Examples of Issues that Have Been Examined using 3-D Modeling

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Some Examples of Calculations Using 3-D Models

- There are many models out there...
- Full 3-D Models- different calculational approaches
- How does the assumed nature of foundation breaches affect results?
- Diffusion dominated profiles of COCs in soil vs. predicting actual contaminant entry rates
- The role of advection
Examples (Continued)

- What do models say about subslab sampling?
- Exploring complex geologies
- Safe distances and monitoring well placement
- Do you need to worry about soil moisture? Capillary zone? Rainfall events during soil gas sampling?
- Predicting transients
- Comparison to JE analysis
- Biodegradation

Modeling Approach

- A finite element computational package (Comsol) used to describe transport processes.
  - Set finite element model domain.
  - Typically assume a perimeter crack in the foundation.
  - Assume “Stack Effect” creates an in-house negative pressure of 5 Pa.
Lots of mathematical models of VI already in use worldwide


Need to make important choices about how to handle above-ground effects.
Typically model 5 mm perimeter cracks

3-step solution method

1. Solve for gas flow through soil (Darcy’s Law).
2. Solve for species transport via advection and diffusion.
3. Indoor air concentration is calculated using the species flow rate into the structure.

\[ q = -\frac{\nabla \cdot \mathbf{J}}{\mu} \]

\[ \mathbf{J} = q \mathbf{C} \]

\[ D_a = d_a = \frac{\eta}{\ell} \]

\[ C_{\text{inlet}} = \frac{J_{\text{in}}}{A \cdot V_t + Q} \]

Not the only 3-D model; Abreu and Johnson have developed a finite difference model.
Really does not make much difference what sort of “cracks”, i.e., foundation breaches, are selected.


Slab-on-grade COC entry rate \( (M_{ck}) \) is much more sensitive to capping around building than is basement foundation (10m x 10 m foundation, 5 m apron).

Groundwater at 8 m bgs
Basement depth 2m
GW TCE Concentration 54 µg/L

Steady state contaminant concentration gradient in soil mainly determined by diffusion

IN action level 1.2 µg/m³

Diffusion Controlled Gradients

Note drawing in of air from surface Sink for air at foundation crack
Interplay of advection and diffusion critical

$k = 10^{-10} \text{ m}^2$
Draws in lots of air

$k = 10^{-11} \text{ m}^2$
Draws in some air, but most of “circle of influence” is contaminated soil

$k = 10^{-12} \text{ m}^2$
less of the “circle of influence” is in contaminated soil

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Second Scenario Modeled: Active Sampling and Different Sampling Locations

Photos from O’Brien and Gere
Third Scenario: Effect of Different Soil Layers
Complexity of different permeability soil layers.

High permeability top layer gives 2 orders of magnitude higher indoor air concentration than low permeability top layer (despite the latter “looking worse” in soil gas concentration).

Clay layers and lenses can really cause problems in understanding field results.

Lots of empirical data that “defy explanation”-need a good quantitative modeling analysis/good CSM.
Structure on an open field is fine...

But what about urban environments?

Adjacent capping and structures
\[ k = 10^{-14} \text{ m}^2 \]
5 m driveway increases \( C_{\text{indoor}} \) by 30%, and adjacent house decreases it by 7%; for \( k = 10^{-14} \), driveway has same effect but adjacent house has none.

Parking lots, driveways

How far is far enough??

Solved simple 2-D Laplace Equation

\[ D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) = 0 \]

Lowell and Eklund, 2004

Echoed in various guidance documents, but challenged by Abreu and Johnson, 2005 for homogeneous soils.
How close should GW Source measurements be?

Consider 2 m deep basement, 4 m deep source, sampling GW at r = 5 i.e., 20 m away, can lead to significant extra attenuation

Unusually high source to slab attenuation can have an origin in GW sources that are not really that “close”

Redfield (Denver) Site

Indoor TCE levels for homes as a function of distance from measured groundwater plume edge (defined by DCE concentration)

Depending upon action level, 100 ft may or may not be enough.
Low permeability top layer\[\frac{C_{\text{indoor}}}{C_{\text{source}}} = 0.0185\]

High permeability top layer\[\frac{C_{\text{indoor}}}{C_{\text{source}}} = 0.29\]

Capillary zone resistance is very important

From Shen et al., *Env. Engineering Sci.,* 2013

**Capillary Zone**

- Shows extent to which open porosity filled with water; diffusion through water layer slow
- Shows how dramatically COC concentration drops through capillary zone - big part of AF$_{\text{soil}}$

Relates to critical issue - the role of GW vertical concentration profiles
Capillary resistance probably needed to explain range of AF values in EPA database.

Predictions without capillary fringe (blue lines)

Yao et al., Env. Sci. Tech., 47, 1425-1433 (2013)

Predictions with capillary fringe (blue/green bars)

Simple approaches to handling the capillary resistance do not work well.

In clay, moisture profile smooth, looks like uniform soil

In sand, narrow high resistance capillary layer

Results using true soil moisture profile

Results using 2-layer soil moisture profile approach of JE-type analysis


In clay, high resistance forced in capillary layer

In sand, more uniform resistance forced
AF = 1.58 x 10^{-5} for actual capillary zone calculation

AF = 1 \times 10^{-3}
(uniform loamy sand)

**Rainfall Events**


- **Soil moisture profiles**
  - In a week, moisture profile approaches initial profile

- **COC soil gas profiles**
  - Hardly any effect on COC soil gas profile; bigger effect comes from rise in GW table
  - 1 m depth of probes generally OK
  - Larger effect - air exchange rate?
Transient Situations

Darcy’s Law

\[ \frac{\partial}{\partial t} \left( r_c (1 - \eta_s) + r_s \eta_s \right) \frac{\partial}{\partial t} = \nabla \cdot \left( \rho_s \theta \nabla \eta_s + \nabla \rho_s \right) \]

Advection and Diffusion

\[ \frac{\partial C_\alpha}{\partial t} + \nabla \cdot (\alpha \nabla C_\alpha) + D_\alpha \nabla C_\alpha + K_\alpha = 0 \]

With sudden appearance of a source at 8 m shows typical response is diffusion rate determined.

Note subsoil profiles take months/years to develop.

Note the very long timescales of response to “remediation”
Variation in Heating Season-Driven Stack Effect

Not a large seasonal variation

Base case S.S. calculation - 3 minutes
Transient calculation - 3 hours
EPA Screening Model Approach

• Based upon a 1-dimensional (1-D) model developed by Paul Johnson and Robbie Ettinger in 1991, based on earlier Radon work of Nazaroff and others.

\[
\text{\text{Q}_{\text{building}} = L_{\text{ck}} w_{\text{ck}} D_{\text{ck}} C_{\text{ck}}}
\]

Everything leaving the source enters the house—may not be realistic, but a consequence of 1-D.

Attenuation factor depends upon Q\text{building}

Comparison of EPA JE results with full 3D

Yao et al., EST, 45 2227-2235 (2011).

Neither calculation shown here took full account of capillary zone effects.

No consistent trend of over or underprediction. Often of same O.O.M., but not always...

Basement cases  Slab-on-grade cases

Deeper sources
Biodegradation Can be Handled


Yao, 2012

No agreement on if $c_0$ should be explicit in models

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