Update on Brown University’s 3D Vapor Intrusion Model

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Vapor Intrusion Workshop
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As part of the Superfund Basic Research Program (SBRP) Brown developed a 3-D mathematical representation of vapor intrusion. VI is one of eight other projects being researched within the SBRP.

www.brown.edu/sbrp
Vapor Intrusion: Not part of original SBRP

- Need for vapor intrusion research was communicated by T. Gray (RIDEM) to Brown’s SBRP.
- NIEHS and EPA/ORD highlighted vapor intrusion research needs during conference in 2006
- NIEHS awarded Brown provided supplemental funding
- Research began late-Fall 2006

Early 2007 - Terry Gray (RIDEM) meets the vapor intrusion graduate student…
Overall Research Objective

Provide a quantitative tool to guide field investigations and mitigation efforts such that VI risks are better characterized and managed.
A finite element model (Comsol) is used to evaluate vapor intrusion using conventional fate and transport processes.

The model solves the problem in 3 steps:
1. Gas flow through soil (Darcy’s Flux)
2. Species transport
3. Indoor air concentration is calculated as a function of building exchange rate, soil gas flow into the building and concentration at the crack

\[ \Delta P = -5 \text{ Pa} \]

Perimeter foundation
crack present.
Modeling Approach (cont.)

Step 1: Assign site characteristics
- Soil characteristics
- CER location/dimensions
- Define domain dimensions
- Building details
- Disturbance Pressure
- Ground cover characteristics
- Etc.

Step 2: Define geometries to incorporate areas of interest for finer meshing
Step 3: Mesh domain
Step 4: Solve Soil Gas Continuity Equation (eq 1)

Are boundary conditions satisfied (as discussed in text)?

Step 5: Investigate sensitivity of CER and adjacent areas to element size

Did the CER flow change with smaller element sizes?

Step 6: Calculate pressure drop across crack, $\Delta p_{ck}$ (eq 2)

Is $\Delta p_{ck}$ negligible?

Step 7: Assign chemical properties
Step 8: Solve Chemical Transport Equation (eq 3)

Are there concentration instabilities (i.e., negative concentrations)?

Step 9: Calculate Indoor Air Concentration (eq 4)
Gas Flow Through Soil

\[ q = -\frac{\kappa \rho dP}{\mu} \frac{dx}{dx} \]

Darcy’s Law for one dimensional incompressible flow

\[ q = -\frac{\kappa \rho \nabla \phi}{\mu} \]

Darcy’s Law for 2D or 3D incompressible flow

\[ \phi = gz + \int_{P_0}^{P} \frac{dP}{\rho} \]

\( q \): specific discharge \((L/T)\)

\( \kappa \): permeability of the soil \((L^2)\)

\( \mu \): viscosity of the fluid \((M/LT)\)

\( \rho \): density of the fluid \((M/L^3)\)

\( \phi \): fluid potential

\( P \): pressure of the fluid \((M/LT^2)\)

\( z \): elevation \((L)\)

\( g \): gravitational acceleration \((L/T^2)\)

\( P_{High} \)

\( P_{Low} \)

Soil

Air
\[ \vec{J}_T = \vec{q}C - D_{\text{eff},i}^{\text{gas}} \nabla C \]

\[ D_{\text{eff},i}^{\text{gas}} = D_i^{\text{air}} \frac{\eta_g^{10/3}}{\eta_T^2} + \frac{D_i^{\text{water}}}{K_H} \frac{\eta_w^{10/3}}{\eta_T^2} \]

Non-aqueous liquids (NAPL) and residual contamination in groundwater and/or soil can act as the source for vapor contamination.
Indoor air concentration is a function of building operations. The mass flow rate of the contaminant into the house ($M_{ck}$) is affected by building depressurization (but few other building parameters).
Model Scenarios
(Homogenous Geology)
Various Site Features

Pennell et al. 2008
Journal of the AWMA
Soil Gas Concentrations (Homogenous Geology)
Various Site Features

(a) Scenario 1: Single Building
(b) Scenario 2: Parking Lot Around Bldg.
(c) Scenario 3: Detached Garage
(d) Scenario 4: Porous Subbase
(e) Scenario 5: Adjacent Buildings

Notes:
Concentration plots are shown as centerline cross-sections (A-A' Figure 1).

Pennell et al. 2008
Journal of the AWMA
<table>
<thead>
<tr>
<th>k (m²)</th>
<th>Scenario</th>
<th>Q (m³/sec)</th>
<th>Conc. at the Crack&lt;sup&gt;a&lt;/sup&gt; (mg/m³)</th>
<th>Subslab Conc.&lt;sup&gt;c&lt;/sup&gt; (mg/m³)</th>
<th>Indoor Air Conc.&lt;sup&gt;2&lt;/sup&gt; (mg/m³)</th>
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<th>Indoor Air Conc./Subslab Conc. (α&lt;sub&gt;subslab&lt;/sub&gt;)</th>
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*Diffusion K=10<sup>14</sup>*

1. Single building, 2-Single building surrounded by 5 m parking lot, 3-Single building with detached garage, 4 - Single building with 10-inches of porous subbase, 5 - Two buildings separated by 4m (data shown for Building A. Due to symmetry, data for Building B should be identical).

The concentration at the crack was determined by integrating over the entire surface of the CER. The CER concentration is not constant over the CER surface.

The subslab concentration location is the center of the building footprint at foundation:soil interface.

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Pennell et al. 2008

Journal of the AWMA
Sensitivity Analysis
(Permeability vs. Diffusivity)

\[
D_{\text{eff},i}^\text{gas} = D_i \frac{\eta_g^{10/3}}{\eta_T^2} + D_i^w \frac{\eta_w^{10/3}}{K_H \eta_T^2}
\]

\[
q = -\kappa \rho \frac{dP}{\mu} dx
\]
More Advanced Model Scenarios (Various Geologic Features)

Bozkurt et al. (submitted GWMR, 2008)
No Pressurization

A. Homogenous  
B. & C. Layered

Bozkurt et al.  
(submitted GWMR, 2008)
Three Layers of Soil (Pressurized)

Which case has highest indoor air? Which case has highest soil gas concentrations?

High Permeability/Diffusivity
\[ k_{\text{High}} = 10^{-10} \text{ m}^2, D_{\text{eff,High}} = 1.05 \times 10^{-6} \text{ m}^2/\text{s} \]

Medium Permeability/Diffusivity
\[ k_{\text{Medium}} = 10^{-12} \text{ m}^2, D_{\text{eff,Medium}} = 8.68 \times 10^{-7} \text{ m}^2/\text{s} \]

Low Permeability/Diffusivity
\[ k_{\text{Low}} = 10^{-14} \text{ m}^2, D_{\text{eff,Low}} = 4.37 \times 10^{-7} \text{ m}^2/\text{s} \]

Bozkurt et al. (submitted GWMR, 2008)
Layered Soil

Results

High (top) highest indoor air
Low (top) highest soil gas concentrations

Bozkurt et al. (submitted GWMR, 2008)
**Other Geologic Features**

<table>
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<th>Soil surrounding clay/obstructions, $K=10^{-11} \text{ m}^2$</th>
<th>Indoor Air (mg/m³)</th>
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<td>Discontinuous Clay</td>
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<td>Obstructions (Plain)</td>
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Bozkurt et al. (submitted GWMR, 2008)
Conclusions

- Vapor intrusion potentials are difficult to predict if soil gas concentrations are used by themselves.
- Modeling can be used as a tool to interpret field results.
- Field verification/calibration/validation are being conducted as a next step…
Current Efforts

Newly Constructed High School
Mesh generation is complex. Proper mesh geometry is critical to accuracy of model results.

Iterative Process:
Evaluate instabilities in concentration and re-mesh.
Soil Gas Concentrations (2m bgs)
Domain Slices Showing Soil Gas Concentrations

C

B

A
Next Steps

• Continue to exercise model and evaluate which site features should be included
• Compare model results with field data
• Consider a separate site, for which a PRP is providing additional data
• Evaluate how model should be improved based on validation efforts.
Overall Research Plan and Longer Term Goals

Model development based on current theoretical understanding

Connect/Revise model using existing field data (model verification and calibration)

Future Research Goal
Bench Scale Experimentation and Model Re-design

LONG TERM GOAL...
Field study
• Have a site that might be a good candidate for model verification?
• Have questions about our research?

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