

Thesis Title
Brown University

Jonathan G. V. Ström

Spring 2020

Abstract

Abstract goes here

Dedication

To mum and dad

Declaration

I declare that..

Acknowledgements

I want to thank...

Contents

1	Introduction	7
2	Topic 1	8
3	Modeling Methodology	9
3.1	Modeling Flow and Mass Transfer in the Vadose Zone	9
3.1.1	Water Flow in Unsaturated Porous Media	9
3.1.2	Vapor Transport in Unsaturated Porous Media	9
3.1.3	Mass Transport in Unsaturated Porous Media	9
3.2	References	9
3.2.1	Soil Moisture Retention Curves	10
3.3	Temperature & Pressure Dependent Properties	10

Chapter 1

Introduction

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

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

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

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

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

Chapter 2

Topic 1

Chapter 3

Modeling Methodology

3.1 Modeling Flow and Mass Transfer in the Vadose Zone

3.1.1 Water Flow in Unsaturated Porous Media

Soil-Water Potential

Soil-Water Retention Curve

3.1.2 Vapor Transport in Unsaturated Porous Media

3.1.3 Mass Transport in Unsaturated Porous Media

3.2 References

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

$$\vec{u} = -\frac{\kappa}{\mu}\nabla p \quad (3.1)$$

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

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

In VI-modeling, the first assumption is fulfilled, but the second is not. Most of the contaminant vapor transport takes place in the partially saturated vadose zone and thus, (3.1) needs modification.

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

$$\kappa_{\text{eff}} = k_r \kappa_s \quad (3.2)$$

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

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

$$\vec{u} = -\frac{k_r \kappa_s}{\mu} \nabla p \quad (3.3)$$

3.2.1 Soil Moisture Retention Curves

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

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

The soil moisture content, θ is given by.

$$\theta = \begin{cases} \theta_r + \text{Se}(\theta_s - \theta_r) & H_p < 0 \\ \theta_s & H_p \geq 0 \end{cases} \quad (3.4)$$

The saturation is given by.

$$\text{Se} = \begin{cases} \frac{1}{(1+|\alpha H_p|^m)^m} & H_p < 0 \\ 1 & H_p \geq 0 \end{cases} \quad (3.5)$$

$$C_m = \begin{cases} \frac{\alpha m}{1-m} (\theta_s - \theta_r) \text{Se}^{\frac{1}{m}} (1 - \text{Se}^{\frac{1}{m}})^m & H_p < 0 \\ 0 & H_p \geq 0 \end{cases} \quad (3.6)$$

$$k_r = \begin{cases} \text{Se}^l [1 - (1 - \text{Se}^{\frac{1}{m}})]^2 & H_p < 0 \\ 0 & H_p \geq 0 \end{cases} \quad (3.7)$$

3.3 Temperature & Pressure Dependent Properties