPs are assessing the building leakage or airtightness and the metric used is the normalized leakage (NL). AER and NL can be related using the scaling factor (SF) model (Chan et al. 2005) (e.g., Empirical models, see AER Models). None of the AER datasets statistically represent the characteristics of houses in the US as a whole (USEPA 2011); however these data have been collected at locations across the US located in key geographic areas and provide considerable insight about how AER values vary across the US. Within the indoor air quality community, many research analyses have been published (Table 3.3) to evaluate these datasets recognizing that AERs are a key determinant in understanding inhalation exposures.

Characteristic examples of US residential AER distributions are presented in Table 3.3 and Figure 3.2. In Figure 3.2, Isaacs’ study is presented with curves for Detroit as the data for this case account for the greatest variability in AER values. Values for the other cities, indicating similar trends, are included in Table 3.3. The data for Murray and Burmaster (1995) and Koontz and Rector (1995) are shown for region 2 and Midwest cities, respectively, which include Detroit data. Koontz and Rector (1995) data was not reported
for different seasons. Murray and Burmaster (1995) data for region 2 summer was not available.
Table 3-2: Summary of database sources for AER distribution.

<table>
<thead>
<tr>
<th>Source</th>
<th>Description</th>
<th>Method</th>
</tr>
</thead>
</table>
| Brookhaven National Laboratory (BNL) (Murray and Burmaster 1995, USEPA 2011) | • Containing over 4,000 measurements for single and multifamily dwelling units.  
• Collected during the period of 1982-1987.  
• Various projects. | PFT |
| Detroit Exposure and Aerosol Research Study (DEARS) (Isaacs et al. 2013) | • Homes in Wayne County Michigan.  
• Collected during the period of 2004-2007.  
• Two seasons: Summer (Jul-Aug), winter (Jan-Mar).  
• A total of 128 homes:  
  - Summer: 105 homes  
  - Winter: 90 homes  
  - Both seasons: 67 homes.  
• 24 h monitoring period. | PFT |
| Relationships in Indoor, Outdoor, and Personal Air (RIOPA) (Isaacs et al. 2013) | • Three US metropolitan cities located in different climate zones: Elizabeth NJ, Houston TX, and Los Angeles, CA.  
• Collected during the period of 1999-2001.  
• Four seasons  
• 300 houses (about 100 homes in each city).  
• Two seasons at each house.  
• 48 h monitoring period. | PFT |
| Lawrence Berkley National Laboratory (LBNL) (Chan et al. 2005) | • Containing 73,000 measurement.  
• Collected in 2001 and earlier.  
• Contributors to the database:  
  – Ohio Weatherization Program that include houses occupied by low income households (77%)  
  – Energy-efficiency program in Alaska (11%)  
  – Wisconsin Energy Conservation Corporation (3%).  
  – Thirty-one other organizations from 30 states (9%). | Air leakage<sup>a</sup> |

<sup>a</sup>NL values were converted to AER using Equation 3.13  
PFT - perfluorocarbon tracer method
Table 3-3: Typical Residential AER distribution studies.

<table>
<thead>
<tr>
<th>Study</th>
<th>AER distribution</th>
<th>Database</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Koontz and Rector 1995)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>All regions</strong></td>
<td><strong>Category</strong></td>
<td><strong>Value (1/h)</strong></td>
<td><strong>10th</strong></td>
</tr>
<tr>
<td>West region</td>
<td>0.18</td>
<td>0.45</td>
<td>1.26</td>
</tr>
<tr>
<td>Midwest region</td>
<td>0.20</td>
<td>0.43</td>
<td>1.25</td>
</tr>
<tr>
<td>Northeast region</td>
<td>0.16</td>
<td>0.35</td>
<td>1.49</td>
</tr>
<tr>
<td>South region</td>
<td>0.23</td>
<td>0.49</td>
<td>1.33</td>
</tr>
<tr>
<td>• Analyzed 2971 measurements.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(Murray and Burmaster 1995)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Cold region (1)</strong></td>
<td><strong>Category</strong></td>
<td><strong>Value (1/h)</strong></td>
<td><strong>10th</strong></td>
</tr>
<tr>
<td>Winter</td>
<td>0.11</td>
<td>0.27</td>
<td>0.71</td>
</tr>
<tr>
<td>Spring</td>
<td>0.18</td>
<td>0.36</td>
<td>0.80</td>
</tr>
<tr>
<td>Summer</td>
<td>0.27</td>
<td>0.57</td>
<td>2.01</td>
</tr>
<tr>
<td>Fall</td>
<td>0.10</td>
<td>0.22</td>
<td>0.42</td>
</tr>
<tr>
<td><strong>Warmest region (4)</strong></td>
<td><strong>Category</strong></td>
<td><strong>Value (1/h)</strong></td>
<td><strong>10th</strong></td>
</tr>
<tr>
<td>Winter</td>
<td>0.24</td>
<td>0.48</td>
<td>1.13</td>
</tr>
<tr>
<td>Spring</td>
<td>0.28</td>
<td>0.63</td>
<td>1.42</td>
</tr>
<tr>
<td>Summer</td>
<td>0.33</td>
<td>1.10</td>
<td>3.28</td>
</tr>
<tr>
<td>Fall</td>
<td>0.22</td>
<td>0.42</td>
<td>0.74</td>
</tr>
<tr>
<td>(Chan et al. 2005)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Whole US</strong></td>
<td><strong>Category</strong></td>
<td><strong>Value (1/h)</strong></td>
<td><strong>5th</strong></td>
</tr>
<tr>
<td>Low income</td>
<td>0.27</td>
<td>0.65</td>
<td>1.62</td>
</tr>
<tr>
<td>Conventional</td>
<td>0.49</td>
<td>1.22</td>
<td>2.74</td>
</tr>
<tr>
<td>(Isaacs et al. 2013)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Cold, newer homes</strong></td>
<td><strong>Category</strong></td>
<td><strong>Value (1/h)</strong></td>
<td><strong>5th</strong></td>
</tr>
<tr>
<td>Cold, older homes</td>
<td>0.38</td>
<td>0.62</td>
<td>1.64</td>
</tr>
<tr>
<td>Warm, central AC</td>
<td>0.16</td>
<td>0.31</td>
<td>3.57</td>
</tr>
<tr>
<td>Warm, no central AC</td>
<td>0.42</td>
<td>1.82</td>
<td>6.10</td>
</tr>
<tr>
<td><strong>Cold, older homes</strong></td>
<td><strong>Category</strong></td>
<td><strong>Value (1/h)</strong></td>
<td><strong>5th</strong></td>
</tr>
<tr>
<td>Cold, newer homes</td>
<td>0.39</td>
<td>0.56</td>
<td>1.03</td>
</tr>
<tr>
<td>Cold, older homes</td>
<td>0.32</td>
<td>0.76</td>
<td>4.14</td>
</tr>
<tr>
<td>Warm, central AC</td>
<td>0.11</td>
<td>0.72</td>
<td>1.04</td>
</tr>
<tr>
<td>Warm, no central AC</td>
<td>0.30</td>
<td>1.04</td>
<td>3.40</td>
</tr>
<tr>
<td><strong>Cold, newer homes</strong></td>
<td><strong>Category</strong></td>
<td><strong>Value (1/h)</strong></td>
<td><strong>5th</strong></td>
</tr>
<tr>
<td>Cold, older homes</td>
<td>0.18</td>
<td>0.66</td>
<td>2.29</td>
</tr>
<tr>
<td>Warm, central AC</td>
<td>0.13</td>
<td>0.38</td>
<td>1.10</td>
</tr>
<tr>
<td>Warm, no central AC</td>
<td>0.23</td>
<td>0.56</td>
<td>2.74</td>
</tr>
<tr>
<td><strong>Los Angeles, CA</strong></td>
<td><strong>Category</strong></td>
<td><strong>Value (1/h)</strong></td>
<td><strong>5th</strong></td>
</tr>
<tr>
<td>Cold, newer homes</td>
<td>0.17</td>
<td>0.42</td>
<td>1.32</td>
</tr>
<tr>
<td>Cold, older homes</td>
<td>0.32</td>
<td>0.80</td>
<td>2.24</td>
</tr>
<tr>
<td>Warm, central AC</td>
<td>0.26</td>
<td>0.71</td>
<td>2.70</td>
</tr>
<tr>
<td>Warm, no central AC</td>
<td>0.21</td>
<td>1.45</td>
<td>4.35</td>
</tr>
</tbody>
</table>
Figure 3-2: Characteristic examples of residential AER distribution curves.

Measured AER varies by an order of magnitude among 90% (5th to 95th percentile) of US homes due to a number of factors, including housing characteristics and meteorological conditions. AER distribution depends mainly on house age, the central air condition (AC) status and weather (e.g. season, ambient temperature and humidity, wind speed and direction, and climate zone). Older (Chan et al. 2013, Isaacs et al. 2013) and low income (Chan et al. 2005) homes, tend to have higher AERs. Conversely, homes that are newer (Chan et al. 2013, Isaacs et al. 2013) and conventional (Chan et al. 2005) tend to have lower AERs. AERs in homes with central AC is much lower compared to homes without central AC (Isaacs et al. 2013). The lower AER curves were obtained in the cold weather (Figure 3.2). Homes without central AC in warm weather tend to have the highest
AERs (Isaacs et al. 2013). Regression analyses (Chan et al. 2013) on updated LBNL database with home built more recently predicts for whole US a slightly (15-30%) higher NL values compared to previous study (Chan et al. 2005), as well as some between-state differences that can be explained by the climate zones and the year built. USEPA’s median residential AER of 0.45 is based on Koontz and Rector (1995). However, this median value is not representative of more recent datasets, as shown in Figure 3.2 and Table 3.3.

Factors Controlling Between-House AER Variations

The AER variations across residences in the same geographical region are due to differences in occupant behavior (e.g., opening windows, operating mechanical ventilation, indoor temperature from thermostat setting during heating and cooling seasons), and building characteristics (e.g., leakage of building envelope, type of mechanical ventilation) (Breen et al. 2010, Breen et al. 2014, Breen et al. 2014). For residences in different geographical regions, the AER variations can also include differences in wind speed (near coast versus inland) and outdoor temperature (Breen et al. 2014).

Continuous measuring of AER in single home during a VI study indicated slow seasonal oscillation accompanied by daily brief transients (e.g., positive and negative spikes) (Holton et al. 2013). The seasonal AER temporal variations are primary due to variations of the indoor-outdoor temperature differences while the spikes correspond primarily to the wind speed variations, and secondarily to indoor-outdoor temperature difference variations. Generally, temporal AER variability of individual homes tends to decrease with decreasing median AER (e.g., tighter building envelop) (Breen et al. 2014). In the following section, we calculate variable indoor air concentrations considering
various geologies and AER values reported in building science literature. The results support the need to consider the implications of AERs when making decisions at VI sites.

3.4. Relevance for VI Studies

Indoor air concentrations calculated using Equation 3.8 with recent AER values (Table 3.3) and 3D VI model simulations ($\dot{m}_i$) demonstrate the importance of AER uncertainty on VI exposure risks.

Equation 3.8 is a slight revision to Equation 3.1, reflecting the new understanding that $Q_{ck}$ in Equation 3.1 is included in the formal definition of AER as defined by the ASHRAE Handbook – Fundamentals (ASHRAE 2013). Equation 3.8 also explicitly accounts for chemical entry via exchanged air, if chemicals are present.

$$C_{\text{indoor}} = \frac{\dot{m}_i}{AER \cdot V_b} = \frac{\dot{m}_i}{Q_b}$$

(3.8)

Where, the mass flowrate of “i” into building ($\dot{m}_i$) (M/t) is given by;

$$\dot{m}_i = JTA_{ck} + C_{i,ex} AER \cdot V_b + \dot{m}_{i,other}$$

(3.9)

Where,

$Q_b$ – total flowrate through the building, which as discussed previously includes a combination of infiltration and ventilation (both mechanical and natural) (L$^3$/t).

$C_{i,ex}$ – chemical “i” concentration in exchanged air (M/L$^3$)

$\dot{m}_{i,other}$ – Mass flowrate of “i” into the building from sources other than VI and exchanged air. Similar formulation for $\dot{m}_i$ was provided by others (Luo 2009).

For the purpose of the current study we assume that the only source of chemical “i” is the soil gas mass entry rate ($JTA_{ck}$) and the chemical concentration in exchanged air or from other sources is equal to zero ($C_{i,ex} AER \cdot V_b + \dot{m}_{i,other} = 0$). As discussed above,
AER (in the denominator of Equation 3.8) is notably influenced by the stack and wind effects. The mass entry rate of contaminant into buildings (the numerator in Equation 3.8) is theoretically influenced by these two factors, as well. However, there are currently no VI models that adequately account for stack and wind effects in both the numerator and the denominator in Equation 3.8. In fact, this is an active area of research for the authors and others. Therefore, to gain the mass entry rate, the research herein used a VI modeling approach that has been widely published (Pennell et al. 2009) and has been compared to field data (Pennell et al. 2016).

3.4.1. **Single Building and Single Geology Evaluation**

Figure 3.3 illustrates the effect of AER on a hypothetical single VI site where the geology is modeled as sandy soil ($K = 10^{-11} \text{ m}^2$). Indoor air concentrations were calculated using Equation 3.8 and the AER values in this equation were taken from (Isaacs et al. 2013) for Detroit, MI (Table 3.3 and Figure 3.2). The soil gas mass entry rate was calculated using a 3-D VI model for the base scenario described by (Pennell et al. 2009) that includes a single building (10 m x 10 m) with a basement (2 m deep) located in the center of an open field and depressurized (-5Pa). Therefore, the mass entry rate in Equation 3.8 was a constant across all scenarios in Figure 3.3. The results show greater $C_{\text{indoor}}/C_{\text{source}}$ variability for warm weather compared to cold weather. The age of the house affected $C_{\text{indoor}}/C_{\text{source}}$ by an order of magnitude ($1.9 \times 10^{-3}$ to $2.4 \times 10^{-4}$), indicating the older homes had lower $C_{\text{indoor}}/C_{\text{source}}$ due to higher AERs. AC operational status resulted in more than one order of magnitude variability of $C_{\text{indoor}}/C_{\text{source}}$ ($4.4 \times 10^{-3}$ to $1.2 \times 10^{-4}$). Previously field study data has reported similar observations for indoor air concentrations and AC status (Johnston and Gibson 2014).
3.4.2. AER Distribution and VI Field Data Comparison

Figure 3.4 illustrates the combined effect of an AER distribution that considers important building features within four geographic areas; and compares AER values to the USEPA VI Database. The need for a geographically diverse AER distribution that is a product of different home types, climate regions and weather conditions in US was a consequent of our goal to compare theoretical evaluations to USEPA VI database (USEPA 2012). The soil gas mass entry rate was calculated using a 3-D VI model described above and considered sand, sandy loam, and clay loam geologies with a building depressurized (-5Pa). In addition, it considered a diffusion only VI scenario depressurization (0Pa).
The AER distribution, presented in Figure 3.5, combines the sixteen final categories distributions, given in (Isaacs et al. 2013) and summarized in Table 3.3, using the weighted average formulation:

\[
A_j = \frac{\sum_{i=1}^{16} A_{i,j} N_i}{\sum_{i=1}^{16} N_i}
\]  

(3.10)

Where,

\(A_j\) - Combined AER value corresponding to percentile j (5, 25, 50, 75, 95),

\(A_{i,j}\) - AER value for case i (1-16) and percentile j,

\(N_i\) – Number of observation in case i.

Currently, USEPA’s VI Database represents the largest collection of VI data for chlorinated VOCs in the US; containing 2929 paired measurements from 42 vapor intrusion sites across the country though the majority of sites are from the North-east and Western portions of the country (USEPA 2012). Groundwater attenuation factor \((C_{\text{indoor}}/C_{\text{source}})\) distribution (5th to 95th percentile) with a filter of groundwater VOCs 1000 times greater than background VOCs (Table 7 in (USEPA 2012)), presented in Figure 3.6, show that 90% of groundwater attenuation factors vary over three orders of magnitude.

The results shown in Figure 3.4 suggests that the combined effect of AER and geology provide a possible explanation for 90% of the variability in the EPA database; and strongly supports the need to consider the implications of AERs when making decisions at VI sites. The simplest approach is to select AER measured value based on various factors (e.g., building characteristics, season, and geographical region) most similar to the investigated case. The main limitation is the uncertainty of using AER measurements from other buildings and from sampling periods with different weather conditions, natural ventilation, and mechanical ventilation.
Figure 3-4: Combined effect of AER distribution and geology on $C_{\text{indoor}}/C_{\text{source}}$ in comparison to USEPA VI database range (shaded area). Error bar present maximum and minimum values.
Figure 3-5: AER distribution that considers important building features within four geographic areas. The error bar show maximum and minimum values.

Figure 3-6: USEPA VI database groundwater attenuation factor ($C_{\text{indoor}}/C_{\text{source}}$) distribution (5th to 95th percentile) for a filter of groundwater VOCs 1000 times greater than background VOCs.
3.5. AER Measurement Methods

Building science and air quality science provide well established methods for estimating single home AER (Sherman and Grimsrud 1980, Sherman 1992, Koontz and Rector 1995, Murray and Burmaster 1995, Sherman 1995, ASHRAE 1998, ASTM 2000, Chan et al. 2005, Breen et al. 2010, ASHRAE 2013, Chan et al. 2013, Isaacs et al. 2013, Sherman et al. 2013, Breen et al. 2014, Breen et al. 2014, Baxter et al. 2017) that can be implemented as part of VI site investigations. One of the more robust techniques for measuring the actual AER of a building is using a tracer gas dilution method (ASTM 2000, USEPA 2011, ASHRAE 2013), but measuring the actual AER is often limited due to costs of collecting site-specific field data, participant burden, and building access restrictions (Breen et al. 2010, Breen et al. 2014). Further, these methods are sensitive to current weather conditions (Breen et al. 2014). Alternatively, AER can be estimated using “equivalent leakage area” methods, which compared to AER measuring methods are typically less expensive (Breen et al. 2010, Breen et al. 2014), easier and are similar to methods being implemented to measure VI fluxes into buildings (McHugh et al. 2007, Guo et al. 2015, Dawson 2016). However, leakage area methods only capture infiltration rates; therefore in order to estimate the total AER, numerical models must be incorporated. The section below describes leakage area measurement methods for a single-zone approach based on the assumption of a single, well mixed enclosure. Airflow between internal zones and between the exterior and individual internal zones has led to the development of multi-zone measurement techniques. A recent study suggests that multi-zone air leakage considerations may play important roles in indoor air quality models (Guyot et al. 2016);
however, these multi-zone measurement techniques are complex and beyond the scope of this review.

3.5.1. Air Leakage Area Measuring Method

The air leakage of a building characterizes the relationship between pressure difference ($\Delta P$) across the building envelope and the airflow through it; and is an indication of building tightness. Leakier buildings will require higher airflow rates to pressurize the building to a certain level, whereas tighter buildings will require lower flow rates.

Air leakage of a building is measured with a pressurizing test known as “Blower Door” test (Sherman 1995, ASTM 2010, ISO9972:2015 2015). A large fan or blower is mounted in a door or window and induces a large, roughly uniform $\Delta P$ across the building shell. This test is performed with natural ventilation openings closed and mechanical ventilation turned off. Airflow (through a calibrated orifice) is adjusted to generate various indoor–outdoor pressure difference ($\Delta P$). The experimental results provide an estimate of the area of an opening which would be equivalent in size to lumping all the combined openings throughout the structure into one opening. This opening area is used in AER models described below.

Most commonly, airflow is measured at $\Delta P=50$ Pa, which is insensitive to the influence of wind variation during the test, and therefore provides reproducible data sets. The resulting AER at 50 Pa (AER50) is calculated by dividing the resulting flow rate by the building volume. AER50 is a useful metric for comparing houses of different sizes and is used as an input for the SF leakage model.

The Lawrence Berkeley Laboratory (LBL) infiltration model (Sherman and Grimsrud 1980) and its extended version that include natural ventilation (LBLX)(Breen et
al. 2010) uses the Effective Leakage Area (ELA) of a building, wind speed, and inside-outside temperature differences to estimate the AER. The LBLX model will be described in a later section. The ELA of a building is defined as the area of a calibrated orifice that would have the same air flowrate as the house at a reference standard pressure of 4 Pa. ELA is an estimate of the combined size of all the leaking areas in the building.

ELA is measured using the multipoint test where blower door flowrates, at a series of ΔPs ranging from about 10-70 Pa, are measured to determine the relationship between ΔP and leakage rate for the test home (Qf). Equation 3.6 is used to find κ and n based on the best fit of the data. Since ELA depends on the indoor–outdoor ΔP, it is necessary to extrapolate experimental results to determine the ELA at the reference pressure (P_r).

The relationship between the airflow rate through the fan orifice and the ΔP can be expressed as:

\[ Q_f = ELA \sqrt{2\Delta P / \rho} \quad (3.11) \]

Combining and rearranging Equations 3.6 and 3.11 allow determination of ELA at standard reference pressure:

\[ ELA = (\sqrt{\rho / 2}) \kappa P_r^{(n-0.5)} \quad (3.12) \]

There is uncertainty in ELA estimation which is due to 1) measurement errors and 2) model specification. Wind can be a source of measurement errors when pressure and flowrate are measured during pressurization test. The model specification error can be created by extrapolation to measure the flowrate at 4 Pa (Sherman 1992, Sherman and Palmiter 1995). Walker et al. (2013) compared single point and multipoint testing approaches and showed that the multipoint testing described above is recommended for the conditions when there is a wind speed less than 6 m/s during the test. For wind speeds
greater than 6 m/s, they suggest a single point testing at ΔP=50 Pa with a fixed pressure exponent (n=0.65) which is less sensitive to wind pressure fluctuations and cause reduction in experimental errors (Walker et al. 2013).

3.5.2. AER Estimation Models

AER estimation models can be distinguished broadly into two categories; empirical models (e.g., data-driven approaches) and physically based models (e.g., based on fundamental physical theory). The physically-based models have been classified into: 1) single zone models and 2) multi-zone models. Various AER models have been described in the literature (ASHRAE 2013, Breen et al. 2014). Selected models are described briefly below.

**Empirical model**

The SF model is an empirical model that relates the AER at 50 Pa (AER50) to AER at typical natural conditions (4 Pa) using a scaling factor (F) as:

$$AER_{SF} \ [h^{-1}] = \frac{AER50}{F}$$ \hspace{1cm} (3.13)

Chan *et al.*\(^{20}\) found that F = 16 gives the best fit for the national data. A commonly used metric for building leakage is the Normalized Leakage, NL, defined as:

$$NL = 1000 \cdot \frac{ELA}{A_{floor}^{2.5}} H^{0.3}$$ \hspace{1cm} (3.14)

Where,

- \(A_{floor}\) – Floor area (L\(^2\))
- \(H\) - The height of the building (L)

NL is ELA normalized with the building floor area and a correction factor for the building height. It describes the relative leakage for a wide range of building sizes (Chan
et al. 2005). To describe AER₅₀ in terms of NL, Equations 3.6, 3.11, and 3.14 are combined to yield:

$$AER₅₀ \ [h^{-1}] = 48 \left(\frac{2.5m}{H}\right)^{0.3} \frac{NL}{H}$$

(3.15)

NL can also be estimated from leakage area model such as (Chan et al. 2005):

$$NL = \exp(\beta_0 + \beta_1y_{built} + \beta_2A_{floor})$$

(3.16)

Where,

- $y_{built}$ – year of construction
- $\beta_0$, $\beta_1$, and $\beta_2$ - regression parameters, which were estimated for three housing types: low income, conventional, and energy efficient (Chan et al. 2005).

A comparison of AER distribution curves measured with the PFT method (Isaacs) and AER₅₀ based on air leakage method (Chan et al. 2005), given in Figure 3.7, show a good agreement between the two distributions; Isaacs’s newer homes curve is very close to Chan’s conventional curve, and Isaacs’s older homes curve is very close to Chan’s low income curve. Figure 3.7 supports the use of the SF model with air leakage measurement. Additionally, the SF model was evaluated with data from 642 daily (e.g., 24 h average) AER measurements across 31 detached homes in central North Carolina collected on seven consecutive days during each of four consecutive seasons and showed a median absolute difference of 50% (0.25 l/h), a slightly higher compared to physical based more sophisticated models (e.g., a median absolute difference of 43% (0.17 l/h) and 40% (0.17 l/h) for the LBL and LBLX models, respectively) (Breen et al. 2010). The main limitation of this simple model is the absent of sensitivity for meteorological conditions (e.g., stack and wind effects) and thus for hourly variations as well.
Figure 3-7: A comparison of AER distribution curves measured with the PFT method (Isaacs et al. 2013) and the air leakage method (Chan et al. 2005).

**Simplified single-zone models**

*LBL and LBLX model*

The LBL model is widely used as a tool for predicting residential infiltration rates (ASHRAE 2013, Breen et al. 2014). Stack and wind effects, the driving forces for infiltration, are calculated separately, and then combined using superposition (Sherman 1992). The LBL model has been compared to AERs measured by tracer gas technique, which were measured during different time periods and different seasons. These comparisons showed that the LBL model predictions resulted in mean absolute errors of 25–46% (Palmiter and Francisco 1996, Wang et al. 2009, Breen et al. 2010, Breen et al. 2014).
LBLX model is an extended version of LBL model that includes natural ventilation airflow through large intentional openings (e.g., windows, doors) (Breen et al. 2010). The LBLX model predicts the AER due to infiltration and natural ventilation. The median absolute difference between LBLX model prediction, using Equation 3.16 for leakage area, and data from 642 daily AER measurements across 31 detached homes in central North Carolina, with corresponding window opening and meteorological data was 40% (0.17 l/h) (Breen et al. 2010), and 29% (0.19 l/h) for data from a subset of 24 study homes on five consecutive days during two seasons in Detroit, MI (Breen et al. 2014).

**Multizone air flow models**

Several multizone computational models have been developed to calculate air flows and contaminant distribution in multizone buildings (Wang and Zhai 2016). In multizone models the building is divided into several zones (e.g. rooms) and each zone is assumed as a well-mixed zone to have uniform temperature, pressure and contaminant concentration. Zones are connected to each other by flow paths (e.g. cracks, openings, ducts). Two examples of well-known multizone air flow models are CONTAM and COMIS. CONTAM (Dols and Polidoro 2015) was developed by the “Building and Fire Research Laboratory of the National Institute of Standards and Technology” (NIST). COMIS (Feustel 1999) was developed by an international group of experts (the Energy Performance of Buildings Group) at the Lawrence Berkeley National Laboratory. In both of these models, wind effect, stack effect and mechanical ventilation are taken into account in building air flow estimation.
COMIS (Feustel 1999), like CONTAM (Dols and Polidoro 2015), uses a similar procedure in solving air flowrates through openings of a building. Both models use a conservation of mass in all zones to calculate the zonal pressures and air flow rates through flow paths. CONTAM and COMIS use dimensionless pressure coefficients and Bernoulli’s equation to gain the pressure distribution on building surfaces induced by wind speed and direction. These two models are widely used in indoor air quality studies and could be used in VI studies to estimate the total air exchange rate of the building and also indoor air concentration of contaminant considering air flows through the building induced by infiltration, natural and mechanical ventilation (Wang and Zhai 2016).

3.6. Conclusions and Implications

AERs commonly referenced in VI literature (Table 3.1) are not representative of the wider range of values present in indoor air quality literature (Table 3.3 and Figure 3.4). Indoor air concentration data collected during VI investigations should be interpreted by considering how AERs may influence the measured indoor air concentration data. As show in Equation 3.8, indoor air concentrations may be diluted by high AERs; if building operation is modified by a building occupant behavior and the AER is decreased, the indoor air concentration may respond by increasing.

An inaccurate assumption that AERs fall within USEPA’s conservative screening range (0.18-1.26 1/h) could result in a false understanding that residential buildings across the US have AERs within this narrow range. However, as shown on Figure 3.4, recent literature reports a broader range (up to 6.1 1/hr). While the majority of AERs do not deviate substantially from USEPA’s conservative screening range, careful consideration is
warranted by the VI scientific community when evaluating and interpreting measured indoor air concentrations as part of VI site assessments.

VI communities continue to be impacted by decisions at VI sites, even after VI site specific risk assessments are completed. Therefore, as part of the USEPA multiple lines of evidence approach, practitioners and regulators should consider how building characteristics may influence AERs and VI exposures risks. The *ASHRAE Handbook – Fundamentals (ASHRAE 2013)* highlights several building features that are known to influence AERs. For instance, older windows and doors, building penetrations, fireplaces, etc. are features that may increase infiltration. Bailly *et al.* (2015) summarizes the results of 65,000 air tightness tests conducted in Europe and reports several leak-prone characteristics for various building-types. Practitioners should consider these qualitative factors when making decisions and communicating risks at VI sites. In the absence of well-known ventilation rates, specific trends about the building’s AER cannot be easily extracted based on leakage information alone. However, leak-prone building features may play a role in potentially decreasing indoor air concentrations and these features can be identified and evaluated as part of VI investigations.

Mechanical and natural ventilation are also an important part of AERs. The exact contribution of ventilation to the total AER is not easily estimated. There may be a need to consider the role of occupant behavior on natural (*e.g.* open windows and doors) and mechanical ventilation systems, such as bathroom and kitchen exhaust fans. The VI community has not routinely considered the variability of ventilation systems during VI investigations. Most indoor air sampling is conducted during heating seasons, when windows and doors are closed to limit natural ventilation and when AERs are thought be
low (most conservative); however even during “cold seasons” some regions of the US have been shown to have AERs > 4 l/hr (see New Jersey data, Table 3.3).

Further, AERs of buildings can vary considerably based on age and construction. Isaacs et al. (2013) showed that AERs for newer and older homes during heating seasons (e.g. “cold” data) varied as much as a factor of 4 for the 95 percentile (see New Jersey data, Table 3.3), with the older homes have the higher AERs (less conservative values). Importantly, Chan et al. (2005) (Table 3.3) showed “low income” homes had higher AERs (less conservative values). These are important implications to consider when evaluating VI exposure risks at VI sites.

Risk management and communication at VI sites should continue to highlight the dynamic nature of VI exposure risks. Decisions that do not consider the possibility of higher AERs to decrease indoor air concentrations, may not be conservative in terms for future VI exposure risks. For example, energy-efficiency initiatives that target older homes and low-income areas (e.g. (Cluett et al. 2016)) may reduce AERs at buildings after VI assessments have deemed indoor air concentrations are below risk levels. With many energy efficiency programs being implemented in neighborhoods, these types of temporal changes in AERs (and ultimately changes in VI exposure risks) should be considered. If a homeowner makes future modifications, perhaps as part of a weatherization program (or any other optional home improvement), the indoor air concentration may change. VI practitioners should engage in risk communication plans that communicate these types of related building issues to homeowners and regulators should consider follow up sampling requirements.
Field measurements could provide information to contextualize indoor air concentration data. VI practitioners may consider measuring building air leakage area to calculate infiltration in homes where vapor intrusion may be occurring. This information combined with knowledge about, or measurements of, building ventilation may inform vapor intrusion decisions. However, occupant behaviors that could influence building ventilation rates and influence indoor air concentrations should also be considered.

As discussed above, building features and other factors that influence AER should be taken into account when evaluating indoor air concentrations as part of the multiple lines of evidence approach at VI sites. Decisions about whether to qualitatively, and/or quantitatively consider AERs can be made on a case-by-case basis within the framework of the specific context of the exposure scenario.

Lastly, AERs are influenced by some of the factors that influence soil gas entry into buildings (wind and indoor-outdoor temperature differential (stack effect)). More research is needed to understand how above-ground and subsurface processes are coupled. This is an active area of research. While research results continue to emerge, VI practitioners can use multiple lines of evidence to make the best decisions possible given the information and evidence currently available.
CHAPTER 4: BACKGROUND

Building air exchange rate (AER) is influenced by various factors such as wind and stack effects, building characteristics, and occupant behavior. These factors not only influence AER but also influence indoor and outdoor pressures, which is the driving force for convective transport of contaminant into the building through foundation cracks. As shown in Equation 2.1 in Chapter 2 and Equation 3.1 in Chapter 3, the indoor air concentration of the contaminant is a function of mass entry rate of contaminant (MER) and building AER. In Chapter 3, we explained the importance and effect of AER on changing indoor air concentration, however, how to quantitatively account for wind and stack effects; and building characteristics was not thoroughly discussed in that chapter. In this chapter, we review the models commonly used in the VI community. These models have not given consideration to complexity of aboveground processes when predicting indoor air concentrations. We also discuss the importance and advantages of incorporating indoor air quality models into VI studies to better understand indoor air concentration variability.

4.1. Models used in VI studies

Over the past two decades, several VI models have been developed to predict vapor transport through soil into indoor spaces (Johnson and Ettinger 1991, Abreu 2005, Abreu and Johnson 2005, Abreu and Johnson 2006, Bozkurt et al. 2009, Pennell et al. 2009, Shen et al. 2012, Diallo et al. 2013, Shen et al. 2014, Diallo et al. 2015). Johnson and Ettinger’s (J&E) one-dimensional VI model assumes that diffusion is the dominant mechanism in vapor migration through the soil and advection is only significant near the foundation cracks (Johnson and Ettinger 1991). Based on J&E assumptions, Abreu and Johnson simulated vapor intrusion using a three-dimensional finite difference numerical model in
which a continuity equation had been coupled with a chemical transport equation to calculate the soil gas pressure, velocity and chemical concentration in soil and indoor air (Abreu 2005, Abreu and Johnson 2005, Abreu and Johnson 2006). Pennell et al. (2009) developed a three-dimensional finite element numerical model and simulated soil vapor transport into buildings under constant negative basement under-pressurization (Pennell et al. 2009). Most of the above-discussed studies use a spatially uniform ground surface atmospheric pressure as boundary condition in VI simulations. These models have focused on subsurface transport processes, however it is been shown that some aboveground factors such as wind flow and temperature have a significant effect on vapor transport in subsurface and also indoor air concentration distribution (Riley et al. 1996, Riley et al. 1999, Luo 2009, Song et al. 2013, Shen and Suuberg 2016). Wind flow not only affects the AER and air pressure inside a building, but also influences on the ground surface pressure adjacent to the building which consequently alters the soil gas flow and concentration under the building (Riley et al. 1996, Riley et al. 1999, Luo 2009). Riley et al. (1996) used the mean ground-surface pressure coefficients obtained from a wind tunnel experiment on a single-family structure to investigate the effect of wind speed and direction on radon concentration in soil and indoor. Wind and stack effect both influence on pressure difference between indoor and outdoor, however they left the effect of temperature on indoor air pressure out of account (Riley et al. 1996). Stack effect has been shown as an important factor that influence on indoor air pressure and AER of a building (Sherman 1992). Sherman (1992) stated that stack effect is more effective than wind effect in changing the radon entry rate through a building. In a VI investigation, Song et al. (2013) assessed the influence of stack effect, wind effect on soil gas entry rate and outdoor air
flowrate through the building, however the authors did not consider the effect of these factors, and also wind direction on indoor air pressure which influence on both soil gas entry rate and building air flowrate (Song et al. 2013). Shen and Suuberg (2016) showed that the AER and indoor air pressure variation cause a significant variation in indoor air contaminant concentration, however they did not indicate how wind and temperature impacted AER and indoor air pressure variation (Shen and Suuberg 2016). In a site study in Wyoming, Lou et al. (2009) showed that wind flow is an essential factor that affects contaminant and oxygen concentration in the soil under a building. The results showed low concentration of contaminant and high concentration of oxygen at the windward side of the building, while the high concentration of contaminant and depleted oxygen was reported at the leeward side of the building (Luo 2009, Luo et al. 2009). Lou et al. (2009) concluded that the oxygen that had been taken into the soil by wind in the windward side caused aerobic biodegradation of contaminant. The sampling results also showed that pressure difference between soil and indoor air pressure in the upwind side of the building was 5-10 Pa higher than the downwind side of the building. Based on these observations, Lou et al. (2009) evaluated the effect of wind flow on contaminant indoor air concentration by modifying the numerical model that Abreu and Johnson (Abreu 2005, Abreu and Johnson 2005, Abreu and Johnson 2006) had used in simulating VI process. The modified model account for the influence of wind flow on ground surface pressure and combination of wind and stack effects (ΔT=10 °K) on building under pressurization. The model did not consider the effect of air flow and stack effect on AER and used a constant value of 0.5 hr⁻¹ in calculating the indoor air concentration (Luo 2009, Luo et al. 2009). AER in a building is an important factor in calculating the indoor air concentration of contaminants which is a
function of building leakage characteristics, natural and mechanical ventilation (Moradi et al. 2015). To date, fewer analytical studies have been conducted to understand the combination effect of temperature, wind speed and direction on under-pressurization and AER in a building which are essential factors in estimating indoor contaminant concentration.

4.2. Modeling Tools in Building Science for Vapor Intrusion Studies

This section includes an “in press” article in Reviews on Environmental Health (E. Shirazi, S. Ojha K. G. Pennell, June 2019). “Building Science Approaches for Vapor Intrusion Studies”.

Indoor air concentrations are susceptible to temporal and spatial variations and have long posed a challenge to characterize for vapor intrusion scientists; in part, because there was a lack of evidence to draw conclusions about the role that building and weather conditions played in altering vapor intrusion exposure risks. Importantly, a large body of evidence is available within the building science discipline that provides information to support vapor intrusion scientists in drawing connections about fate and transport processes that influence exposure risks. Modeling tools developed within the building sciences provide evidence of reported temporal and spatial variation of indoor air contaminant concentrations. In addition, these modeling tools can be useful by calculating building AERs using building specific features. Combining building science models with vapor intrusion models provide new insight to facilitate decision making by estimating indoor air concentrations and building ventilation conditions under various conditions. This review highlights existing building science research and summarizes the utility of building science models to improve vapor intrusion exposure risk assessments.
4.2.1. Introduction

The World Health Organization (WHO) has guidelines for indoor air quality for nine chemicals for which toxicological and epidemiological data suggest health concerns exist at relevant environmental exposure levels (WHO 2010). Three of the nine chemicals (e.g. benzene, trichloethylene, tetrachloroethylene) are directly relevant to the problem of volatile organic compound (VOC) vapor intrusion. Vapor intrusion is the process by which vapors emanating from groundwater plumes or contaminated soils migrate upward in the subsurface and ultimately enter indoor air spaces. VOC concentrations in indoor air resulting from vapor intrusion can vary spatially and temporally (e.g. (Folkes et al. 2009, Holton et al. 2013)). There are many possible explanations for these variations, but above ground processes including environmental and structural conditions, occupant activities and climate variability are important factors that influence variability; and these factors have not been systematically considered as part of vapor intrusion exposure risk assessments.

Many of these above ground processes are impacted by building conditions that change over disparate timescales. Variations in building mechanical ventilation systems or weather conditions are examples of variations that could occur over short time scales, and subsequently influence indoor air quality. Over longer time scales, for instance when a building ages, variations in a building’s tightness will influence the building’s infiltration, exfiltration and ventilation rates (Reichman et al. 2017). Song et al. highlights the importance of building tightness and climate variability on vapor intrusion exposure risks (Song et al. 2018). They indicated that air-tight houses (energy-efficient) in different climate zones in U.S. may be more prone to vapor intrusion compared to the less air-tight
houses ("conventional" and "low-income") because energy-efficient houses have building characteristics that likely result in lower AERs (Song et al. 2018). Folks et al. suggest that ventilation caused by depressurization and AER contribute to spatial variation in indoor air more than building foundation type (Folkes et al. 2009). Brewer et al. highlight the role of climate data, building specific designs and AERs for on subslab vapor concentrations and vapor intrusion exposure risks (Brewer et al. 2014). These recent studies emphasize to account for season variability in building ventilation process as important for vapor intrusion studies.

Multizone indoor air quality models commonly used in building science studies can account for not only weather conditions but also building features (such as, layout, opening size and location, mechanical ventilation) and occupant behavior to calculate building AERs and indoor air concentrations (Feustel 1999, Dols 2001, Dols and Polidoro 2015, Wang and Zhai 2016). Integrating building science into exposure risk assessments at vapor intrusion sites, will assist vapor intrusion scientists by being able to account for climate variability (the climate that building is located in), seasons effect and occupant behavior in buildings which eventually influence the building condition and air quality. This review discusses the importance of building science in vapor intrusion processes and introduces multizone indoor air quality models that can be used to evaluate vapor intrusion exposure risks.

4.2.2. Building Science Modeling Techniques

Modeling approaches in building science have focused on a variety of goals, but commonly aim to reduce energy consumption and improve indoor air quality (Nguyen et al. 2014). Since the late 1980s, considerable effort has been placed on modeling building
ventilation processes (Wang and Zhai 2016). Coupling building science models and vapor intrusion models can be a promising way to create an indoor environment that accomplishes the goals of building science (i.e. reduce energy consumption and improve air quality) and vapor intrusion (i.e. healthy indoor air quality). In building science and vapor intrusion research, various simulation models and techniques are employed.

For building science, the analytical models widely used in natural ventilation usually consider wind and stack effect or a combination of these forces in buildings (Li and Delsante 2001, Li et al. 2001, Chen and Li 2002, Andersen 2007). The analytical solutions used in indoor air quality usually consider both diffusive and convective transport of air contaminant in buildings (Mazumdar and Chen 2009, Parker et al. 2014). Computational fluid dynamics (CFD) methods started gaining interest in building science research to predict detailed information of airflow, pressure, temperature and contaminate distribution in buildings (Li and Nielsen 2011, Wang and Zhai 2012, Wang 2013, Nielsen 2015). The CFD models used in indoor environment modeling are computationally expensive but are able to predict spatial contaminant, pressure and temperature distribution in a zone.

Multizone indoor air quality models are faster than CFD models. Multizone computational models usually solve a conservative of mass and concentration to calculate zonal air pressure, contaminant concentration; and interzonal airflows. In multizone approaches the building is divided into various zones relative to building layout with specific characteristics. Each zone is assumed as a well-mixed zone in which temperature and contaminant concentration is homogenously distributed. Zones are connected through flow paths and multizone model is able to calculate flowrate and pressure difference through these flow paths (Dols and Polidoro 2015).
Various multizone software have been developed in building research including: CONTAM, COMIS, AIRNET, BREEZE and ASCOS (Wang and Zhai 2016). CONTAM and COMIS are two of the more popular multizone airflow programs. CONTAM was developed by the “Building and Fire Research Laboratory of the National Institute of Standards and Technology” (NIST) in 1993. CONTAM is freely available software though the Building and Fire Research Laboratory of NIST with a relatively user-friendly interface and the results in post processing are easy to understand and follow. The first version was CONTAM 93 developed from AIRNET (1989) (Emmerich et al. 1994). After Version 3.0, CONTAM was developed to be integrated with CFD models to account for non-uniform mixing within buildings and wind flow effects around the building envelop.

COMIS (Conjunction of Multizone Infiltration Specialists) (Feustel 1999) was developed by an international group of experts (The Energy Performance of Building Group) at the Lawrence Berkeley National Laboratory (LBNL). Both CONTAM and COMIS account for wind, stack, and mechanical ventilation effect in changing building airflow and indoor contaminant distribution. These multizone modeling approaches have been validated in different studies that predict air flow rates or contaminant transport in buildings. Li (2002) reported good agreements between the model predictions and experimental data collected in a controlled environment test laboratory and field measurement data (Li 2002, Haghghat and Li 2004). Wang et al. demonstrated that the multizone model predictions agreed well with the field measurements (Wang et al. 1998).

CFD approach can calculate contaminant spatial variability in a zone while multizone models consider a uniform value of contaminant and temperature in each zone. CFD methods are computationally expensive which can be a main disadvantage of this
approach (Figure 4-1). Coupling CFD models and multizone models is a promising way to take advantages of each method and reduce the disadvantages. The CFD model introduced by NIST to be integrated with CONTAM is CFD0 which is able to incorporate turbulence models to CONTAM.

![Building simulation tools diagram](image)

**Figure 4-1: Advantages (pros) and disadvantages (cons) of various building simulation tools**

In coupled CONTAM and CFD0 program, CFD0 applies to the zone where the multizone assumption fail and CONTAM applies to the rest of zones. Wang and Chen (2007) validated the results of the coupled CONTAM and CFD0 programs with experimental data from a four-zone facility at Purdue University (Wang and Chen 2007). The results indicated that the coupled program (CONTAM-CFD0) calculated more accurate airflow rates compared to CONTAM and used less computing time compared to CFD0. Coupled CONTAM-CFD0 program reduced computational time up to one order of
magnitude compared to CFD0 and were able to correctly predict the airflow and contaminant distribution in all zones (Wang and Chen 2007).

CFD0 is a CFD program originally developed for the American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) project RP-927 (Chen et al. 1999) which is currently freely available through NIST. CFD0 solves a set of partial differential equations for pressure, air velocity, temperature and species concentration calculations (Wang et al. 2010). CFD0 can be internally and externally coupled to CONTAM (Wang et al. 2010, Dols and Polidoro 2015). In internal coupling method the CFD zone is a zone assumed poorly mixed in a well-mixed multizone building. Spatial variation of contaminant and temperature is calculated in the CFD zone and remaining zones behave like a well-mixed zone. In the internally linked method, CONTAM gives pressure boundary conditions to CFD0, and CFD0 gives the pressure boundary condition back to CONTAM until both the inputs and outputs stabilize, and solution converge (Wang and Chen 2005).

In the externally coupled method, which is the method of interest in this study, outdoor air is considered as the CFD zone and building zones (rooms) are considered as well-mixed zones in CONTAM. The outdoor CFD zone accounts for wind pressure effect as a function of, wind direction, wind speed, building configuration and local terrain effects. CFD0 calculates pressure coefficients ($C_p$) on building envelope for each leakage path for a range of wind directions. Pressure coefficient values are a function of location of the paths on a building surface and wind direction, thus CFD does not need to run whenever wind speed changes which considerably saves computational time in coupling method. After pressure coefficient ($C_p$) values are calculated by CFD0 for different wind
directions, CONTAM will be linked to CFD0 and uses appropriate pressure coefficient values for each flow path defined on building envelope in CONTAM. To calculate building airflows, zonal pressure, AER and indoor air concentration, CONTAM uses conservative mass and concentration equations (Wang et al. 2010, Dols and Polidoro 2015). In following sections, the possibility and advantage of an external link of CONTAM and CFD0 in vapor intrusion studies is discussed.

4.2.3. CONTAM-CFD0 Application in vapor intrusion studies

Early versions of CONTAM has been used in some radon transport studies to predict radon concentration and interzone airflow rates in a large multizone buildings (Persily 1993, Fang and Persily 1995). Persily investigated the effect of radon source terms, indoor and outdoor temperature difference and exterior and interior walls’ leakage characteristics and mechanical ventilation operation on airflow rates and radon concentration distribution in a twelve-story residential building (Persily 1993). Persily reported that radon distribution within the building is not only affected by radon entry rate but also affected by the airflow pattern in the building (Persily 1993).

Existing vapor intrusion models (Johnson and Ettinger 1991, Abreu and Johnson 2005, Pennell et al. 2009) typically focus on problem identification in single family residential buildings and the subsurface soil, without considering above ground processes effect (such as weather condition, building configuration, climate effect and occupant behavior) on contaminant concentration distribution and dynamic building AER and pressure (Table 4-1). Coupling vapor intrusion models with CFD0-CONTAM program is a potential field of study in vapor intrusion investigations that introduce the ability of CFD and multizone indoor air quality programs in considering weather and building condition.
effect on contaminant concentration distribution to vapor intrusion community (Table 4-1 and Figure 4-2). Additionally, multizone indoor air quality models can predict contaminant concentration in multiple zones of buildings, while previous vapor intrusion models usually predict indoor concentration in a single zone of building (typically the basement).

Table 4-1: Advantages and disadvantages of models used in vapor intrusion and building science

<table>
<thead>
<tr>
<th>Models/methods</th>
<th>Proposed by</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Vapor intrusion</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J&amp;E</td>
<td>Johnson and Ettinger (35)</td>
<td>Faster than finite element and finite difference methods</td>
<td>Do not account for above ground processes such as weather and building condition in calculating indoor air concentration</td>
</tr>
<tr>
<td>Finite difference methods</td>
<td>Abreu and Johnson (33)</td>
<td>Gives details of soil concentration and pressure</td>
<td></td>
</tr>
<tr>
<td>Finite element methods</td>
<td>Pennell et al. (34)</td>
<td>Gives details of soil concentration and pressure</td>
<td></td>
</tr>
<tr>
<td><strong>Building science</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CONTAM</td>
<td>NIST (8)</td>
<td>Accounts for building characteristics in calculating indoor air concentration and faster than CFD models</td>
<td>Not able to give details of concentration and temperature distribution</td>
</tr>
<tr>
<td>CFD models</td>
<td>NIST (8)</td>
<td>Calculates indoor air concentration in details</td>
<td>Computationally expensive</td>
</tr>
<tr>
<td>CFD0-CONTAM</td>
<td>NIST (8)</td>
<td>Accounts for building characteristics and weather condition in calculating indoor air concentration and faster than CFD models, results are more accurate than CONTAM only model</td>
<td>Not as fast as CONTAM only method</td>
</tr>
</tbody>
</table>
Notes: Inputs and outputs are shown for each model. Wind pressure coefficients are the output of CFD0, which is required as input for CONTAM. CONTAM requires contaminant flux as the input to predict indoor air concentration. Contaminant flux can be estimated by vapor intrusion models or from field site measurements.

Figure 4-2: Combination of vapor intrusion models, CFD and multizone indoor air quality programs to predict indoor air quality impacted by vapor intrusion sites.

In CONTAM, we need to identify an appropriate representation of the building as a collection of zones that exchange air with each other through the air flow paths with appropriate leakage characteristics between the zones (zones can be the building rooms or outdoor area). Leakage characteristics can be measured using the air leakage measuring methods (Breen et al. 2014, Reichman et al. 2017) or can be specified using the suggested air leakage area (Effective leakage area (ELA)) values in ASHRAE Handbook of Fundamentals (ASHRAE 2001). In general, there are too many leakage paths in a building to be measured, therefore the range of ELA values for different kind of pathways suggested by ASHRAE Handbook of Fundamentals are a reliable source of ELA values to be used in multizone indoor air quality programs (ASHRAE 2001).
CONTAM can account for an unlimited number of contaminants and sources within a given building model (Dols and Polidoro 2015). The rate at which contaminant enters a building is the link between vapor intrusion models and CFD0-CONTAM program (Figure 4-2). The entry rate of a contaminant is an input value in multizone indoor air quality models that can be determined using vapor intrusion models (Johnson and Ettinger 1991, Abreu and Johnson 2005, Pennell et al. 2009) or measured in a building located on vapor intrusion sites. Shirazi and Pennell linked a 3D vapor intrusion model to CFD0-CONTAM to improve previous vapor intrusion modeling approaches and predicted building AER, indoor pressure and indoor air concentrations based on weather conditions and building characteristics (See chapter 5)(Shirazi and Pennell 2017).

Table 4-2 indicates the advantages of new developed vapor intrusion model (which is a combination of previous vapor intrusion models with CFD0-CONTAM) (Shirazi and Pennell 2017) compared to previous vapor intrusion models. As shown in Table 4-2, the building AER’s and pressure difference between indoor and outdoor was a user defined value in previous vapor intrusion models, however building AER and pressure difference between indoor and outdoor is a function of many factors including, weather conditions, building characteristics and occupants behavior. Shirazi and Pennell indicated that vapor intrusion models can be improved by being coupled with building science programs and predict building AER and indoor air concentration considering above ground processes (Shirazi and Pennell 2017).
### Table 4-2: Values calculated in previous vapor intrusion models compared to values calculated in vapor intrusion model linked to CFD0-CONTAM programs

<table>
<thead>
<tr>
<th>Values</th>
<th>Previous vapor intrusion models</th>
<th>Vapor intrusion model linked to CFD0-CONTAM programs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Indoor pressure</td>
<td>User defined</td>
<td>Calculated Based on building and weather condition</td>
</tr>
<tr>
<td>Outdoor air pressure profile</td>
<td>Not calculated</td>
<td>Calculated</td>
</tr>
<tr>
<td>Building air exchange rate</td>
<td>User defined</td>
<td>Calculated Based on building and weather condition</td>
</tr>
<tr>
<td>Mass entry rate</td>
<td>Calculated</td>
<td>Calculated</td>
</tr>
<tr>
<td>Soil concentration profile</td>
<td>Calculated</td>
<td>Calculated</td>
</tr>
<tr>
<td>Soil pressure profile</td>
<td>Calculated</td>
<td>Calculated</td>
</tr>
<tr>
<td>Indoor air concentration</td>
<td>Calculated</td>
<td>Calculated</td>
</tr>
</tbody>
</table>

Indoor air concentration variations in vapor intrusion studies have multiple explanations including mass entry rate variation, building and weather condition variations, climate zone in which the building is located, etc. Considering building simulation technique capabilities in estimating indoor air concentration and building airflow rates, this review suggests incorporating building simulation tools at vapor intrusion studies could provide useful information. The new developed model by Shirazi and Pennell calculated AER and indoor air concentration under different weather conditions and compared the model results with previous models (Abreu and Johnson 2005, Pennell et al. 2009) in vapor intrusion studies (Shirazi and Pennell 2017). Shirazi and Pennell reported that their model compares qualitatively well with field data collected by (Luo et al. 2009).

#### 4.2.4. Conclusion

Vapor intrusion is well-known to be difficult to characterize using field data because indoor air concentrations exhibit considerable temporal and spatial variability throughout impacted communities. Using building science information, vapor intrusion
scientists can evaluate how weather and building conditions may impact vapor intrusion exposure risks, in particular indoor air concentrations. Incorporating building science perspectives and tools is advantageous over focusing primarily on subsurface fate and transport processes. Figure 4-2 and Table 4-2 highlight that by integrating building science into vapor intrusion modelling approaches, the role that building and weather conditions play in altering vapor intrusion exposure risks can be better understood.
CHAPTER 5: WIND AND STACK EFFECTS COMBINATION ON INDOOR, ATMOSPHERIC, AND SUBSURFACE DOMAINS IN VI STUDIES (Published Article)

This chapter includes an article that is published in the Environmental Science Processes & Impacts journal (E. Shirazi and K. G. Pennell, 2017). “Three-dimensional vapor intrusion modeling approach that combines wind and stack effects on indoor, atmospheric, and subsurface domains.” DOI: 10.1039/c7em00423k

Existing vapor intrusion modeling approaches, although extensively used and published, lack sophistication to directly calculate building air exchange rates and building pressures. Consequently, vapor intrusion modeling has focused predominantly on subsurface domains. This paper provides a new modeling approach that combines three domains—indoor air, atmospheric air and subsurface soil gas. The modelling approach accounts for building-specific features and weather conditions to determine air exchange rates, indoor air pressures and contaminant concentrations in the soil gas and indoor air. It is advantageous over previous vapor intrusion models because it incorporates information known to influence indoor air exposure risks, but that has not been adequately incorporated into previous VI models.

5.1. Abstract

Vapor intrusion exposure risks are difficult to characterize due to the role of atmospheric, building and subsurface processes. This study presents a three-dimensional VI model that extends the common subsurface fate and transport equations to incorporate wind and stack effects on indoor air pressure, building air exchange rate (AER) and indoor
contaminant concentration to improve VI exposure risk estimates. The model incorporates three modeling programs: 1) COMSOL Multiphysics to model subsurface fate and transport processes, 2) CFD0 to model atmospheric air flow around the building, and 3) CONTAM to model indoor air quality. The combined VI model predicts AER values, zonal indoor air pressures and zonal indoor air contaminant concentrations as a function of wind speed, wind direction and outdoor and indoor temperature. Steady state modeling results for a single-story building with a basement demonstrate that wind speed, wind direction and opening locations in a building play important roles in changing the AER, indoor air pressure, and indoor air contaminant concentration. Calculated indoor air pressures ranged from approximately -10Pa to +4Pa depending on weather conditions and building characteristics. AER values, mass entry rates and indoor air concentrations vary depending on weather conditions and building characteristics. The presented modeling approach can be used to investigate the relationship between building features, AER, building pressures, soil gas concentrations, indoor air concentrations and VI exposure risks.

5.2. Introduction

Vapor intrusion (VI) is a process by which volatile organic compounds (VOCs) migrate through the soil from a subsurface vapor source into the indoor air of nearby buildings. Exposure risks related to VI has been a growing concern in recent years and the United States Environmental Protection Agency (USEPA) recently established VI guidance (USEPA 2015). While indoor air targets exist for many contaminants of concern at VI sites, regulatory standards do not currently exist for soil vapor concentrations. Therefore, USEPA recommends non-traditional data sets (i.e. multiple lines of evidence) to evaluate the potential for VI exposure risks (USEPA 2015). The multiple lines of
evidence approach provides a flexible framework for investigating vapor intrusion; however, there is a need to improve the understanding of how building operation and atmospheric conditions affect VI exposure risks.

Professional judgement and inclusion of multiple lines of evidence when conducting VI site assessments is widely acknowledged as valuable (USEPA 2015). Since no other published VI modeling approach has attempted to predict AERs or indoor air concentrations based on weather conditions or specific building features, the model presented here is meant to help inform about processes that are not yet well understood within the VI community. The number of field studies to compare the results of VI models is small, and practically speaking, model verification using field data is not currently feasible and presently there is no VI model that has been fully validated in the field. However, it is important that new models are compared to previously well-established modeling approaches. The results of the model developed as part of this research was compared to two previously published models (Abreu and Johnson 2005, Pennell et al. 2009) for select cases. In addition, the model was qualitatively compared to field data from (Luo et al. 2009).

VI processes. With few exceptions, VI models are commonly employed as screening tools. Screening models provide information about whether additional site investigation is warranted. A widely employed screening tool is based on the efforts of Johnson and Ettinger (Johnson and Ettinger 1991). This model (known as the Johnson and Ettinger, or J&E model) is a one-dimensional (1-D) approximation, and has been adapted as a spreadsheet program by several regulatory agencies for risk-based screening purposes (e.g. (USEPA 2004)). More recently, USEPA has developed a screening level calculator that relies on empirically-based data to establish screening levels for VOCs at VI sites (USEPA 2014). The screening VI models primarily focus on soil gas entry, with little emphasis on complex role aboveground processes play in the VI process.

The emergence of three-dimensional (3-D) vapor intrusion models has provided considerable insight into the VI process and are an important tool within the multiple lines of evidence framework for assessing vapor intrusion exposure risks (Pennell et al. 2016). One of the first 3-D VI models incorporated a finite difference numerical code in which a continuity equation was coupled with a chemical transport equation to calculate the soil gas pressure, velocity and chemical concentration in soil and indoor air (Abreu 2005, Abreu and Johnson 2005, Abreu and Johnson 2006). Later, Pennell et al. (2009) developed a similar 3-D VI model, but incorporated a commercially-available finite element numerical code (Pennell et al. 2009). Most 3-D VI models have focused on subsurface transport process; however only a few have considered aboveground processes (e.g. (Luo et al. 2009)).

(Reichman et al. 2017) reviewed the importance of considering building air exchange rates (AERs) when evaluating VI exposure risks; and, other VI researchers have
also highlighted the role that factors such as wind flow and temperature can have on contaminant transport in subsurface and also indoor air concentration distribution (Riley et al. 1996, Riley et al. 1999, Luo 2009, Luo et al. 2009, Song et al. 2013, Shen and Suuberg 2016). (Reichman et al. 2017) noted that existing VI models require users to input generic building pressures and AERs even though indoor air science research provides tools to determine AERs and building pressures based on building characteristics, occupant behavior and weather conditions.

In this study, we improve existing VI models by incorporating wind and stack effects, and building characteristics to calculate indoor air pressures, AERs, and indoor air concentrations. We present a theoretical basis, overall governing equations, a general modeling approach that combines subsurface VI model approaches with a multizone indoor air quality model coupled with an outdoor atmospheric model and provide illustrative results.

5.3. Theory and Methods

This manuscript presents a framework for a new modeling approach that advances current VI models by linking existing subsurface VI models to an aboveground computational fluid dynamic (CFD) program and a multizone indoor air quality modeling program. Multizone indoor air quality programs predict infiltration and exfiltration through openings of different building zones under given weather conditions (Feustel and Dieris 1992, Dols 2001). These programs are especially valuable because they can calculate the airflow and relative pressures between different building zones and AER values (Haghighat and Li 2004, Wang and Zhai 2016). They have been used for indoor air quality, including radon intrusion studies (Persily 1993). Recently multizone programs have been improved
by coupling with CFD programs to combine the effect of indoor and outdoor air quality on pressure gradients and air flow rate distribution in a building (Wang 2007, Wang et al. 2010).

5.3.1. Background

AERs are known as an important parameter that control indoor air quality. Weather condition and building condition and operation (air conditioning status and occupant preference) are factors that can affect AERs. Recently, (Reichman et al. 2017) reviewed several indoor air quality studies and highlighted important considerations for including accurate estimates of AERs during VI assessments. In addition, they summarized methods for estimating AERs.

Wind and stack effects are two driving forces that influence AER, indoor-outdoor pressure differences, and consequently VI exposure risks. Stack effect is caused by air density differences that result from temperature differences between indoor and outdoor air. Wind flow not only influences AER and air pressure inside a building, but also influences the ground surface pressure adjacent to the building, which consequently alters the soil gas flow and subsurface soil gas concentrations under the building (Riley et al. 1996, Riley et al. 1999, Luo 2009). Previous radon research has highlighted the importance of wind and stack effects for radon intrusion. For instance, Riley et al. (1996, 1999) used the mean ground-surface pressure coefficients obtained from a wind tunnel experiment on a single family structure to investigate the effect of wind speed and direction on radon concentration in soil and indoor air (Riley et al. 1996, Riley et al. 1999). While Riley et al. (1996, 1999) models did not account for stack effect on indoor air pressure, Sherman
(1992) stated that stack effect is more effective than wind effect in changing the radon entry rate into a building.

A few vapor intrusion models have specifically investigated the role of stack and wind effects. Song et al. (2013) assessed the influence of stack and wind effects on soil gas entry rate and outdoor air flowrate through the building, however the authors did not consider wind effect (or wind direction) on subsurface pressure, which influences on soil gas entry rate (Song et al. 2013). Shen and Suuberg (2016) showed that the AER and indoor air pressure variation can result in substantial variation in indoor air contaminant concentration; however they did not indicate how wind and temperature influence AER or indoor air pressure (Shen and Suuberg 2016). Although these studies are important in highlighting the importance of aboveground processes on VI, these studies have not considered how AER and indoor air pressure are directly connected to wind and stack effects, and how together all of these parameters collectively alter VI exposure risks.

To date, one of the most comprehensive VI studies to investigate wind and stack effects involved a site in Evansville, Wyoming (Luo 2009, Luo et al. 2009). The findings showed that wind flow is important in influencing (an aerobically biodegradable) contaminant and oxygen concentrations in the soil under a building. The results showed low concentration of contaminant and high concentration of oxygen at the windward side of the building, while a high concentration of contaminant and depleted oxygen was reported on the leeward side of the building (Luo 2009, Luo et al. 2009). The study concluded that the oxygen delivered to the soil by wind on the windward side enhanced aerobic biodegradation of the contaminant. Luo (2009) developed a numerical model that modified the 3-D VI model previously developed by Abreu and Johnson (2005) to account
for the influence of wind and stack effects; however the modified model did not consider the effect of wind and stack effects on AER when calculating the indoor air concentration (Luo 2009).

The research described herein presents a modeling framework that advances previous modeling efforts by accounting for the influence of wind and stack effects on AER, indoor-outdoor pressure differences, ground surface pressures, and predicts indoor air contaminant concentrations using a multizone model.

5.3.2. Model Methods

This study relies on three modeling programs: 1) a three dimensional finite element Multiphysics program known as COMSOL Multiphysics, 2) CFD0 which is a CFD program, and 3) CONTAM which is a multizone indoor air quality and ventilation analysis computer program developed by the Building and Fire Research Laboratory of the National Institute of Standards and Technology (NIST). CFD0 and CONTAM are both freely available software through the Building and Fire Research Laboratory of NIST.

In VI studies, most existing VI models incorporate a user defined value for indoor air pressure as a boundary condition; however, indoor air pressure is influenced by wind and stack effect (ASHRAE 2013). To investigate wind and stack effects, this research uses an indirect coupling approach between CONTAM and CFD0 through the air flowrates at the interfaces. Indirect coupling used by Wang (2007) is a one-step strategy in which CFD0 and CONTAM run sequentially.

CONTAM runs two times in this study: One time to calculate basement pressure and AER (CONTAM (1)). The basement pressure is used as boundary condition in COMSOL; and one time to calculate indoor air contaminant concentration (CONTAM (2))
after the mass entry rate of contaminant through the cracks is obtained by COMSOL. 

Figure 5.1 illustrates a step by step overview of the modeling process used in the present study. In Step 1, the user inputs the building characteristics and the wind direction range (0-360°). CFD0 solves the Reynolds Averaged Navier-Stokes (RANS) equations to calculate the distribution of wind pressure on building surface. Then, CFD0 converts the wind pressures on the building envelope to wind pressure coefficients (C_p) using Bernoulli’s equation (Step 1, Figure 5.1) (Wang et al. 2010).

In step 2(a) and 2(b) (Figure 5.1), C_p values are assigned to each flow path (any small or large opening) of the building for variable wind directions in wind pressure profile (WPP). Small openings around windows, doors, or walls can be considered as small flow paths, and open window and doors can be considered as large flow paths. The user defines the path locations in Step 2a which depends on building characteristics. CONTAM (1) calculates the AER, the zonal indoor air pressures and air mass flowrates through the paths by solving the mass balance equations for all the zones considering wind effect (by C_p values) and stack effect (Step 3, Figure 5.1) (Wang et al. 2010).

In step 4, zonal pressures obtained in step 3 are used as boundary conditions for foundation cracks in COMSOL. Unlike previous VI models (e.g. (Pennell et al. 2009)), where the pressure at the foundation cracks were defined by the user, in this model, the boundary condition at the crack is defined by the results from CONTAM (1) and is influenced by stack and wind effects. The influence of wind flows on the pressure outside of the building in the surrounding air and soil domains, as well as the contaminant concentration in soil domain, is determined by COMSOL. COMSOL calculates the mass entry rate of contaminant near the foundation cracks which is used as inputs in step 5.
(Figure 5.1). In step 5, CONTAM (2) calculates the indoor air concentration of contaminant considering the zonal pressures, infiltration and exfiltration rates and AER obtained in step 3. Both COMSOL and CFD0 solve for the wind pressure. COMSOL solves for the wind pressure in atmospheric air and on the ground surface. COMSOL links the ground surface pressure created by wind to the subsurface soil pressure to investigate how wind flow influences subsurface soil pressure and consequently soil gas concentration. CFD0 is used to calculate the pressure coefficients on the building surface. CFD0 is then coupled to CONTAM to calculate indoor pressure and building AER based on wind and stack effects. The COMSOL and CFD0 wind pressure results in the atmospheric domain are compared to ensure agreement between modeling approaches.

Turbulent (wind) flows are solved using a segregated approach to prevent the solution from becoming ill-conditioned. Each iteration of the RANS group involves a sub-iteration of two or three repetitions conducted for the turbulence transport equations. Specifically, the sub-iteration is required to assure the balance of the very non-linear source term in the turbulence transport equations before the next iteration for the RANS group. The default iterative solver for the turbulence transport equations in COMSOL is GMRES accelerated by Geometric Multigrid.
In the present study, there is no external contaminant source, so the \( C_c \) values in WPC file are equal to zero.

*(2) WPC file for each path contains building envelope \( C_p \) values for all assigned wind directions.

**WPP file: Wind Pressure Profile

Figure 5-1: Overview of modeling process

The overall governing equations used in this modeling process are as follows:

CONTAM calculates indoor air pressure by solving mass balance equations for all the zones (Dols and Polidoro 2015). In a steady state condition the principle of conservation of mass states that:

\[
\sum_j F_{ji} = 0 \quad (5.1)
\]
where $F_{ji}$ (kg/s) is the air mass flow rate between zones j and i which is a function of the pressure drop between these two zones. A positive value for $F_{ji}$ shows that air is flowing from zone j to zone i and a negative value indicates an opposite direction from i to j.

In this study, CONTAM calculates the air mass flow rate ($F_{ji}$) through a crack or opening in a building envelope based on the power law equation for different types of air flow paths:

$$F_{ji} = C(\Delta P)^n$$  \hspace{1cm} (5.2)

where $\Delta P$ (Pa) is the pressure difference across a flow path between zones j and i, $C$ (kg/s.Pa$^n$) is the flow coefficient, and n (dimensionless) is the flow exponent which, theoretically, lies between 0.5 and 1 values. (Orme et al. 1994) showed that n varies between 0.6 and 0.7 in houses. In this study we use 0.65 for n value (for closed windows, doors and external walls) which is a typical value for small crack-like openings. For cracks, CONTAM uses equation 5.3 (Dols and Polidoro 2015):

$$n = 0.5 + 0.5\exp\left(-\frac{W}{2}\right)$$  \hspace{1cm} (5.3)

In which W is the crack width in mm.

Using equation 5.4, CONTAM converts the parameters that describe an opening to flow coefficient ($C$) in equation 5.2:

$$C = LC_d \sqrt{2} (\Delta P_r)^{\frac{1}{2}-n}$$  \hspace{1cm} (5.4)

where $C_d$ (dimensionless) is the discharge coefficient, $\Delta P_r$ (Pa) is the reference pressure difference on a pressurization test. The set of reference condition used in this study
is $C_d = 1$ and $\Delta P_r = 4 \text{ Pa}$. $L$ (cm²/m² or cm² per item) is the effective leakage area of an opening in the building. Typical leakage areas for residential buildings have been provided in chapter 26 of 2001 ASHRAE Handbook of Fundamentals (see table 1 of (ASHRAE 2001)).

In equation 5.2, pressure difference between two zones ($\Delta P$) for each air flow path is calculated using equation 5.5 which includes three components: 1) wind effect, 2) stack effect, and 3) zone pressure difference.

$$\Delta P = P_j - P_i + P_s + P_w \quad (5.5)$$

where $P_j$ (Pa) and $P_i$ (Pa) are total pressure at zones $j$ and $i$, respectively. $P_s$ (Pa) is the pressure difference due to stack effect and $P_w$ (Pa) is the pressure difference induced by wind effect. Pressure difference caused by stack and wind effect at height $H$ is computed using the equations 5.6 and 5.7, respectively, based on 2013 ASHRAE Handbook of Fundamentals (ASHRAE 2013).

$$P_s = \rho g (H_{NPL} - H) \frac{T_{in} - T_{out}}{T_{in}} \quad (5.6)$$

where $\rho$ (kg/m³) is outdoor air density, $g$ (m/s²) is gravitational acceleration, $H_{NPL}$ (m) is the location in the building envelope where there is no indoor-to-outdoor pressure difference, and $T_{in}$ (°C) and $T_{out}$ (°C) are the indoor and outdoor temperatures, respectively.

$$P_w = \frac{1}{2} \rho U_H^2 C_p \quad (5.7)$$

where $U_H$ (m/s) is the wind velocity at the reference height $H$ (m) that can be calculated as follows:
\[ U_H = U_{\text{met}} \left( \frac{\delta_{\text{met}}}{H_{\text{met}}} \right)^{a_{\text{met}}} \left( \frac{H}{\delta} \right)^{\alpha} \]  \hspace{1cm} (5.8)

In which, \( U_{\text{met}} \) (m/s) is the wind velocity at the height of \( H_{\text{met}} \) (m); \( H_{\text{met}} \) is the reference height at the meteorological station (Usually 10m above ground level); \( \delta_{\text{met}} \) (m) and \( a_{\text{met}} \) (dimensionless) are the atmospheric boundary layer thickness and the exponent at meteorological station, respectively. \( \delta \) (m) and \( \alpha \) (dimensionless) are the corresponding values for the local building terrain which can be found in chapter 24 of 2013 ASHRAE Handbook of Fundamentals (see table 1 of (ASHRAE 2013)).

To calculate \( C_p \) (the wind pressure coefficient for the airflow path), CONTAM is coupled with a CFD program (CFD0) through the airflow rates or pressure drops at the interfaces. CFD0 solves the Reynolds Averaged Navier-Stokes equations to calculate the distribution of wind pressure on building surface. Then wind pressure coefficients will be calculated using Bernoulli’s equation (Equation 5.9):

\[ C_p = \frac{P_D}{\frac{1}{2} \rho U_H^2} \]  \hspace{1cm} (5.9)

where \( C_p \) (dimensionless) is the wind pressure coefficient at a point on the building surface, \( P_D \) (Pa) is the difference between wind pressure on the building surface and the free-stream pressure. \( C_p \) values will be calculated by CFD0 for a specific local terrain feature and different wind directions. \( C_p \) values are a function of location of the paths on a building surface and wind direction. (Wang et al. 2010) compared the predicted wind pressure coefficients (using CFD0) with measured data (Holmes 1986, Holmes 1994) and the results showed that the calculated values are in good agreement with measured data.

Based on the equations above, equation 5.1 is a nonlinear function of \( P_i \) and \( P_j \):
\[
\sum_j F_{ji} = \sum_j f(P_j, P_i) = 0
\] (5.10)

Regarding equation 5.10, the steady state mass flow analysis for multiple zones requires the simultaneous solution of nonlinear equations by Newton-Raphson method until a convergent solution of the set of zone pressures is attained \((P_j, P_i, \ldots, P_n)\).

Zones can be defined in CONTAM with either known or unknown pressures. Unknown pressure zones are linked by pressure dependent flow paths to a constant pressure zone, like an ambient zone (when there is no wind flow the ambient pressure would be equal to zero and in case wind is blowing, ambient pressure will be calculated using CFD0).

Once the zonal pressures are computed, the air mass flow rates are calculated using equation 5.2. Contaminant concentration in each zone then can be calculated based on conservation of mass in each zone. CONTAM uses the following conservation of mass equation in steady state condition to compute the contaminant concentration in each zone (Dols and Polidoro 2015):

\[
0 = \sum_j F_{j\rightarrow i} C_j^\alpha + G_i^\alpha - \sum_j F_{i\rightarrow j} C_i^\alpha - R_i^\alpha
\] (5.11)

\(C_i^\alpha\) represents the contaminant air concentration as a mass ratio (mass of contaminant \(\alpha\) in zone \(i\) / mass of air in zone \(i\)) and is reported as kg/kg. The first term in Equation 5.11 accounts for contaminant entry by inward flows \((F_{j\rightarrow i})\) through paths from nearby zone \(j\) to zone \(i\). The third term indicates contaminant removal by outward airflows from zone \(i\) \((F_{i\rightarrow j})\) (Dols and Polidoro 2015).

In this study, the contaminant is added or removed from a zone in a building by inward or outward airflows \((F_{j\rightarrow i}\) and \(F_{i\rightarrow j}\)), which are a function of wind and stack effect.
Inward and outward air flows include air from outside the building as well as interzonal flows.

The second and last terms allow the contaminant to be added or removed from a zone at a constant generation ($G_{i\alpha}$) or removal ($R_{i\alpha}$) rates (kg/s of contaminant $\alpha$). The COMSOL multiphysics program computes the mass entry rate and contaminant concentration near the foundation cracks solving a chemical transport equation which is coupled with a soil gas continuity equation. The resulting VI entry rate corresponds to $G_{i\alpha}$ in equation 5.11. Although not included in this study, CONTAM includes $R_{i\alpha}$, which allows removal of the chemical from a zone at a given rate.

The general approach, for computing mass entry rate, has been well described previously (Pennell et al. 2009). COMSOL uses weak constraints to obtain accurate estimates of soil gas entry rates through the crack; and, then mass flux, a combination of advective and diffusive flux, into the building is calculated assuming 1D transport through the crack. Unlike previous studies, the COMSOL Multiphysics software is used to investigate the influence of wind/stack effects in both atmospheric and subsurface domains. In the current model application, Darcy’s law equation is coupled with RANS equations with turbulence models (k-ε) to solve turbulent wind flow above and around a building to obtain the mass entry rate by considering both wind and stack effects. The application of this model can be expanded to include contaminant mass entry through other entry points besides foundation cracks (i.e. preferential pathways). The mass entry rates from other sources would be combined with the mass entry rate determined for vapor intrusion (via cracks) by COMSOL and added to CONTAM as $G_{i\alpha}$.
5.3.3. COMSOL Multiphysics

Simulations in this study are carried out on a residential single story building with basement that extends 2m below ground surface (bgs). The air and soil domain dimensions are 200 m (Length) ×200 m (Width) ×50 m (Height) and 200 m (Length) ×200 m (Width) ×8 m (Height), respectively. The single-story building has a 10m×10m area with 3 m (Height) walls aboveground. The building has a roof that has an additional height of 1.8 m (≈20° slope) making the total building height 4.8 m above grade (Figure 5.2). The building is located in the center of soil and air domains. A perimeter crack with 0.005 m width and 0.1999 m² area is located around the basement foundation and serves as the entry point for contaminant vapors. All simulations are modeled for steady state conditions.

It is assumed that the subsurface domain consists of homogeneous soil. The source of the contaminant is assumed to be trichloroethylene (TCE) (MW=131.4 g/mol) located at 8 m bgs along the bottom of the entire modeling domain. The vapor source concentration is defined as 2.014×10⁻³ mol/m³ which is consistent with the source concentration used in previous modeling studies (Pennell et al. 2009). This concentration was selected for ease of comparison between previous and current studies. The total soil porosity and soil permeability to soil gas flow are 0.35 (m³ voids)/(m³ soil) and 1×10⁻¹² m², respectively. The overall effective diffusion coefficient for transport in the porous media is 8.68×10⁻⁷ m²/s in models. The diffusivity of TCE in air is equal to 7.4×10⁻⁶ m²/s. In addition, one scenario with 10⁻¹⁴ m² soil permeability and 0.45 (m³ voids)/(m³ soil) total soil porosity is studied to investigate the influence of soil permeability and soil gas diffusion coefficient on contaminant concentration distribution in soil while wind blows above ground. The overall effective diffusion coefficient for transport in the porous media equals to 4.37×10⁻⁷ m²/s in
the latter scenario, which is consistent with the soil properties used in previous modeling studies (Pennell et al. 2009).

The element shape was tetrahedral. The minimum element size is 0.1 mm and the maximum element size is 2 m. The element growth rate is 1.5. The number of elements for the no wind flow scenario is $4.3519 \times 10^6$ elements. The number of elements for scenarios with wind flow is $1.0086 \times 10^7$ elements. All scenarios were run using the University of Kentucky high performance computing cluster (DLX2/3), which is a traditional batch-processing institutional cluster, with high-speed interconnects and a shared filesystem. The DLX cluster provides over 4800 processor cores, 18TB of RAM, and 1PB of high-speed disk storage. Model run times for scenarios with wind flow typically ranged from 1 to 4 hours.

5.3.4. **CONTAM coupled with CFD0**

This study is not meant to be representative of an actual building but to present a VI model that couples a multizone and CFD programs and is capable of generating soil vapor entry rates, indoor pressures, AERs and indoor concentrations in the presence of wind and stack effects. In the multizone model, all zones are assumed as well-mixed zones, which means each zone has been considered as a single node wherein air has uniform temperature, pressure and contaminant concentration. The building modeled in this study has two zones, the basement and the first floor which are connected by a stairway. The cross-sectional area of the stairs is equal to 10 m$^2$ and the stair treads are assumed to be closed. All simulations are modeled for steady state conditions.

The building is connected to outdoor area by a door in south and one window on each north and south sides of the building. There is no window or door on the east and west
side of the building. Windows and doors are assumed to be closed and the only pathways through the building are the leakage areas in windows, doors and external walls. The plan view of the 1st floor and profile view of the building is shown in Figure 5.2.

![Diagram of a) First Floor Plan and Wind Directions and b) Single Story Building With Basement]

Figure 5-2: a) 1st floor plan view and wind directions blew on building b) elevation of the modeled building

In the present study, airflow through various pathways is modeled using powerlaw relationship (described in Model Method section). Perimeter cracks (5mm wide) allow soil gas to enter the building. The leakage characteristics for external walls, windows and doors
can be gained based on range of leakage values for various components in chapter 26 of ASHRAE Handbook of Fundamentals, 2001 (ASHRAE 2001). The values of leakage areas used in this study are shown in Table 5.1 which are the best estimate values of leakage ranges suggested by ASHRAE Handbook of Fundamentals, 2001 (ASHRAE 2001). All leakage areas are based on a reference pressure ($P_r$) of 4 Pa and a discharge coefficient ($C_d$) of 1.0. Indoor air temperature in models is equal to 23°C which is a value inside the comfort zone (see Chapter 9, Figure 5 of (ASHRAE 2013)). Using Lexington, Kentucky as a representative case and considering 99.6% confidence, the maximum and minimum outdoor air temperatures are assumed to be 33°C and -12°C, respectively (see Chapter 9 of (ASHRAE 2013)).

Table 5-1: Effective air leakage areas used in this study (best estimate values in (ASHRAE 2001)

<table>
<thead>
<tr>
<th>Path</th>
<th>Type</th>
<th>Units</th>
<th>Best Estimate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Door frame</td>
<td>General</td>
<td>cm²/ea</td>
<td>12</td>
</tr>
<tr>
<td>Door</td>
<td>Single, not weather-stripped</td>
<td>cm²/ea</td>
<td>21</td>
</tr>
<tr>
<td>Exterior walls</td>
<td>Precast concrete panel</td>
<td>cm²/ m²</td>
<td>1.2</td>
</tr>
<tr>
<td>Window framing</td>
<td>Masonry, uncaulked</td>
<td>cm²/ m²</td>
<td>6.5</td>
</tr>
<tr>
<td>Windows</td>
<td>Awning, not weather-stripped</td>
<td>cm²/ m²</td>
<td>1.6</td>
</tr>
</tbody>
</table>

Atmospheric boundary layer thickness ($\delta_{met}$) and the exponent at meteorological station ($\alpha_{met}$) are equal to 270m and 0.14, respectively (see Table 1, Chapter 24 of ASHRAE, 2013). Assuming that the building is located in an urban and suburban location, $\delta$ and $\alpha$ values in equation 5.8 are equal to 370 m and 0.22, respectively. The CFD0 models simulate the wind flow with a range of 0° to 360° for wind direction with 15° increment. Wind flow above and around a building can affect the pressure distribution on the ground.
surface and under surface around the building. Figure 5.3 shows the daily wind speed fluctuations in Lexington, KY, in 2014 year (minimum and maximum wind speed are 0.9 to 9.4 m/s, respectively). Using Lexington as a representative case, we investigate the influence of wind speeds in the range of 1-10 m/s on atmospheric, subsurface and indoor air pressure, concentration of contaminant in the subsurface, AER and indoor air concentration.


Ventilation (natural and mechanical) is another important factor that affects indoor air pressure and contaminant concentrations in the building. However, these effects, are not included explicitly in the application of this model. Inclusion of ventilation in VI modeling is a topic of ongoing and future research. The AER values calculated in this study are specific for the conditions modeled and are fairly low when considered in the context of typical US residential AER values, which often include the contribution of ventilation (Reichman et al. 2017).
5.4. Results and Discussion

The sections below present several scenarios to highlight key aspects of this modeling approach. A simplified building was used to illustrate the model, therefore the results are not meant to necessarily represent a particular “real-world” building. As the subsequent sections will highlight, a key advantage of the modeling approach presented here, is that it can capture the influence of weather conditions and building features when calculating indoor air concentrations. Many previous VI models (e.g. (Abreu and Johnson 2005, Pennell et al. 2009) apply a user-defined AER value of 0.5 l/hr. However, for the building modeled herein with few features prone to leakage (e.g. concrete external walls, 2 windows and a door), the resulting AER is appropriately low for the no wind scenario (0.06 l/hr). A building with different characteristics and different weather conditions, a different AER would be expected. (Reichman et al. 2017) discuss the variability of AERs in US residential buildings and highlight factors that influence building-specific AERs. The modeling approach presented here directly estimates an AER that is representative of the building and weather (e.g. wind and stack effects) and provides a more informed estimate of the VI exposure risk.

5.4.1. Indoor air pressure and AER

This study investigates how wind speed (WS) (0, 1m/s, 5m/s and 10 m/s), wind direction (WD) (0° to 360° with 15° increment), temperature difference (i.e. stack effect) between outdoor and indoor (ΔT = T_{out} - T_{in}) equal to +10°C (33°C-23°C), 0°C (23°C-23°C), -15°C (8°C-23°C) and -35°C (-12°C-23°C) and building characteristics (window and door layout) affect indoor pressure and corresponding AER. Figure 5.4 (a) shows the effect of the above-mentioned parameters on AER values for all the scenarios.
To investigate the influence of stack effect, different $\Delta T$ values were defined, while maintaining $WS=0$. For the scenario with no wind speed ($WS=0 \text{ m/s}$) and $\Delta T=0^\circ \text{C}$, the AER value is equal to 0 (see Figure 5.4 (a) green line with x symbols). The results show increasing trend for AER as the absolute value of $\Delta T$ increases. Consequently, the scenario with the largest temperature difference ($\Delta T=-35^\circ \text{C}$) resulted the highest AER value among the scenarios, regardless of wind speed (see Figure 5.4 (a) blue line--all symbols).

Wind speed is another factor that can influence AER value in a building. The results indicate that when wind speed increases, the building AER value increases. In addition, wind direction can influences AER values, especially for a 10 m/s wind speed. As shown in Figure 5.2 (a), north side ($0$ to $45^\circ$ and $315^\circ$ to $360^\circ$ wind direction) and south side ($135^\circ$ to $225^\circ$ wind direction) of the building are leakier than the east and west walls ($45^\circ$ to $135^\circ$ and $225^\circ$ to $315^\circ$ wind directions, respectively). $90^\circ$ and $270^\circ$ wind directions blow perpendicularly on the tight side of building. For a constant wind speed, AER reaches the highest values when wind blows on the leakier (north and south) side of the building and lowest values when wind blows on the tighter (east and west) side of the building. Figure 5.4 (a) shows that stack effect is typically small compared to wind effect in changing AER values for the conditions modeled here.
Figure 5.4 (b) shows the influence of wind speed, wind direction and stack effect on basement pressure. The horizontal lines show the influence of stack effect (WS≤1 m/s). When WS≤1 m/s and ΔT is equal to zero, the basement pressure is near to zero. For scenarios with WS≤1 m/s (horizontal lines) and when outdoor temperature is less than indoor temperature (ΔT= -15°C and ΔT= -35°C), the basement is under-pressurized; however when outdoor temperature is higher than indoor temperature (ΔT= +10°C) the basement is over-pressurized.

For WS≥5m/s, the basement is over-pressurized when wind blows on the leaky side of the building, but the basement is under-pressurized when wind blows on the tight
side of the building. These results are for the specific building modeled; however they emphasize that wind direction and opening locations play an important role in estimating basement pressure. Depending on wind direction and opening location, a building can be under-pressurized or over-pressurized at the same wind speeds and $\Delta T$ values. Other wind speeds may also be of interest; however the overall effect will depend on building features, wind directions and temperature differences.

5.4.2. Pressure and concentration profiles

COMSOL Multiphysics program is used to couple the outdoor atmospheric air and soil domains to investigate the influence of wind flow above- and below ground. Two different scenarios were defined to study the wind effect (WS=10 m/s and 0 m/s). Both scenarios were modeled for $\Delta T = -35^\circ C$. Soil properties in both scenarios are 0.35 (m$^3$ voids)/(m$^3$ soil) total soil porosity and $1\times10^{-12}$ m$^2$ soil permeability. The overall effective diffusion coefficient for transport in the porous media is $8.68\times10^{-7}$ m$^2$/s in both scenarios. Figure 5.5 (a-1) shows the pressure profile when WS=10 m/s. The wind flow produces an asymmetric pressure profile in both air and soil domains. The pressure is higher on the windward side and lower on the leeward side.

The plan view of the pressure profiles indicates that the lowest pressure happens on the lateral sides of the building (Figure 5.5 (a-1)). The pressure reaches +30 Pa on the windward side and -45 Pa on the lateral sides of the building. This pressure gradient around building influences the pressure difference between indoor and outdoor, which is an important feature that was not previously identified by VI models (Song et al. 2013, Shen and Suuberg 2016).
Figure 5.5 (a-2) shows the pressure profile for WS=0 m/s, which is the same scenario that has been most commonly modeled by previous VI models (Yao et al. 2013). The pressure profile is symmetric and basement air pressure is determined (due to stack effect only) to be -5.2 Pa for $\Delta T= -35^\circ C$.

Figure 5.5 (b) shows the concentration profiles for the same scenarios (WS=10 m/s and 0 m/s, $\Delta T= -35^\circ C$). The concentration profile is symmetric when WS=0 m/s; however
for WS=10 m/s, the concentration profile is slightly asymmetric (Figure 5.5 (b-2)). To investigate the influence of wind on soil gas concentrations in a less permeable soil (10^{-14} m^2 soil permeability, see COMSOL Multiphysics section). The results indicate that for this case, wind does not have an effect on contaminant concentration distribution for WS\leq 10 m/s. Therefore, the influence of wind is most likely important due to the role it plays on pressure profiles, and for soil gas concentrations for high permeability soils or possibly when wind speeds are high (>10m/s).

5.4.3. Indoor air concentration

Table 5.2 and Figure 5.6 summarize the results of twelve (12) different modeled scenarios. The influence of ΔT, WD, and WS are considered with respect to AER, contaminant mass entry rate and indoor concentration.

Figure 5.6 (a) shows that mass entry rate of the contaminant through the foundation crack is inversely related to the basement pressure for all scenarios. In addition, scenarios with low (negative) basement pressures and high mass entry rates have higher C_C/C_S values (Table 5.2). As with other previous modeling efforts, a decrease in basement pressure causes the contaminant to enter the basement at a higher rate. Air flow due to contaminant entry/exit through the crack and wind flow around the building can dilute contaminant concentrations near the foundation. The basement pressure for all scenarios modeled here (Figure 5.6 (a) and Table 5.2) is obtained by coupling indoor and outdoor domains, rather than a user defining a specific basement pressure.

Scenario 11 (ΔT=0, WD=0, WS=10 m/s) is the most over pressurized scenario and has the lowest mass entry rate (among the scenarios modeled). In this scenario, wind blows on the leaky side of the building and outdoor temperature is higher than the indoor
temperature, which results in a higher basement pressure than other scenarios. The external (asymmetric) pressure profile around the building caused by wind can still result in a pressure differential between the outdoor and indoor domains that allows soil gas to enter the building; however it results in the lowest VI exposure risks due to the relatively high basement pressure, as well as a high AER value. The highest AER values were obtained for scenarios when WD=0 (wind was blowing on the leaky side of the building) and WS=10 m/s. The results show that when WS=0 (stack effect only), the AER values are the lowest among all of the scenarios modeled.

Table 5-2: Summary of Model Results

<table>
<thead>
<tr>
<th>Scenario #</th>
<th>Scenario WD-WS-(ΔT)</th>
<th>Basement Pressure (Pa)</th>
<th>Flow Direction</th>
<th>AER (1/hr)</th>
<th>Mass entry rate (μg/s)</th>
<th>CC/CS*</th>
<th>CB/CS*</th>
<th>CFF/CS*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>N/A-0-(-35)</td>
<td>-5.2</td>
<td>B to FF</td>
<td>0.06</td>
<td>1.03</td>
<td>0.289</td>
<td>4.79E-3</td>
<td>4.50E-4</td>
</tr>
<tr>
<td>2</td>
<td>0-5-(-35)</td>
<td>-4.0</td>
<td>B to FF</td>
<td>0.19</td>
<td>0.86</td>
<td>0.276</td>
<td>4.79E-3</td>
<td>1.14E-4</td>
</tr>
<tr>
<td>3</td>
<td>0-10-(-35)</td>
<td>-1.2</td>
<td>B to FF</td>
<td>0.47</td>
<td>0.48</td>
<td>0.220</td>
<td>5.72E-3</td>
<td>2.60E-5</td>
</tr>
<tr>
<td>4</td>
<td>90-5-(-35)</td>
<td>-6.4</td>
<td>B to FF</td>
<td>0.13</td>
<td>1.10</td>
<td>0.294</td>
<td>4.49E-3</td>
<td>2.17E-4</td>
</tr>
<tr>
<td>5</td>
<td>90-10-(-35)</td>
<td>-10.0</td>
<td>B to FF</td>
<td>0.28</td>
<td>1.24</td>
<td>0.290</td>
<td>3.82E-3</td>
<td>1.15E-4</td>
</tr>
<tr>
<td>6</td>
<td>N/A-0-(-15)</td>
<td>-2.1</td>
<td>B to FF</td>
<td>0.03</td>
<td>0.79</td>
<td>0.268</td>
<td>6.94E-3</td>
<td>6.51E-4</td>
</tr>
<tr>
<td>7</td>
<td>0-5-(-15)</td>
<td>-1.2</td>
<td>B to FF</td>
<td>0.18</td>
<td>0.67</td>
<td>0.257</td>
<td>8.57E-3</td>
<td>9.68E-5</td>
</tr>
<tr>
<td>8</td>
<td>0-10-(-15)</td>
<td>+1.3</td>
<td>FF to B</td>
<td>0.44</td>
<td>0.39</td>
<td>0.209</td>
<td>4.84E-3</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>90-5-(-15)</td>
<td>-3.2</td>
<td>B to FF</td>
<td>0.11</td>
<td>0.84</td>
<td>0.273</td>
<td>5.62E-3</td>
<td>2.00E-4</td>
</tr>
<tr>
<td>10</td>
<td>90-10-(-15)</td>
<td>-6.6</td>
<td>B to FF</td>
<td>0.25</td>
<td>0.96</td>
<td>0.272</td>
<td>4.06E-3</td>
<td>9.82E-5</td>
</tr>
<tr>
<td>11</td>
<td>0-10-(0)</td>
<td>+3.0</td>
<td>FF to B</td>
<td>0.41</td>
<td>0.33</td>
<td>0.200</td>
<td>2.39E-3</td>
<td>0</td>
</tr>
<tr>
<td>12</td>
<td>90-10-(0)</td>
<td>-4.3</td>
<td>B to FF</td>
<td>0.24</td>
<td>0.81</td>
<td>0.260</td>
<td>4.59E-3</td>
<td>8.70E-5</td>
</tr>
</tbody>
</table>

*CC: Foundation crack TCE concentration, CB: TCE concentration in basement indoor air, CFF: TCE concentration in first floor indoor air and CS: TCE (vapor) concentration of source (modeled as 2.014×10⁻³ mol/m³ (See COMSOL Multiphysics Section))
Figure 5.6 (b and c) shows the relationship between AER and $C_{FF}/C_S$ and $C_B/C_S$. The results show AER appears to be a dominant factor in controlling $C_{FF}$; however, AER is not the dominant factor that controls $C_B$. This VI modeling approach uses a multizone model to calculate indoor air concentrations in different zones. In this model, no windows were included in the basement zone; however a stairway connected the first floor to basement and allowed air flow between the first floor and basement. AER is not the dominant factor that controls the indoor air concentration in the basement. Other factors such as basement pressure and mass entry rate of contaminant through the cracks directly influence the basement air concentration.

The AER reported in Table 5.2 is calculated as a value for the entire house. Since the first floor has more openings, the AER value is more representative of the first floor, than it is of the basement. However, $C_B$ is calculated based on the mass balance equations (see Model Method section), which is considerably different than previous VI modeling approaches. Here, indoor air concentrations are determined for different zones based on the air flow characteristics of specific zones.
Figure 5-6: a) The mass entry rate of contaminant through the crack vs. basement pressure, b) Normalized contaminant concentration in first floor vs. AER and c) Normalized contaminant concentration in basement vs. AER
5.5. Special considerations and limitations

The following subsections discuss several special considerations and limitations of the current modeling approach. Table 5-3 summarizes comparisons between previous modeling approaches (Abreu and Johnson 2005, Pennell et al. 2009) and the current model, as well as the special consideration of paving around a building.

Table 5-3: Comparison of Model Results for Select Cases

<table>
<thead>
<tr>
<th>Scenario WD-WS-(ΔT)</th>
<th>Paved</th>
<th>Basement Pressure (Pa)</th>
<th>AER (1/hr)</th>
<th>Soil gas flow (L/min)</th>
<th>Mass entry rate (μg/s)</th>
<th>C_{in}/C_{S}</th>
<th>C_{B}/C_{S}</th>
<th>CFF/CS</th>
<th>New approach</th>
<th>New approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Wind</td>
<td>N</td>
<td>-5 user defined</td>
<td>user defined</td>
<td>0.40</td>
<td>NR</td>
<td>2.22E-4</td>
<td>NA</td>
<td>NA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Abreu and Johnson (2005)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>No Wind</td>
<td>Y</td>
<td>-5 user defined</td>
<td>user defined</td>
<td>0.47</td>
<td>1.25</td>
<td>1.46E-4</td>
<td>NA</td>
<td>NA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pennell et al. (2009)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>No Wind</td>
<td>N</td>
<td>-1.2 model result</td>
<td></td>
<td>0.47</td>
<td>0.48</td>
<td>NA</td>
<td>5.72E-3</td>
<td>2.60E-5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Y</td>
<td></td>
<td>-1.2 model result</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Current Study</td>
<td>N</td>
<td>-10 model result</td>
<td>model result</td>
<td>0.65</td>
<td>1.24</td>
<td>3.82E-3</td>
<td>1.15E-4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0-10(-35)</td>
<td>Y</td>
<td>-10 model result</td>
<td>model result</td>
<td>0.67</td>
<td>2.16</td>
<td>NA</td>
<td>6.67E-3</td>
<td>2.00E-4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>90-10(-35)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Notes: NR- Not Reported. NA – Not Applicable. Values for Abreu and Johnson (2005) and (Pennell et al. 2009) are provided as reported in the literature. Paving around the building includes 5m of impervious surface around the entire building (as described by (Pennell et al. 2009)) Current Study “No wind” scenario was modeled to approximate the previous modeling approach by (Abreu and Johnson 2005, Pennell et al. 2009). The current study and (Pennell et al. 2009) used the same soil gas effective diffusivity, air diffusivity and vapor source concentrations. Abreu and Johnson (2005) used different values for the diffusivity in soil \((1.036\times10^{-6} \text{ m}^2/\text{s})\), air diffusivity \((8.8056\times10^{-6} \text{ m}^2/\text{s})\) and the vapor source concentration \((200 \text{ mg/L})\).

5.5.1. Comparison with Previous Modeling Studies

The model results for specific scenarios (no wind) were compared to two previously published 3D VI models (Abreu and Johnson 2005, Pennell et al. 2009). It is only possible
to compare the current modeling approach no wind (WS=0) scenarios because the previous models did not include wind flow. (Abreu and Johnson 2005, Pennell et al. 2009) set user-defined values for $\Delta P=5$Pa (under-pressurized inside the building) and AER (0.5 l/hr); however they used different computational methods, finite difference and finite element, respectively. In the current modeling study, the indoor air pressure, outdoor air pressure, and AER are calculated directly by the model.

The results summarized in Table 5.3 for (Abreu and Johnson 2005, Pennell et al. 2009) and the current study agree well. (Pennell et al. 2009) modeled a characteristic entrance region (CER) as 10cm and then assumed all soil gas flowed through the 5 mm crack (due to continuity). Given steep pressure and soil gas concentration gradients in the region of the CER, differences in the soil gas flow rate and soil gas concentrations may be responsible for the reported difference in Table 5.3. The difference between the current study and Abreu and Johnson (2005) model results is likely due to the fact that the soil properties and the computational modeling approach was different (see Table 5.3 notes).

A building surrounded by 5m paved ground was investigated in (Pennell et al. 2009). For comparison purposes, this special case was also investigated using the current modeling approach. For no wind (WS=0) and paved ground, the soil gas flow rate is 0.38 L/min in (Pennell et al. 2009) and 0.32 L/min in this study match well, especially given the difference in modeling approaches (e.g. CER vs crack). The results indicate that the soil gas flow rate decreases when a paved surface is present around the building. The mass entry rate of contaminant through the foundation crack is 1.25 $\mu$g/s and 1.81 $\mu$g/s for unpaved and paved ground in (Pennell et al. 2009), respectively. In the current study, the mass entry rate for unpaved ground is 1.01 $\mu$g/s, compared to 1.56 $\mu$g/s for paved ground.
While these mass flow rates in the current study are lower than the values reported in (Pennell et al. 2009), they follow a similar trend in which the paved ground has a higher mass entry rate. The reason for lower mass entry rates is likely due to the CER vs crack and mesh sizes in finite element study in (Pennell et al. 2009) compared to the current study.

Lastly, an important consideration for model comparison is the indoor air concentration divided by the source concentration ($C_{in}/C_s$). In Table 5.3, $C_{in}/C_s$ values for Pennell et al. (2009) and Abreu and Johnson (2005) are provided as reported in the literature. These values are calculated using the approach described by Pennell et al. (2009) and Abreu and Johnson (2005),

$$C_{in} = \frac{\text{Mass entry rate}}{AER \cdot \text{Volume of enclosed space} + \text{Soil gas flow rate}}$$  (5.12)

The $C_{in}/C_s$ values rely on user-defined AERs and do not incorporate the AERs that are estimated by the current modeling approach. (Pennell et al. 2009) and current study used an enclosed space value of 233 m$^3$ to calculate $C_{in}/C_s$. Abreu and Johnson (2005) used 174 m$^3$ for the volume of the enclosed space and explains the difference in $C_{in}/C_s$ values reported in Table 5.3.

5.5.2. Wind Effects and Paved Ground Surface

Two scenarios with 10 m/s wind speed and two different wind directions (0 and 90 degree) were modeled with and without 5m paved ground surface extending around the building. The scenario with WD=0 (leaky side of the building) is less under-pressurized
with lower soil gas flow rate and mass entry rate compared to no wind flow scenario. The scenario with WD=90 (tight side of building) is more under-pressurized with higher values of soil gas flow rate and mass entry rate compared to the WD=0 scenario.

Wind flow can cause higher soil gas flow or lower soil gas flow for paved ground scenarios depending on the wind direction; however a paved ground around the building causes higher mass entry rates through the crack because the contaminant accumulates under the paved ground and building. Paved surfaces can also cause higher indoor air concentration for both basement and first floor space.

$C_B/C_S$ and $C_F/C_S$ values are determined using CONTAM and rely on the current modeling approach described in Figure 5.1. Like the existing VI models, the paved surface has a higher indoor air concentration due to higher mass entry rates. However, the current modeling approach provides weather and building-specific indoor pressures and AER values, which directly influence the indoor air concentrations. The multi-zone indoor air modeling approach, provides different estimates for indoor air concentrations depending on location. For the building modeled, the data shows that the basement indoor air concentration is higher than the first floor, regardless of whether a paved surface is present around the building.

5.5.3. Comparison with Field Data

The model results in this study were qualitatively compared to field data collected by (Luo et al. 2009). They collected these field data beneath and around a slab-on-grade building overlying a petroleum hydrocarbon impacted soil in Evansville, WY. The field data indicated that dominant wind direction was southwest and the pressure difference (indoor and shallow soil) on the windward side of the building (south west side) was higher
than the leeward side of the building (northeast side). They reported pressure differences in the range of 4.4-17 Pa on windward side for WS=5.1m/s. The model results in the current study show a similar trend to the field study (i.e. higher pressure difference in the windward side and lower pressure difference at the leeward side) in soil. The pressure difference in present study lies in the range of 3.6-10.9 Pa, which is in a good agreement with the field study by (Luo et al. 2009). They also showed that the contaminant and oxygen concentration in soil depend on dominant wind direction in the area. Contaminant and oxygen concentration were lower and higher, respectively, in the windward side of dominant wind direction. An opposite trend was observed at the leeward side which indicates the dominant wind direction is able to influence (through fate and transport processes) the contaminant distribution in soil due to the dominant wind direction.

5.5.4. Steady State Limitations of the Current Study

Additional model simulations were conducted to investigate timescales necessary to reach steady-state pressure profiles in aboveground and subsurface domains. The data (not shown) suggest that times are typically much shorter (e.g. minutes) for pressure profiles in the atmosphere and along the ground surface to reach steady state as compared to times for soil gas concentrations (e.g. days to months to years) to reach steady state in the subsurface. While the time to reach steady state is scenario specific and will depend on many different conditions, steady-state simulations provide useful information, even though wind flows may not be constant.

As discussed above, the results of the field study by (Luo et al. 2009) suggest that soil gas pressure and concentration of an aerobically degradable contaminant are influenced by dominant wind direction. Steady state modeling may be an important
simplification to assist in better understanding VI exposure risks influenced by dominant wind flows. However, transient modeling may be important for AER and indoor pressure estimation and additional research is needed.

5.6. Conclusions

To date, most VI models have focused on subsurface fate and transport processes coupled with stack effects (i.e. user-defined $\Delta P$); in this study we developed a comprehensive model that combines three different domains: the atmospheric domain (outdoor above-ground), indoor domain, and subsurface domain. The results suggest that wind flows can result in asymmetrical pressure profiles; and for permeable soils at moderate to high wind speed scenarios, soil gas concentrations may also exhibit asymmetric profiles.

Asymmetric pressure profiles around buildings can cause infiltration in the windward side and exfiltration on the leeward side of the building, which influences indoor air pressure and the mass entry rate of contaminant. Results show that the indoor air contaminant concentration is influenced by the AER which is a function of wind speed, wind direction and temperature difference. The results also indicate that when the wind speed increases and blows on the leaky side of the building, the indoor pressure and AER increase, which causes a decrease in the contaminant mass entry rate and indoor air concentration. When the wind speed increases and blows on the tight side of the building, the indoor air pressure and AER decreases and mass entry rate and indoor air concentration increases. The VI model presented here provides an improved conceptual understanding of how wind and stack effects influence VI exposure risks due to changes in AER, indoor/outdoor air pressures.
The results for the current modeling approach are for the special case of homogenous soils and steady state conditions. The influence of other factors that can affect VI exposure risks, such as heterogeneous soil in the subsurface, the presence of preferential pathways, and variable soil moisture have not been investigated in this study. However, the modeling approach presented can be used to consider the influence of these effects.

5.7. Supplement Information: Qualitative Model Comparison with Field Data

There are very few data sets to which models can be compared for calibration or validation of models. Rather, VI models are mostly used to inform professional judgments and guide practitioners. To test the modeling approaches developed as part this research, results (Shirazi and Pennell 2017) were qualitatively compared to field data collected by (Luo et al. 2009). Lou et al. collected these field data as part of a study funded by the American Petroleum Institute. The data was collected beneath and around a slab-on-grade building overlying a petroleum hydrocarbon impacted soil in Evansville, WY. The building has a 15m×14m footprint with concrete slab that is about 12.5 cm thick. The field data indicated that dominant wind direction was southwest and the pressure difference between indoor and shallow soil on the windward side of the building (south west side) was higher than the leeward side of the building (northeast side) (Figure 5-7). They reported pressure differences in the range of 4.4-17 Pa on windward side for WS=5.1m/s.
The Shirazi and Pennell model results show a similar trend to the field study (i.e. higher pressure difference on the windward side and lower pressure difference on the leeward side) in soil. The pressure difference in present study for a 5 m/s wind speed on windward side lies in the range of 3.6-10.9 Pa (Figure 5-8), which is in a good agreement with the field study by (Luo et al. 2009).
They also showed that the contaminant (total petroleum hydrocarbon (TPH)) and oxygen concentration in soil depend on dominant wind direction in the area. The contaminant investigated in Lou et al. was a degradable contaminant that could be degraded by oxygen beneath the building. Contaminant and oxygen concentration were low and high, respectively, in the windward side of dominant wind direction which shows TPH was degraded because of high concentration of oxygen in windward side. An opposite trend was observed at the leeward side which indicates the dominant wind direction is able to influence (through fate and transport processes) the contaminant distribution in soil due to the dominant wind direction (Figure 5-9 (Luo et al. 2009)).
Figure 5-9: O$_2$ and TPH soil gas distribution at 1.2 m below ground surface (Luo et al. 2009)

Model results in this study shows an asymmetric concentration distribution 2m below the building when 10 m/s wind is blowing (Figure 5-10), however the contaminant
herein is not degradable and cannot be directly compared with the results in Lou et al. (2009), but still shows the wind direction influences soil gas concentration below and around the building.

Figure 5-10: Normalized TCE concentration 2m below and around building foundation when 10m/s wind is blowing on west side of the building
CHAPTER 6: COMPARISON OF THE MODELED AND MEASURED RESULTS OF A REAL HOUSE OVERLYING VOLATILE ORGANIC COMPOUNDS GROUNDWATER PLUMES

This chapter includes an article that is “in-preparation” for submission to a peer-reviewed journal. (E. Shirazi and K. G. Pennell). “Indoor Air Variability as a function of Wind, Temperature, and Building Characteristics: Modeling and Field Data”

Temporal variability of exposure risks measured as indoor air volatile organic compound (VOC) concentrations in buildings near hazardous waste sites has been a challenge for decision makers for decades. Adding to this challenge is the lack of vapor intrusion models that can account for weather conditions and building characteristics, especially at sites where alternative pathways complicate the vapor intrusion pathway. In this research, a method is presented to incorporate freely-available models, CONTAM and CFD0, to estimate site-specific building air exchange rates (AERs) and indoor air contaminant concentrations by accounting for weather conditions and building characteristics at a vapor intrusion site. The site included in this research is a residential house located south of Hill Air Force Base Superfund site where a trichloroethene (TCE) groundwater plume is present. This site has been the focus of extensive one-of-the-kind field measurements funded by the Department of Defense. Availability of these existing data allowed for model results to be compared to multiple years of field measurements. The maximum modeled AER (33 d⁻¹) was 95% of the maximum measured AER (35 d⁻¹), and the minimum modeled AER (3.2 d⁻¹) was approximate 80% of the minimum measured AER (4 d⁻¹). In addition, the results suggest that temporal variability in the indoor air TCE
concentrations is greatest (modeled and measured) when the alternative pathway was active. The agreement observed between the field data and model results suggests that the modeling approach presented here may be a useful tool for decision makers as they continue to assess complex and variable processes that influence exposure risks at hundreds of thousands of vapor intrusion sites across the United States, and countless more worldwide.

6.1. Background

Hundreds of thousands of hazardous waste sites exist throughout most rural and urban communities in the United States. According to the National Research Council (NRC 2013), some of the most persistent and pervasive legacy contaminants at hazardous waste sites include chlorinated volatile organic compounds (CVOC). A challenge of decision makers at hazardous waste sites who are tasked with managing CVOC exposure risks in communities near groundwater plumes is vapor intrusion—the transport of vapors from subsurface sources into indoor spaces.

Characterizing vapor intrusion risks is a challenge for many reasons: the source of CVOCs can be difficult to identify due to alternative pathways (Pennell et al. 2013, Guo et al. 2015, McHugh et al. 2017, Roghani et al. 2018); variations in indoor air concentrations occur frequently (Holton et al. 2013, Guo et al. 2015); and, weather conditions and building characteristics, including building air exchange rates (AERs), are only recently being better understood within the context of vapor intrusion exposure risk variability (Luo 2009, Reichman et al. 2017, Shirazi and Pennell 2017).

For many years, models have been used to assist decision makers in understanding exposure risks and to inform professional judgement (USEPA 2004, Luo 2009). In
addition, several three-dimensional models (Abreu and Johnson 2005, Luo 2009, Pennell et al. 2009, Shirazi and Pennell 2017) have been developed to inform the vapor intrusion scientific community about fate and transport processes that govern exposure risks and drive risk management decisions. The purpose of this research is to present a modeling approach that considers weather conditions and building characteristics when calculating AERs and indoor air concentrations. The modelling results are in good agreement with field data from one of the most well-studied and documented sites in the United States, and the world.

The “site” has been the focus of a field study research program since 2010 (Holton et al. 2013, Guo et al. 2015, Johnson et al. 2016). The building, referred to as the “study house” (Figure 6-1), is located in the northwest portion of Layton, Utah; and south of Hill Air Force Base Superfund site. The study house is a two-story residential building with approximately 2.5 m elevation drop from back yard to front yard. The building dimensions are 11.7m×8.7m×7.5 m which are length, width and height of building, respectively. Figure 6-2 shows the floor plan. An associated groundwater plume contaminated with 1,1-dichloroethene (1,1-DCE), 1,1,1-trichloroethane (1,1,1-TCA) and trichloroethylene (TCE) is within the vicinity of the study house. Holton et al. (2013) reported 10-50 μg/L average concentration of dissolved TCE in groundwater beneath the building. TCE concentrations detected in indoor air were associated with TCE vapors into the study house from subsurface sources (Holton et al. 2013, Guo et al. 2015).
Figure 6-1: Front yard (a) and backyard (b) of study house.
Photos taken by E. Shirazi, September 28, 2019.
Figure 6-2: Floor plan of study house showing first and second floor.
6.2. Modeling Approach

Figure 6-3 describes the modeling process, including required data input/output for the study house. This research incorporates a multizone indoor air quality computer program (CONTAM) coupled with computational fluid dynamics program (CFD0) which were developed by and are freely available through the Building and Fire Research Laboratory of the National Institute of Standards and Technology (NIST). These programs have been used previously by Shirazi and Pennell (2017) to investigate the influence of weather condition and building characteristics on building air exchange rate (AER) and indoor air concentration. Shirazi and Pennell (2017) determined mass entry rate of contaminant through the foundation cracks using a CFD modeling approach for vapor intrusion and used it as the input in CONTAM to predict indoor air concentration based on weather and building condition (See Figure 1 in Shirazi and Pennell (2017)). Herein, the mass entry rate measured by Holton et al. (2015) is used as input in CONTAM instead of CFD vapor intrusion modeling, as described previously (Shirazi and Pennell 2017).

![Diagram](image)

Figure 6-3: Modeling process by coupled CFD0 and CONTAM for the study house
Model input, such as outdoor temperature, wind speed, and mass entry rate of contaminant are available from previous studies (Holton et al. 2013, Guo et al. 2015, Holton et al. 2015). Other inputs related to building characteristics were collected by the authors. The list of inputs are as follows in Table 6-1. Specific values used in model are summarized in Table 6-2, Table 6-3 and Figure 6-4.

Table 6-1: List of inputs related to study house used in CONTAM

<table>
<thead>
<tr>
<th>Input</th>
<th>Range</th>
<th>Modeled values</th>
<th>Determined by</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outdoor temperature</td>
<td>-13 to 37 °C</td>
<td>-13, 7, 22 and 37°C</td>
<td>Holton et al. (2013 and 2015) and based on ASHRAE Handbook of Fundamentals (2013)</td>
</tr>
<tr>
<td>Indoor temperature</td>
<td>NR*</td>
<td>22°C</td>
<td>Measured by authors and based on ASHRAE Handbook of Fundamentals (2013)</td>
</tr>
<tr>
<td>Wind speed</td>
<td>0-10 m/s</td>
<td>0, 1, 5 and 10 m/s</td>
<td>Holton et al. (2013 and 2015)</td>
</tr>
<tr>
<td>Mass entry rate</td>
<td>$1 \times 10^{-4}$ to $3.2 \times 10^{-1}$ g/d</td>
<td>See Table 6-5</td>
<td>Holton et al. (2015) under natural condition</td>
</tr>
<tr>
<td>Floor height</td>
<td>2-2.5 m</td>
<td>2 and 2.5 m</td>
<td>Measured by authors</td>
</tr>
<tr>
<td>Building dimension</td>
<td>NR*</td>
<td>11.7m $\times$ 8.7m $\times$ 7.5 m</td>
<td>Measured by authors</td>
</tr>
<tr>
<td>Room size</td>
<td>NR*</td>
<td>See Table 6-2 and Figure 6-4 in supporting information</td>
<td>Measured by authors</td>
</tr>
<tr>
<td>Openings’ relative elevation</td>
<td>NR*</td>
<td>See Table 6-3 and Figure 6-4 in supporting information</td>
<td>Measured by authors</td>
</tr>
<tr>
<td>Openings’ effective leakage area (ELA)</td>
<td>Varies based on opening type</td>
<td>See Table 6-4</td>
<td>Suggested by ASHRAE Handbook of Fundamentals (2001)</td>
</tr>
</tbody>
</table>
Table 6-2: Information related to zones

<table>
<thead>
<tr>
<th>Zone</th>
<th>Zone number in Figure 6-4</th>
<th>Height (m)</th>
<th>Area in CONTAM (m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>First floor</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Living area</td>
<td>1</td>
<td>2.5</td>
<td>16.16</td>
</tr>
<tr>
<td>Stairwell</td>
<td>2</td>
<td>2.5</td>
<td>5.76</td>
</tr>
<tr>
<td>Garage</td>
<td>3</td>
<td>2.5</td>
<td>36.25</td>
</tr>
<tr>
<td>Laundry room</td>
<td>4</td>
<td>2.5</td>
<td>5.66</td>
</tr>
<tr>
<td>Closet</td>
<td>5</td>
<td>2.5</td>
<td>1.3</td>
</tr>
<tr>
<td>Bathroom</td>
<td>6</td>
<td>2.5</td>
<td>4.48</td>
</tr>
<tr>
<td><strong>Second floor</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Living room</td>
<td>7</td>
<td>2.5</td>
<td>33.71</td>
</tr>
<tr>
<td>Kitchen</td>
<td>20</td>
<td>2.5</td>
<td>8.32</td>
</tr>
<tr>
<td>Closet in kitchen</td>
<td>17</td>
<td>2.5</td>
<td>1.86</td>
</tr>
<tr>
<td>Bathroom</td>
<td>19</td>
<td>2.5</td>
<td>4.78</td>
</tr>
<tr>
<td>Closet in bathroom</td>
<td>16</td>
<td>2.5</td>
<td>0.5</td>
</tr>
<tr>
<td>Bedroom 1</td>
<td>18</td>
<td>2.5</td>
<td>14.51</td>
</tr>
<tr>
<td>Closet in bedroom 1</td>
<td>13 and 14</td>
<td>2.5</td>
<td>0.76</td>
</tr>
<tr>
<td>Hallway</td>
<td>15</td>
<td>2.5</td>
<td>3.47</td>
</tr>
<tr>
<td>Closet in hallway</td>
<td>8</td>
<td>2.5</td>
<td>0.6</td>
</tr>
<tr>
<td>Bedroom 2</td>
<td>11</td>
<td>2.5</td>
<td>10.07</td>
</tr>
<tr>
<td>Closet in bedroom 2</td>
<td>10</td>
<td>2.5</td>
<td>1.18</td>
</tr>
<tr>
<td>Bedroom 3</td>
<td>12</td>
<td>2.5</td>
<td>8.31</td>
</tr>
<tr>
<td>Closet in bedroom 3</td>
<td>9</td>
<td>2.5</td>
<td>0.49</td>
</tr>
<tr>
<td>Opening type</td>
<td>Connection</td>
<td>Opening number in Figure 6-4</td>
<td>Width (cm)</td>
</tr>
<tr>
<td>------------------</td>
<td>---------------------</td>
<td>------------------------------</td>
<td>------------</td>
</tr>
<tr>
<td>Garage door</td>
<td>Garage to outdoor</td>
<td>3</td>
<td>486</td>
</tr>
<tr>
<td>Window</td>
<td>Garage to outdoor</td>
<td>4</td>
<td>96</td>
</tr>
<tr>
<td>Internal door</td>
<td>Garage to stairwell</td>
<td>10</td>
<td>99</td>
</tr>
<tr>
<td>Internal door</td>
<td>Laundry to stairwell</td>
<td>9</td>
<td>76</td>
</tr>
<tr>
<td>Window</td>
<td>Laundry to outdoor</td>
<td>5</td>
<td>94</td>
</tr>
<tr>
<td>Door†</td>
<td>Living area to stairwell</td>
<td>11</td>
<td>57</td>
</tr>
<tr>
<td>Internal door</td>
<td>Living area to bathroom</td>
<td>8</td>
<td>81</td>
</tr>
<tr>
<td>Window</td>
<td>Living area to outdoor</td>
<td>1</td>
<td>150</td>
</tr>
<tr>
<td>Window</td>
<td>Bathroom to outdoor</td>
<td>6</td>
<td>63.5</td>
</tr>
<tr>
<td>Door</td>
<td>Closet to bathroom</td>
<td>7</td>
<td>150</td>
</tr>
<tr>
<td>Front yard door</td>
<td>Stairwell to outdoor</td>
<td>2</td>
<td>89</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Opening type</th>
<th>Connection</th>
<th>Opening number in Figure 6-4</th>
<th>Width (cm)</th>
<th>Height (cm)</th>
<th>Level from floor (cm)</th>
<th>Relative elevation (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Window</td>
<td>Living room to outdoor</td>
<td>11</td>
<td>150</td>
<td>147</td>
<td>46</td>
<td>119.5</td>
</tr>
<tr>
<td>Backyard Door</td>
<td>Living room to outdoor</td>
<td>18</td>
<td>180</td>
<td>200</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>Window</td>
<td>Kitchen to outdoor</td>
<td>17</td>
<td>119</td>
<td>103</td>
<td>94</td>
<td>145.5</td>
</tr>
</tbody>
</table>

†Door was taken out

†††Window was a circle window with 70cm diameter located above the entrance door
<table>
<thead>
<tr>
<th>Opening type</th>
<th>Connection</th>
<th>Opening number in Figure 6-4</th>
<th>Width (cm)</th>
<th>Height (cm)</th>
<th>Level from floor (cm)</th>
<th>Relative elevation (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Second floor</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Door†</td>
<td>Closet to hallway</td>
<td>29</td>
<td>61</td>
<td>204</td>
<td>0</td>
<td>102</td>
</tr>
<tr>
<td>Internal door</td>
<td>Bedroom 3 to hallway</td>
<td>28</td>
<td>76</td>
<td>204</td>
<td>0</td>
<td>102</td>
</tr>
<tr>
<td>Internal door</td>
<td>Bathroom to hallway</td>
<td>26</td>
<td>71</td>
<td>206</td>
<td>0</td>
<td>103</td>
</tr>
<tr>
<td>Internal door</td>
<td>Bedroom 1 to hallway</td>
<td>23</td>
<td>76</td>
<td>206</td>
<td>0</td>
<td>103</td>
</tr>
<tr>
<td>Internal door</td>
<td>Bedroom 1 to bathroom</td>
<td>19</td>
<td>71</td>
<td>206</td>
<td>0</td>
<td>103</td>
</tr>
<tr>
<td>Door</td>
<td>Closet to bedroom 1</td>
<td>21 and 22</td>
<td>117</td>
<td>202</td>
<td>0</td>
<td>101</td>
</tr>
<tr>
<td>Window</td>
<td>Bathroom to outdoor</td>
<td>16</td>
<td>117</td>
<td>27</td>
<td>175</td>
<td>188.5</td>
</tr>
<tr>
<td>Door</td>
<td>Closet to bathroom</td>
<td>24</td>
<td>61</td>
<td>208</td>
<td>0</td>
<td>104</td>
</tr>
<tr>
<td>Window</td>
<td>Bedroom 1 to outdoor</td>
<td>15</td>
<td>150</td>
<td>120</td>
<td>79</td>
<td>139</td>
</tr>
<tr>
<td>Window</td>
<td>Bedroom 2 to outdoor</td>
<td>14</td>
<td>119</td>
<td>145</td>
<td>48</td>
<td>120.5</td>
</tr>
<tr>
<td>Door</td>
<td>Closet to bedroom 2</td>
<td>31</td>
<td>147</td>
<td>202</td>
<td>0</td>
<td>101</td>
</tr>
<tr>
<td>Door</td>
<td>Closet to bedroom 3</td>
<td>32</td>
<td>61</td>
<td>202</td>
<td>0</td>
<td>101</td>
</tr>
<tr>
<td>Window</td>
<td>Bedroom 3 to outdoor</td>
<td>13</td>
<td>119</td>
<td>150</td>
<td>48</td>
<td>123</td>
</tr>
<tr>
<td>Window††</td>
<td>Stairwell to outdoor</td>
<td>12</td>
<td>70††</td>
<td>70††</td>
<td>264</td>
<td>299</td>
</tr>
</tbody>
</table>

†Door was taken out
†††Window was a circle window with 70cm diameter located above the entrance door
Figure 6-4: Zones and opening numbers related to Table 6-2 and Table 6-3 (openings shown in figures but not numbered are the openings considered for external walls)
Holton et al. (2013) reports windows and doors were kept closed during sampling activities, therefore windows and doors connected to outdoor areas are assumed to be closed in the model and the only pathway through the building is the leakage through windows, doors and external walls. Internal doors that connect different zones (rooms) to each other are observed and modeled as open. Open exterior doors and windows, as well as other occupant behaviors, can influence exposure risks (Reichman et al. 2017, USEPA 2018); and the modeling approach presented herein can account for these factors, as necessary. Effective leakage area is an input in CONTAM that estimates the leakage area for closed openings based on type and size of openings. The values of leakage areas used in this study are provided in Table 6-4.

Table 6-4: Effective leakage area corresponding to openings in study house (best estimate values suggested in ASHRAE Handbook of Fundamentals, 2001)

<table>
<thead>
<tr>
<th>Path</th>
<th>Type</th>
<th>Units</th>
<th>Best Estimate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Door frame</td>
<td>General</td>
<td>cm²/ea</td>
<td>12</td>
</tr>
<tr>
<td>Door</td>
<td>Single, not weather-stripped</td>
<td>cm²/ea</td>
<td>21</td>
</tr>
<tr>
<td>Exterior walls</td>
<td>Precast concrete panel</td>
<td>cm²/ m²</td>
<td>1.2</td>
</tr>
<tr>
<td>Window framing</td>
<td>Masonry, uncaulked</td>
<td>cm²/ m²</td>
<td>6.5</td>
</tr>
<tr>
<td>Windows</td>
<td>Single horizontal slider, aluminum</td>
<td>cm²/ lm²</td>
<td>0.8</td>
</tr>
</tbody>
</table>

CFD0 is coupled with CONTAM to investigate the influence of weather condition (wind and temperature) and building characteristics of study house to predict building AER and indoor air concentration and compare results with measured data in study house. CFD0 solves a turbulence model such as the Reynolds Averaged Navier-Stokes equations to calculate the distribution of wind pressure on building envelop. Then wind pressure will be converted to pressure coefficient (Cp) values using Bernoulli’s equation. In CONTAM
we determine flow path locations and link CFD0 to CONTAM to get the Cp values relevant to each path way. The theoretical method of CONTAM and CFD0 and how these two models are connected is comprehensively explained in Shirazi and Pennell (2017). CFD0 considers building and site characteristics and calculates pressure coefficients (Cp) related to different wind directions on the building envelope. Inputs in CFD0 are related to overall building dimension such as width, length, total height of building including building’s roof (2m height of roof with 20° slope); and local terrain features. Soils that surround part of building’s walls from backyard to front yard are modeled which allows CFD0 to predict pressure coefficients (Cp) on building envelope properly.

In CFD0, atmospheric boundary layer thickness (δmet) and the exponent at meteorological station (αmet) are equal to 270m and 0.14, respectively which is in accordance with category of open terrain with scattered obstructions (see Table 1, Chapter 24 of ASHRAE, 2013). The study house is located in a residential neighborhood with two-story detached buildings. Considering the study house site, it is assumed that the category terrain is an urban and suburban area with numerous closely spaced obstructions. Therefore the δ and α values are equal to 370 m and 0.22, respectively (More description related to δ and α values in Shirazi and Pennell (2017)). Herein, CFD0 simulates different wind directions all around the building from 0° to 360° with 15° increment, considering relative north to be zero wind direction for the study house.

To calculate indoor air contaminant concentration in the study house, mass entry rate of contaminant is used as input as the generation rate of contaminant from a contaminant source (Shirazi and Pennell 2017). This mass entry rate is selected from the data collected by Holton et al. (2015) under natural conditions. Based on a likely vapor
intrusion entry point of the house being a foundation-wall gap in stairwell area at first floor (Holton et al. 2013). The maximum, minimum and average values for the mass entry rate used in this study for each season is indicated in Table 6-5.

Table 6-5: Mass entry rate (g/d) values used as input in models

<table>
<thead>
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<th>Mass entry rate (g/d)</th>
<th>Maximum</th>
<th>Average</th>
<th>Minimum</th>
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<tbody>
<tr>
<td>Winter</td>
<td>3.2×10⁻¹</td>
<td>2×10⁻³</td>
<td>1×10⁻⁴</td>
</tr>
<tr>
<td>Summer</td>
<td>1×10⁻³</td>
<td>2×10⁻⁴</td>
<td>1×10⁻⁴</td>
</tr>
<tr>
<td>Shoulder seasons</td>
<td>1×10⁻²</td>
<td>9×10⁻⁴</td>
<td>1×10⁻⁴</td>
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Figure 6-5 shows the air pressure profile around study house modeled using CFD0. Pressure coefficient (Cp) relevant to each opening in CONTAM will be calculated using Bernoulli’s equation. As an example, Figure 6-6 indicates the pressure coefficient (Cp) calculated by CFD0 for opening number 11 in CONTAM (Figure 6-4 and Figure 6-6).

Figure 6-5: Pressure profile view from west side, 10 m/s is blowing from north side
6.3. Results and Discussions

6.3.1. Study House AER: Modeled and Measured

The model results of the study house provide the whole-house AER estimate based on wind, temperature effects and building characteristics listed in Table 6-1. Figure 6-7 shows the variability in the modeled AER values, with the greatest values occurring when wind is the southern direction ($135^\circ$-$225^\circ$). Based on previous research at the study house, the southern direction is the dominant wind direction (Holton et al. 2013) with most leakage areas. The lowest AERs (for each wind speed) occur when the wind blows on the tight sides of the building ($90^\circ$ and $270^\circ$). Figure 6-7 also indicates that for each specific wind speed and most wind directions, winter results in higher AER values, which is due to higher temperature differentials (indoor compared to outdoor) and summer results in lower AER due to lower temperature differentials.

Figure 6-6: Pressure coefficient (Cp) estimated by CFD0 for opening number 11 in Figure 6-4 (each opening has a specific Cp profile, opening 11 is chosen as an example)
Holton et al. (2013) reported southern wind direction as the dominant wind direction during their sampling activities. Therefore, wind direction from 135° to 225° is considered as southern wind direction for this study.

![Figure 6-7: Modeled air exchange rates under different wind speeds, wind directions and outdoor air temperatures](image)

Straight lines in Figure 6-7 indicate the outdoor air temperature effect with no wind flow (stack effect only) on AER. The blue straight line represents winter with largest AER value compared to other seasons which is due to higher temperature difference between indoor and outdoor. Other straight lines represent summer and shoulder seasons under stack effect only condition. The lowest AER estimated by the model (<0.5 d⁻¹) corresponds to a weather condition with no temperature difference between indoor and outdoor (shoulder...
season with 22°C outdoor temperature with wind speed less than or equal to 1 m/s), which is a rare, nearly impossible, condition to sustain for any length of time. Because these conditions are unlikely to be observed in field settings, the scenario is not plotted in Figure 6-7 for simplification purposes.

AERs relevant to summer and shoulder seasons (e.g. fall and spring) are lower than the AERs calculated for winter due to lower temperature difference between indoor and outdoor in summer and shoulder seasons. Wind direction and building characteristics (such as opening location and or being leaky or tight) are important factors that control building’s AER. Figure 6-7 shows that when 5 or 10 m/s wind blows on tight side of building (90° and 270°) AER drops to values even lower than the values calculated for no wind flow scenario (stack effect). These observations indicate that wind direction and building openings can impact the AER.

The largest AER calculated for the study house corresponds to winter with 10 m/s wind blowing on the south side of the building which is the dominant wind direction. This maximum AER is equal to 33.33 d⁻¹ which agrees well with the largest AER measured in study house equal to 35 d⁻¹. The lowest AER corresponds to summer, and shoulder seasons and the scenarios in which wind blows on tight side of the building. The lowest AER calculated in this study is equal to 3.2 d⁻¹ which agrees well with the lowest AER values (~4 d⁻¹) measured in study house.

To compare the modeled and measured results, box and whiskers plot of modeled AER overlies the range of measured AER in Holton et al. (2013). Comparing the maximum values of AER, winter and shoulder seasons indicate larger AER values compared to summer. Summer indicates lower range of modeled AERs which matches the AER values
measured in study house. Results are shown on Figure 6-8. The modeling approach used here, which accounts for the study house characteristics and weather conditions compares well with field measurements over nearly two years. Additionally, model estimated AERs follow the same trend of seasonal variability as the field measurements—the greatest AER is predicted for winter, then shoulder seasons, with the lowest AERs estimated for summer seasons. AER field measurements were conducted by others (Holton et al. 2013) using SF6 (sulfur hexafluoride) tracer gas method in the study house.

Figure 6-8: AER vs time (a) and (b) AER vs seasons: Modeled (Box and Whisker) and Measured (Shaded)

Note: Figure 6-8a shows the study number days to be consistent with data reported at the study house (Holton et al. 2013, Guo et al. 2015, Holton et al. 2015, Johnson et al. 2016). Raw field measurement data were not available for comparison purposes. Shaded regions were visually interpreted from cited references.

6.3.2. Indoor Air TCE Concentrations: Modeled and Measured

Modeled indoor air TCE concentration compared well with field measured indoor air TCE concentrations, as shown on Figure 6-9. The lowest indoor air TCE concentration was observed (by the model and measured in the field) during the summer, as compared to other seasons. The greatest indoor air TCE concentrations corresponded to the winter season, with up to three orders of magnitude in variation in model estimated concentrations,
as well as field measured values. The lowest indoor air TCE concentrations and variations (modeled and measured) were detected in the summer. Collectively, these results suggest that the modeling approach described here is able to predict temporal variation in indoor air TCE concentrations that agree with field measured values, when building characteristics and weather conditions (such as wind speed, variant wind directions and outdoor temperatures) are considered.

Figure 6-9: Indoor Air TCE Concentrations versus time (a) and versus seasons (b): Modeled (Box and Whisker) and Measured (Holton et al. 2013) (Shaded)

Note: Figure 6-9a shows the study number days to be consistent with data reported at the study house (Holton et al. 2013, Guo et al. 2015, Holton et al. 2015, Johnson et al. 2016). Raw field measurement data were not available for comparison purposes. Shaded regions were visually interpreted from cited references. The dashed horizontal line shown in Figures 6-9a and 6-9b at 0.011 ppbv is the lowest concentration measured (Holton et al. 2013).

6.3.3. Indoor Pressure Variations

Indoor pressure is a function of wind speed, wind direction and temperature difference between indoor and outdoor and varies seasonably. Indoor pressures from the model ranged from -18.8 to +5.7 Pa in the study house (Figure 6-10). Season fluctuations
are important, because winter conditions resulted in the lowest indoor pressure and summer conditions created the highest indoor pressure. Figure 6-10a shows the pressure pattern and suggests that higher mass entry rates may occur in the winter compared to summer and shoulder seasons because of lower indoor pressure. The results illustrate driving forces may cause variations in mass entry rates due to changes in weather conditions. However, the largest variations in mass entry rates was observed due to the connection associated with the alternative pathway (Holton et al. 2015), and is not supported (alone) by pressure fluctuations. Rather, alternative pathways that serve as a source for vapor intrusion exposure risks may experience contaminant flux variations due to connections to other conduits to which they are connected, as reported by Roghani et al. (2018).

Figure 6-10: Indoor pressure variation caused by different weather conditions in study house

6.3.4. Implications for Decision Makers

To predict indoor air concentration, the modeling approach used in this research requires the mass entry rate of contaminant to be input into the model (Figure 6-3). Mass entry rate can be obtained by several methods. Shirazi and Pennell (2017) used a finite element model, which considered weather conditions and building characteristics in the
mass entry rate calculation, but their approach is computationally expensive and likely too complicated to be widely used routinely at vapor intrusion sites. They indicated that mass entry rate of contaminant is linearly related to building indoor pressure. Another method that is more accessible to practitioners is the 2004 EPA version of the Johnson and Ettinger (J&E) model (Johnson and Ettinger 1991, USEPA 2004). The J&E model does not account for the effect of weather conditions when estimating indoor air concentration, and consequently mass entry rate of contaminant. For this research, when the alternative pathway was not active, the J&E model appeared to approximate the mass entry. However, when the alternative pathway is active, considerable temporal variability in mass entry rates occurred; and, higher mass entry rates were required for the model to agree with the measurements.

“Measured” mass entry rates can be obtained indirectly using indoor air contaminant concentrations and air exchange rates. These values were used in herein. We input mass entry rates into the model that ranged from 0.32 g/d and 1x10^{-4} g/d (Table 6-5), which represent the range of mass entry rates measured at the study house (Holton et al. 2015). The highest mass entry rates reported for the study house occurred during the winter, and also during CPM testing when the alternative pathway was open. The lowest and least temporally variable mass entry rates were observed when the alternative pathway was closed (Guo et al. 2015). The mass entry rate reported for this period is similar to the mass entry rate predicted by the 2004 EPA J&E spreadsheet.

For vapor intrusion sites where temporal variability in indoor air concentrations has been observed and a range of indoor air concentrations have been recorded, a similar approach could be used. However, it should be noted that the field measurement data used
herein was high-resolution and availability of this type of data would be rare for a typical site. Nonetheless, decision makers are challenged every day to make decisions in real-world settings with limited data. Incorporating the models used in this research along with the typical data available for a site could provide new insight for understanding exposure risks.

Mass entry rate (range), can be obtained from indoor air VOC concentration measurements within a building.

\[ M_{ER} = C_{\text{indoor air (measured)}} \times AER_{\text{(CONTAM)}} \times V_B \quad \text{Eq. 6.1} \]

Where,

\( M_{ER} \) is the mass entry rate of contaminant (g/d), \( C_{\text{indoor air (measured)}} \) is the indoor air concentration of contaminant that has been measured during different sampling events (g/m³), \( AER_{\text{(CONTAM)}} \) is the range of AER calculated by CONTAM considering weather condition and building characteristics (d⁻¹) and \( V_B \) is the volume of building. As shown on Figure 6-3, AER can be calculated by CONTAM independently of the indoor air concentration. Decision makers could determine a range of mass entry rates and model variability in indoor air concentrations using CONTAM and obtain output similar to that shown in Figure 6-8.

At sites where obtaining mass entry rates using existing indoor air VOC concentrations is not possible, the 2004 EPA spreadsheet version of the J&E model (Johnson and Ettinger 1991, USEPA 2004) is another option for obtaining mass entry rates, but this approach would assume that an alternative pathway does not exist. Mass entry rate of contaminant can be calculated using Equation 6.2.
\[ M_{ER} = C_{J&E} \times AER_{(CONTAM)} \times V_B \]  \hspace{1cm} \text{Eq. 6.2}

Where,

\( M_{ER} \) is the mass entry rate of contaminant (g/d), \( C_{J&E} \) is the indoor air concentration of contaminant calculated by EPA spreadsheet when there is no alternative pathway (g/m³), \( AER_{(CONTAM)} \) is the range of AER calculated by CONTAM considering weather condition and building characteristics (d⁻¹) and \( V_B \) is the volume of building.

Once mass entry rates are obtained, the approach used for modeling the study house in this research would allow decision makers to cost-effectively evaluate variability in exposure risks (e.g. indoor air concentrations) based on weather conditions and building characteristics. In this research, we showed that measured AER values and TCE indoor air concentrations for the study house compared well to modeled values (Figure 6-8 and Figure 6-9). This agreement was dependent on inputting measured mass entry values into CONTAM, which simulated the range of conditions that were present at the site (including an alternative pathway). The modelling approach was able to not only predict the indoor air concentration value, but was also able to predict the range of temporal variability observed at this site.
CHAPTER 7: CONCLUSIONS AND RECOMMENDATIONS

7.1. Findings

The overall research hypothesis that variability in indoor air VOC concentrations can be (partially) explained by variations in building air exchange rate (AER) and pressure differentials between indoor spaces and outdoor spaces is verified based on results from a newly developed model that combined building science and vapor intrusion science concepts. In addition, the model results were compared qualitatively and quantitatively with field data from two different field sites.

Weather conditions such as wind speed and direction; and outdoor temperature all played important roles in the variability of indoor air VOC concentrations. Building characteristics such as opening locations and leakage areas were important in AERs and the resulting indoor air VOC concentrations. Considering these factors, this research illustrated new perspectives for VI science to consider. The new VI modeling approach that is presented herein, for the first time calculates the building air exchange rate (AER), indoor air pressure and indoor air VOC concentration, is advantageous over previous VI models because it incorporates information known to influence indoor air VOC concentration variability.

The results of the research described in Chapters 2 and 3 highlight commonly referenced AER values used by VI regulators and practitioners do not account for the variability in AER values that have been published in indoor air quality studies. Building features, weather conditions and other factors that influence AER should be taken into
account when evaluating indoor air concentrations as part of the multiple lines of evidence approach at VI sites.

Chapters 4 and 5 provide information about how to integrate building science models into VI studies. Importantly, the modelling approach, as discussed in Chapter 5, accounts for building-specific features and weather conditions to determine air exchange rates, indoor air pressures and contaminant concentrations in the soil gas and indoor air. The results suggest that wind flows can result in asymmetrical pressure profiles; and for permeable soils at moderate to high wind speed scenarios, soil gas concentrations may also exhibit asymmetric profiles. Results show that the indoor air contaminant concentration is influenced by the AER which is a function of wind speed, wind direction and temperature difference. The mass entry rate of the contaminant through the foundation crack is inversely related to the basement pressure. It also concludes dominant wind direction and speed, as well as the location of building characteristics prone to leakage, can influence VI exposure risk assessments. The developed model improves the understanding of how outside temperature, wind speeds, building air exchange rates, and building-specific features collectively vary the VI exposure risk.

Freely available indoor air quality models used in the new developed model and field data at a vapor intrusion site were used to estimate site-specific building air exchange rates (AERs) and indoor air contaminant concentrations by accounting for weather conditions and building characteristics at this site. In this research we showed that the model results of AER and indoor air concentration compared well with the measured values in the study house. The modelling approach was able to not only predict the indoor air concentration value, but was also able to predict the range of temporal variability observed
at this site. The agreement observed between the field data and model results suggests that the modeling approach presented here may be a useful tool for decision makers as they continue to assess complex and variable processes that influence exposure risks at hundreds of thousands of vapor intrusion sites across the United States, and countless more worldwide.

7.2. Limitation of the study

Vapor intrusion is well-known to be difficult to characterize because indoor air concentrations exhibit considerable temporal and spatial variability throughout impacted communities. Over the past two decades, several VI models have been developed to predict vapor transport through soil into indoor spaces. This research like most vapor intrusion studies was subject to some limitations. Following are the limitations in this research:

1) Like most vapor intrusion models, each modeling approach has limitations and assumptions. In this research we developed a 3-D VI model that calculates VOC concentration in the steady state condition in soil and indoor. Steady state modeling may be an important simplification to assist in better understanding VI exposure risks influenced by dominant wind flows. However, transient modeling may be important for AER and indoor pressure estimation and additional research could be the focus of future research.

2) As described in Chapter 5, in this research we incorporated three different modeling programs: 1) a finite element Multiphysics program known as COMSOL Multiphysics, 2) CFD0 which is a CFD program, and 3) CONTAM which is an indoor quality model. This modeling approach is computationally expensive and likely too complicated to be widely used routinely at vapor intrusion sites. In this model, COMSOL Multiphysics coupled soil
and outdoor domains to calculate mass entry rate of contaminant (to be input into CONTAM) under various wind speed and directions which was computationally too expensive. To reduce the computational time and make the modeling approach more applicable, the authors decided to use “measured” value of mass entry rate of contaminant to be input into the CONTAM. The model results compared well with the field data at a vapor intrusion site, but to validate the model used in this research we would need to apply a multiple lines of evidence approach. Using this approach requires collecting different data (e.g. indoor air, building air exchange rate, wind speed and temperature during a long time period). Data collection for various buildings and for a long time is expensive and needs a trained person to operate.

7.3. Opportunities for future research

In this research we investigated different factors such as building characteristics, wind direction, wind speed, outdoor temperature effects on VI process that have not been well addressed in previous literature. However due to complexity of the VI process, there still might be other contributing factors to the process that were overlooked. Examples of such factors include, but not limited to, open window and doors, mechanical ventilation operation and occupant behavior that could be investigated in future studies. Below are things that could be conducted as part of future research activities:

1) Collecting field data at sites where indoor air VOC concentrations, time of mechanical ventilation operation, opening window and doors, meteorological records can be characterized to validate computational models.
2) Incorporating a transient model to assess AER and indoor air VOC concentrations in response to short term weather condition variation and seasonal behavior in various buildings in a neighborhood overlying a contaminated site.

3) Using EPA spreadsheet and modeling method described in this research to predict mass entry rate of contaminant and indoor air concentration, respectively, in a building in which there is no alternative pathway and compare the model results with field data.

4) Using CONTAM and CFD0 in VI studies to predict inter-zonal indoor air contamination variations in a building under various weather condition and building characteristics and occupant behavior.
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154


VITA

Elham Shirazi

Place of Birth: Tehran, Iran

Education

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<th>Institution</th>
<th>Location</th>
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<td>University of Tehran, Tehran, Iran</td>
<td>Tehran, Iran</td>
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<tr>
<td>B.S., Civil Eng.</td>
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Experience

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Professional publications


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