Update on Brown University's 3D Vapor Intrusion Model

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Vapor Intrusion Workshop

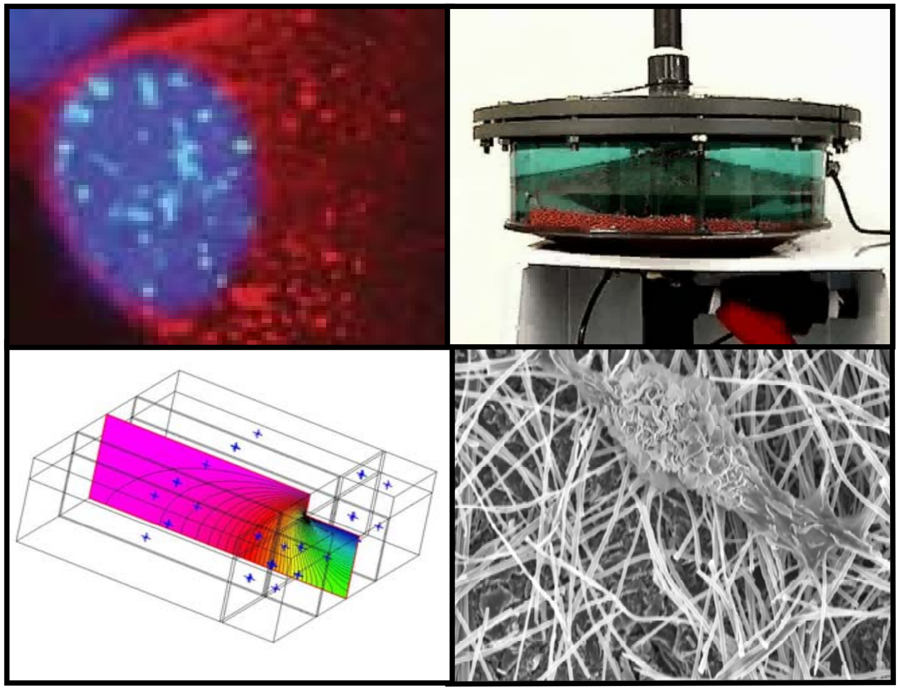
September 2008

Brown's Superfund Basic Research Program (SBRP):
Reuse in Rhode Island

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



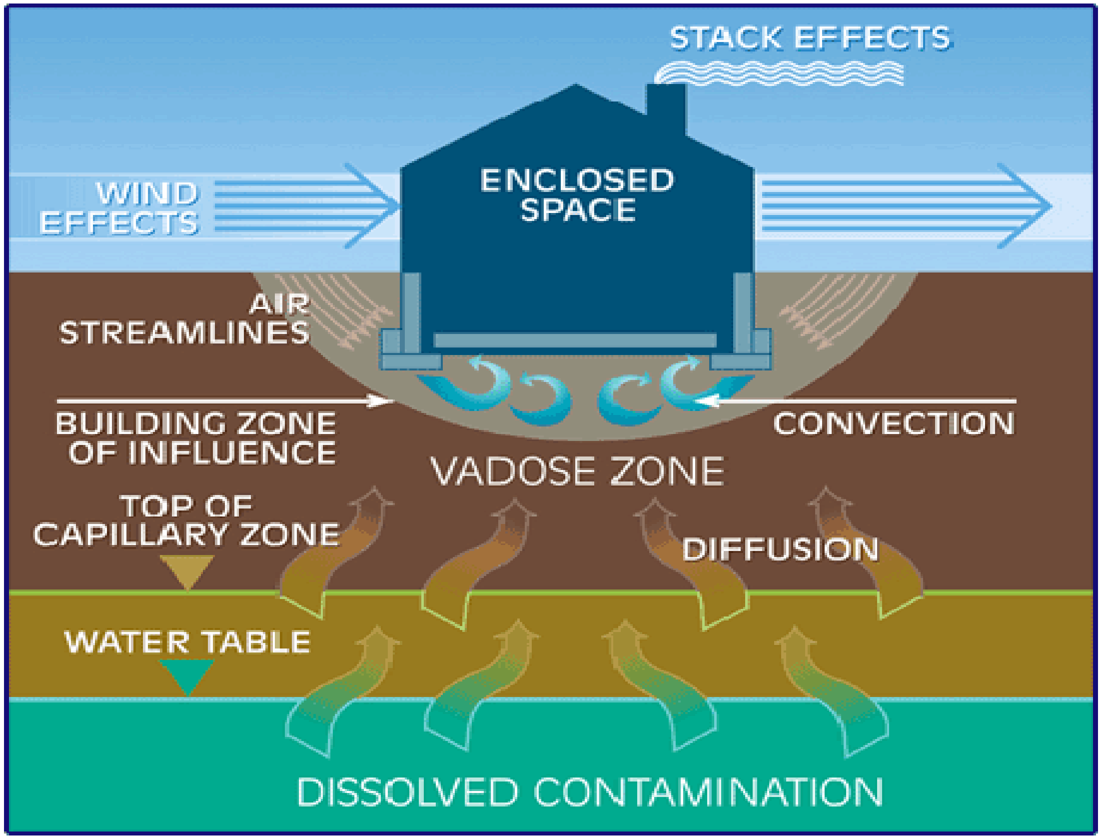
Vapor Intrusion: Not part of original SBRP

- 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.



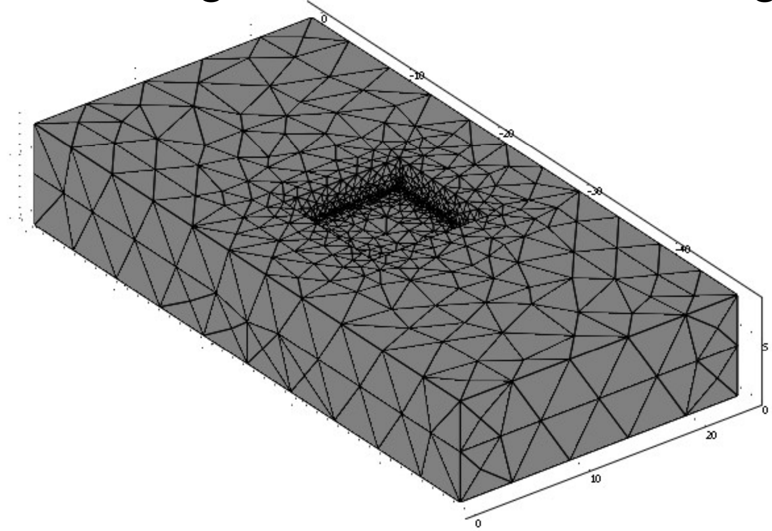
www.vaprotect.com/images/2006/10/17/graphic.gif

Modeling Approach

A finite element model (Comsol) is used to evaluate vapor intrusion using conventional fate and transport processes

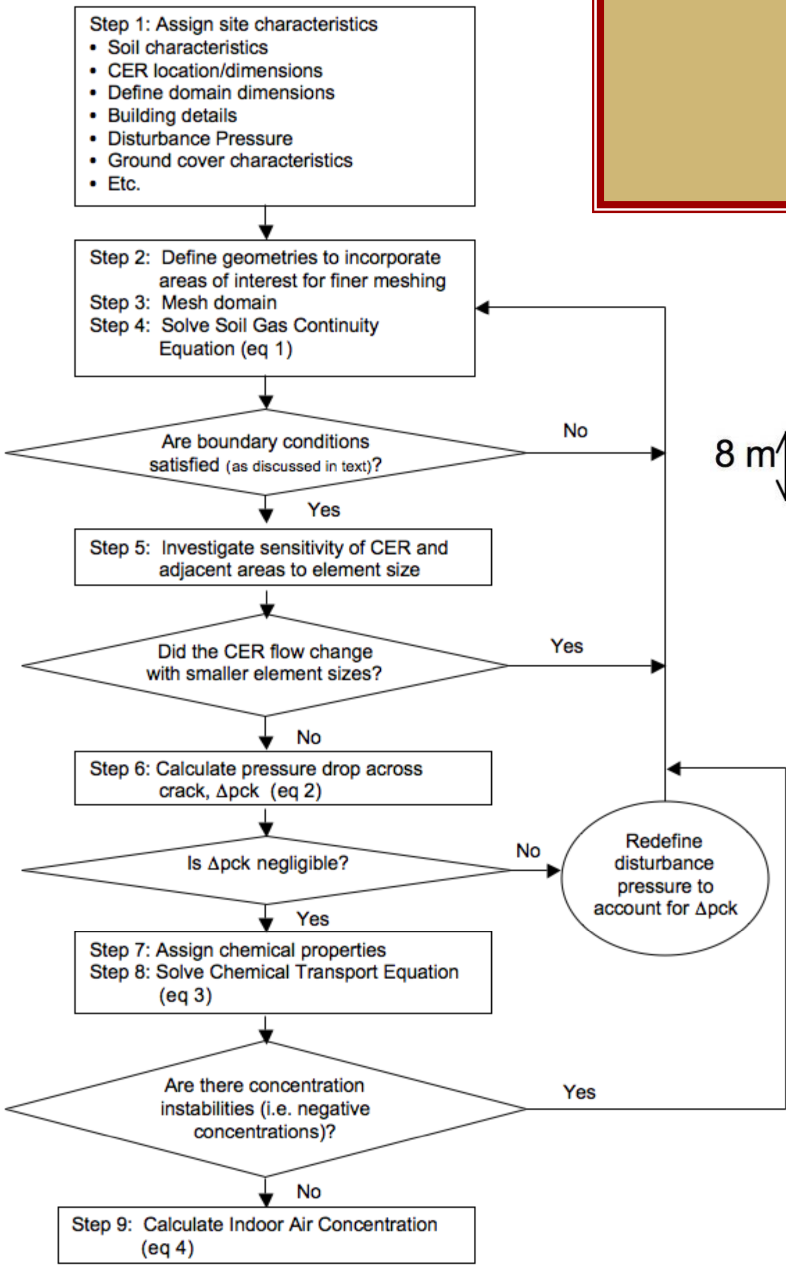
The model solves the problem in 3 steps:

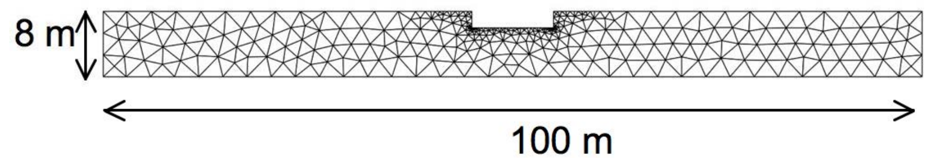
1. Gas flow through soil (Darcy's Flux)
2. Species transport
3. Indoor air concentration is calculated as a function of building exchange rate, soil gas flow into the building and concentration at the crack

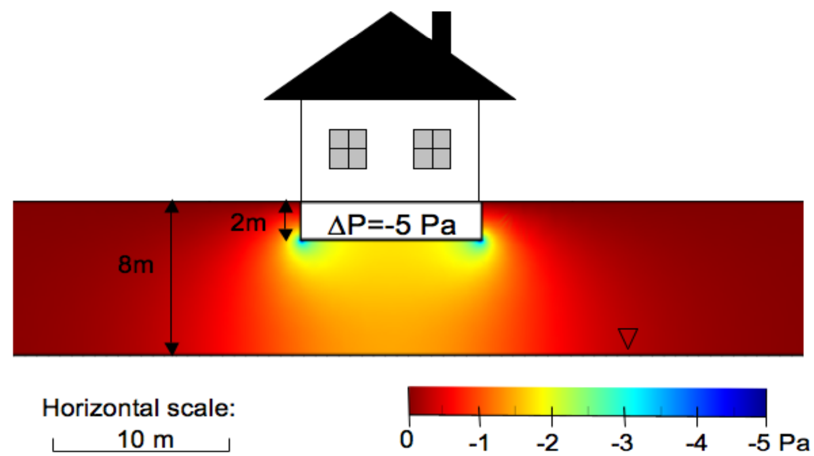


Perimeter foundation crack present.
ΔP= -5 Pa

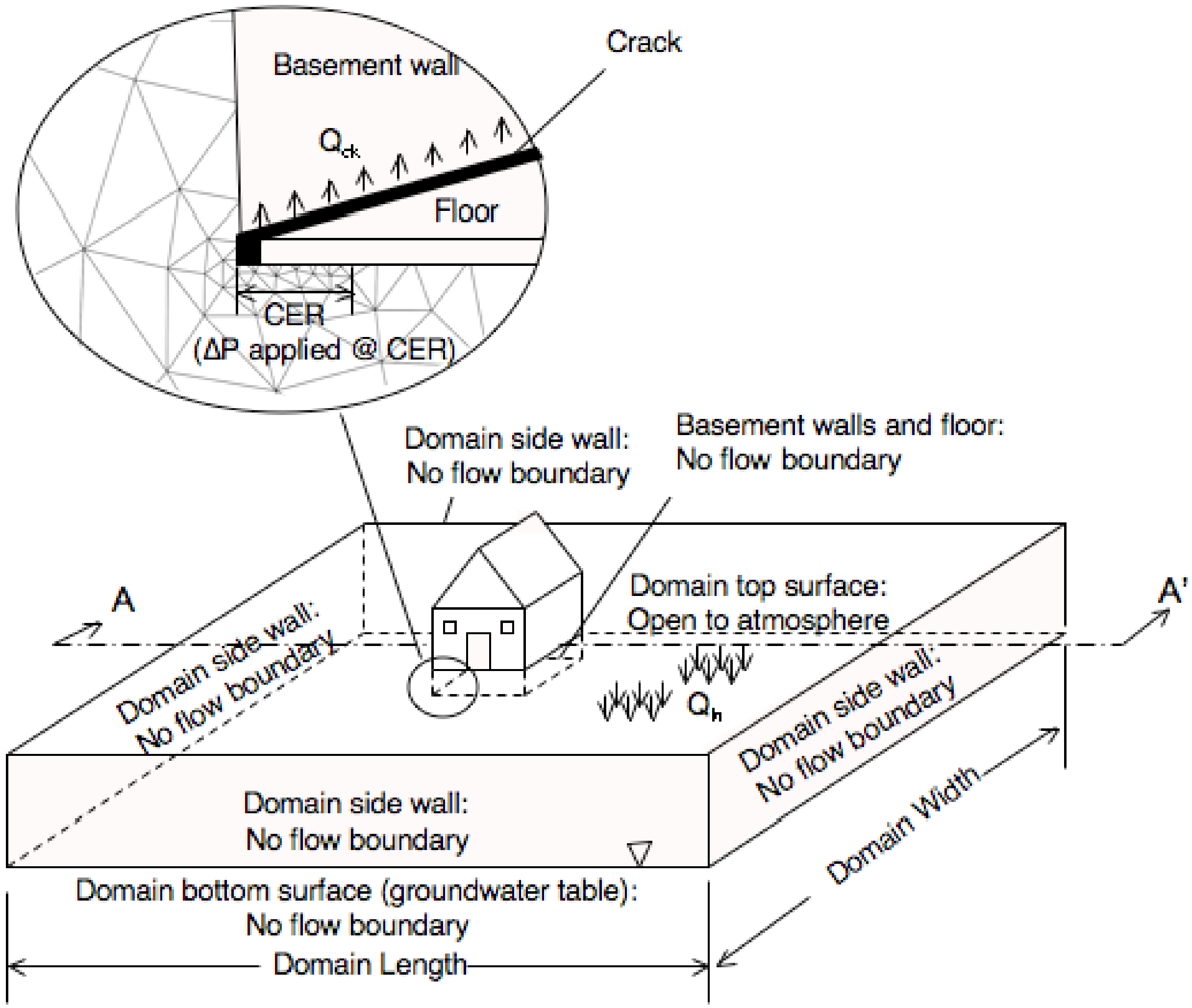
Modeling Approach (cont.)







Sample Model Domain



Gas Flow Through Soil

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

Darcy's Law for one dimensional incompressible flow

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

$$\phi = gz + \int_{Po}^{P}\frac{dP}{\rho}$$

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

q : *specific dischrg* (L/T)

κ : *permeability of the soil* (L^2)

μ : *visc. of the fluid* (M/LT)

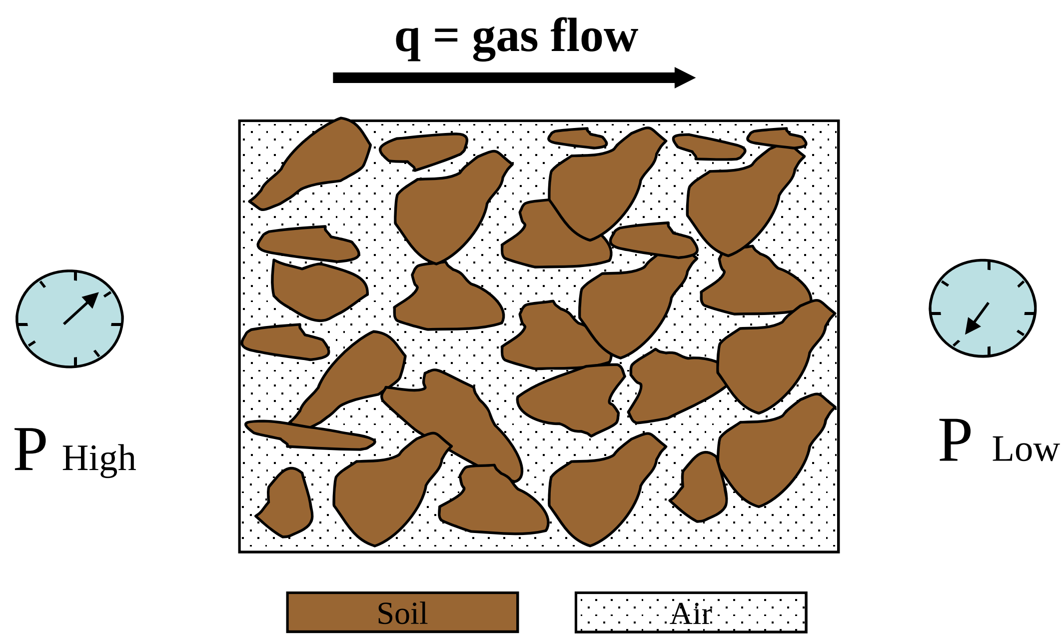
ρ : *density of the fluid* (M/L^3)

ϕ : *fluid potential*

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

z : *elevation* (L)

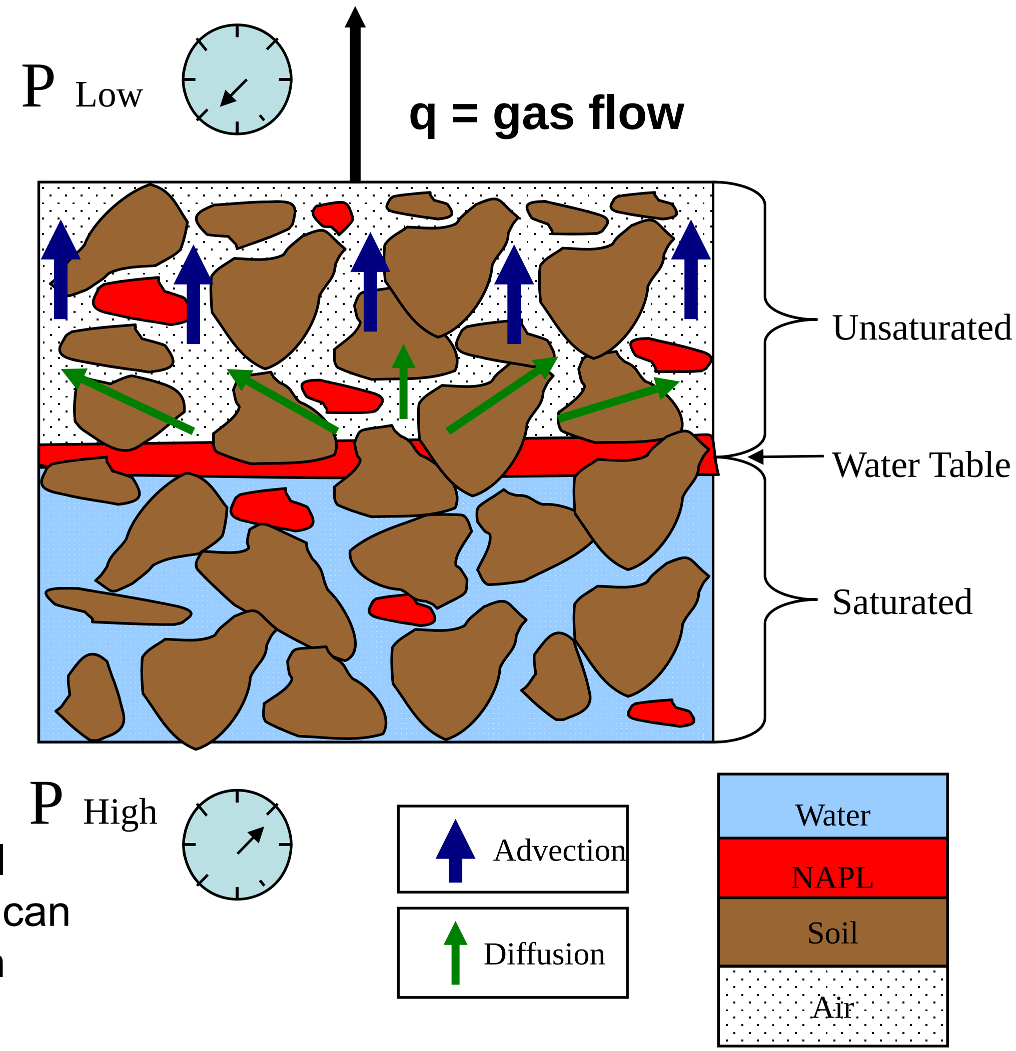
g : *gravitational acceleration* (L/T^2)



Species Transport

$$\vec{J}_T = \vec{q}C - D^{gas}_{eff,i}\nabla C$$

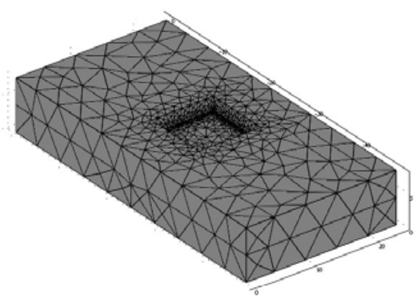
$$D^{gas}_{eff,i} = D_i^{air}\frac{\eta_g^{10/3}}{\eta_T^{2}} + \frac{D_i^{w}}{K_H}\frac{\eta_w^{10/3}}{\eta_T^{2}}$$



Non-aqueous liquids (NAPL) and residual contamination in groundwater and/or soil can act as the source for vapor contamination

Determining Indoor Air Concentration

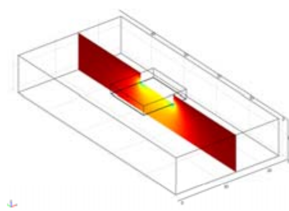
Model Domain



Gas Transport

$$q = \frac{k \cdot \rho_g \cdot d\phi}{\mu_g}$$

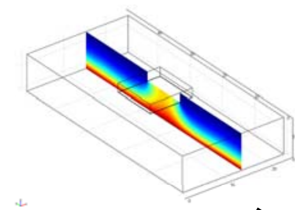
$$d\phi = gz + \int_{P_0}^{P} \frac{dP}{\rho}$$



Chemical Transport

$$J_T = q \cdot C + D_{ig} \nabla C$$

$$D_{ig} = d_i^{air} \cdot \frac{\eta_g^{10/3}}{\eta_T^{2}}$$



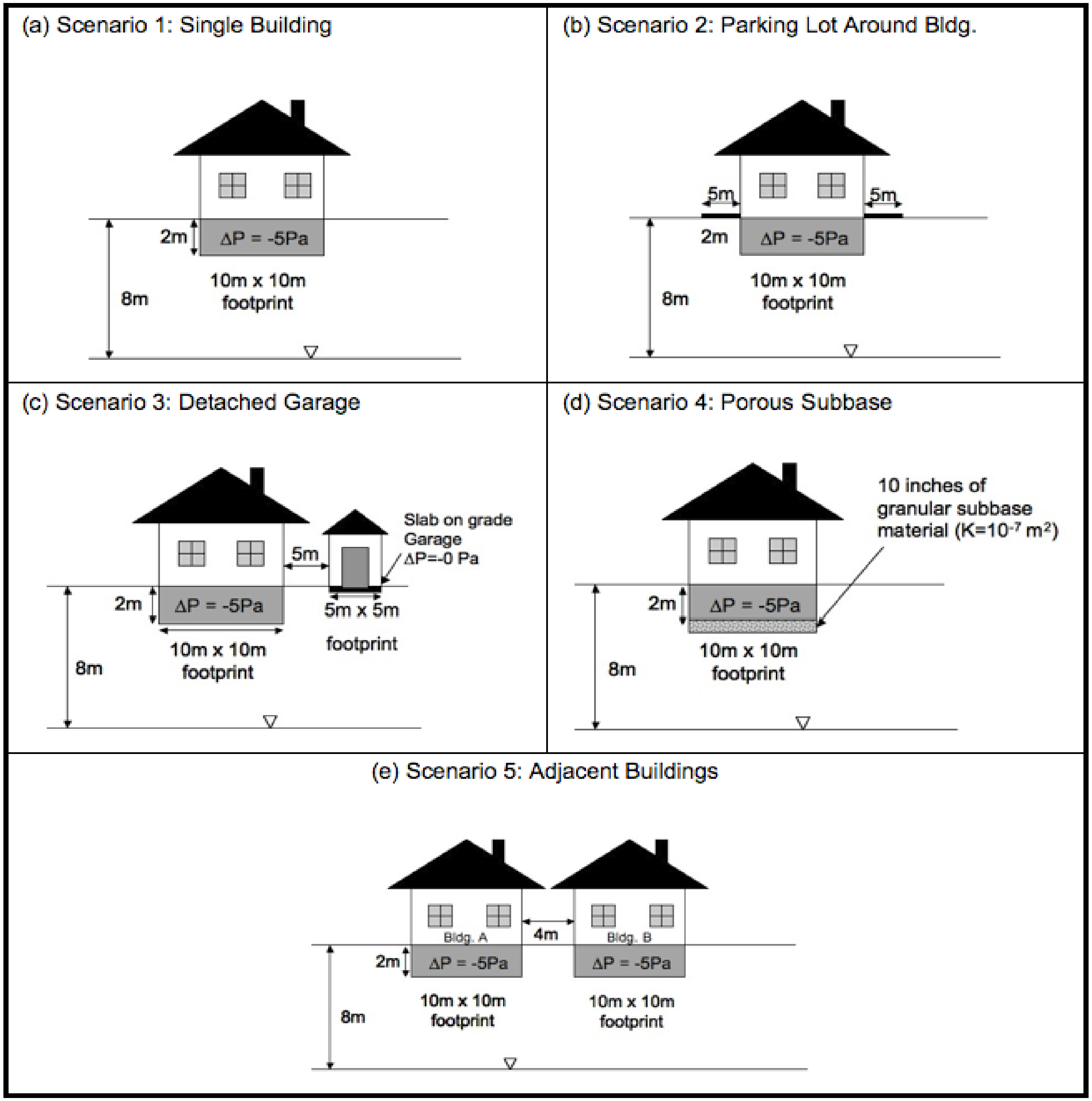
Indoor Air Concentration

$$C_{indoor} = \frac{M_{ck}}{A_e \cdot V_b + Q_{ck}}$$

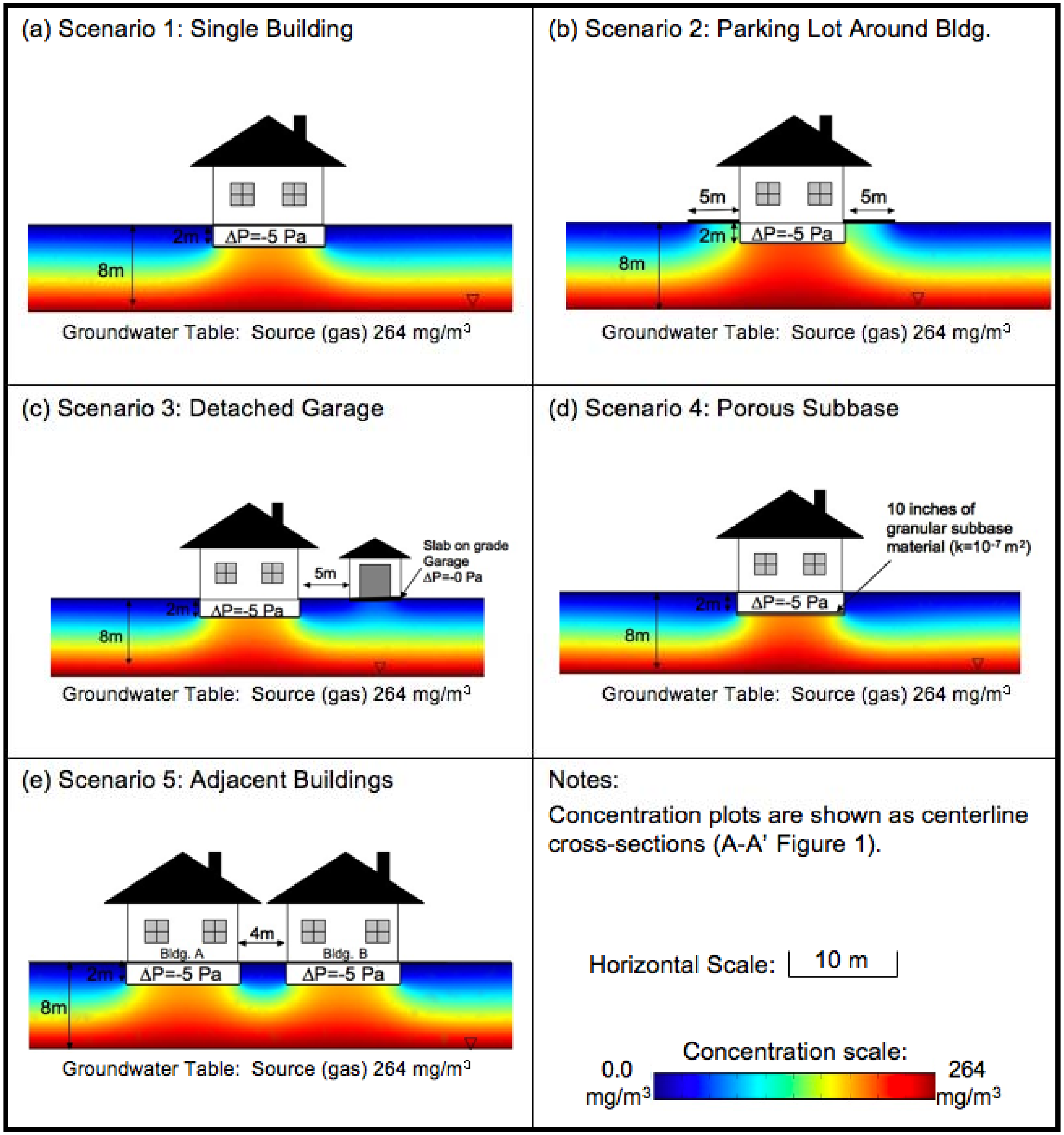
Indoor air concentration is a function of building operations. The mass flow rate of the contaminant into the house (M_{ck}) is affected by building depressurization (but few other building parameters).

Model Scenarios (Homogenous Geology) Various Site Features

Pennell et al. 2008
Journal of the AWMA



Soil Gas Concentrations (Homogenous Geology) Various Site Features



Pennell et al. 2008
Journal of the AWMA

k (m^2)	Scenario[a]	Q (m^3/sec)	Conc. at the Crack[b] (mg/m^3)	Subslab Conc.[c] (mg/m^3)	Indoor Air Conc. (mg/m^3)	Mass Flowrate (mg/s)	Indoor Air Conc./Subslab Conc. ($\alpha_{subslab}$)	Indoor Air Conc./Source (gas) Conc. (α_{gw})
10^{-10}	1	7.91E-04	7.45E+01	2.17E+02	1.78E+00	5.89E-02	8.20E-03	6.72E-03
	2	6.26E-04	1.16E+02	2.26E+02	2.19E+00	7.24E-02	9.69E-03	8.29E-03
	3	7.91E-04	7.44E+01	2.17E+02	1.78E+00	5.88E-02	8.18E-03	6.71E-03
	4	1.31E-03	4.88E+01	2.24E+02	1.90E+00	6.39E-02	8.46E-03	7.17E-03
	5	7.52E-04	6.40E+01	2.07E+02	1.45E+00	4.82E-02	7.03E-03	5.50E-03
10^{-11}	1	7.91E-05	1.10E+02	1.90E+02	2.68E-01	8.70E-03	1.41E-03	1.01E-03
	2	6.26E-05	1.81E+02	2.15E+02	3.49E-01	1.13E-02	1.62E-03	1.32E-03
	3	7.91E-05	1.10E+02	1.90E+02	2.68E-01	8.70E-03	1.41E-03	1.01E-03
	4	1.31E-04	1.00E+02	1.98E+02	4.03E-01	1.31E-02	2.04E-03	1.52E-03
	5	7.52E-05	6.23E+01	1.75E+02	1.88E-02	8.02E-03	1.07E-04	7.09E-05
10^{-12}	1	7.91E-06	8.78E+01	1.81E+02	3.85E-02	1.25E-03	2.13E-04	1.46E-04
	2	6.26E-06	1.37E+02	2.08E+02	5.58E-02	1.80E-03	2.68E-04	2.11E-04
	3	7.91E-06	8.80E+01	1.81E+02	3.86E-02	1.25E-03	2.13E-04	1.46E-04
	4	1.31E-05	9.68E+01	1.81E+02	5.29E-02	1.71E-03	2.91E-04	2.00E-04
	5	7.52E-06	8.82E+01	1.81E+02	3.80E-02	1.23E-03	2.10E-04	1.44E-04
10^{-13}	1	7.91E-07	7.33E+01	1.77E+02	2.29E-02	7.40E-04	1.30E-04	8.65E-05
	2	6.26E-07	1.14E+02	2.02E+02	3.53E-02	1.14E-03	1.75E-04	1.33E-04
	3	7.91E-07	7.34E+01	1.77E+02	2.29E-02	7.42E-04	1.30E-04	8.66E-05
	4	1.31E-06	8.10E+01	1.71E+02	2.60E-02	8.41E-04	1.52E-04	9.82E-05
	5	7.52E-07	7.40E+01	1.78E+02	2.31E-02	7.47E-04	1.30E-04	8.72E-05
10^{-14}	1	7.91E-08	6.17E+01	1.74E+02	1.86E-02	6.01E-04	1.07E-04	7.02E-05
	2	6.26E-08	9.49E+01	1.97E+02	2.86E-02	9.24E-04	1.45E-04	1.08E-04
	3	7.91E-08	6.18E+01	1.74E+02	1.86E-02	6.02E-04	1.07E-04	7.03E-05
	4	1.33E-07	7.34E+01	1.61E+02	2.22E-02	7.17E-04	1.38E-04	8.37E-05
	5	7.52E-08	6.23E+01	1.75E+02	1.87E-02	6.07E-04	1.07E-04	7.09E-05
Diffusion K=10^{-14}	1	0.00E+00	6.16E+01	1.74E+02	1.85E-02	5.97E-04	1.06E-04	6.98E-05
	2	0.00E+00	9.47E+01	1.97E+02	2.84E-02	9.19E-04	1.44E-04	1.07E-04
	3	0.00E+00	6.17E+01	1.74E+02	1.85E-02	5.98E-04	1.06E-04	6.99E-05
	4	0.00E+00	7.32E+01	1.61E+02	2.19E-02	7.10E-04	1.36E-04	8.30E-05
	5	0.00E+00	6.21E+01	1.75E+02	1.86E-02	6.03E-04	1.07E-04	7.04E-05

[a] 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 Š Two buildings separated by 4m (data shown for Building A. Due to symmetry, data for Building B should be identical).

[b] 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.

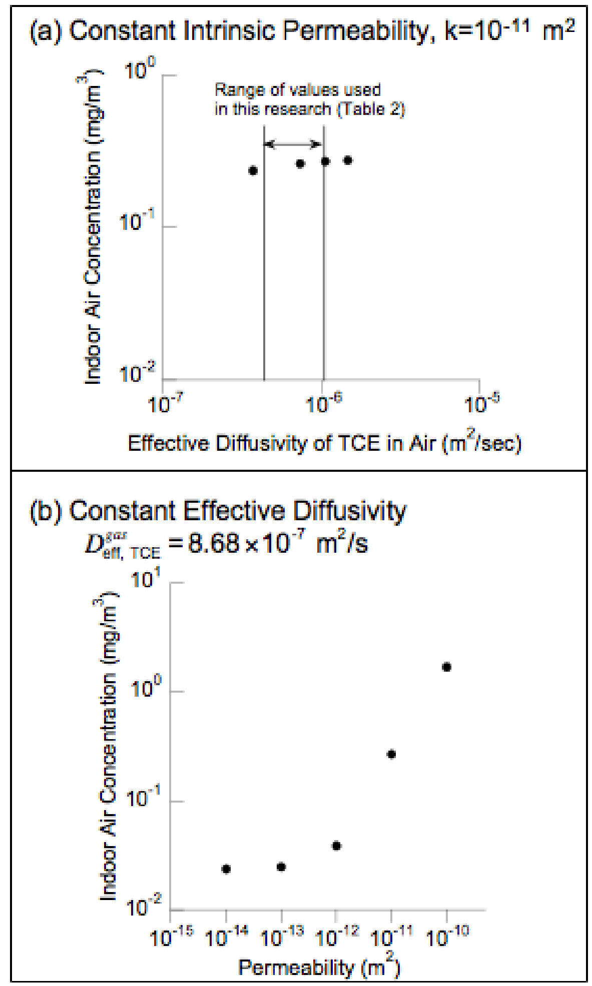
[c] The subslab concentration location is the center of the building footprint at foundation:soil interface.

Pennell et al. 2008
Journal of the AWMA

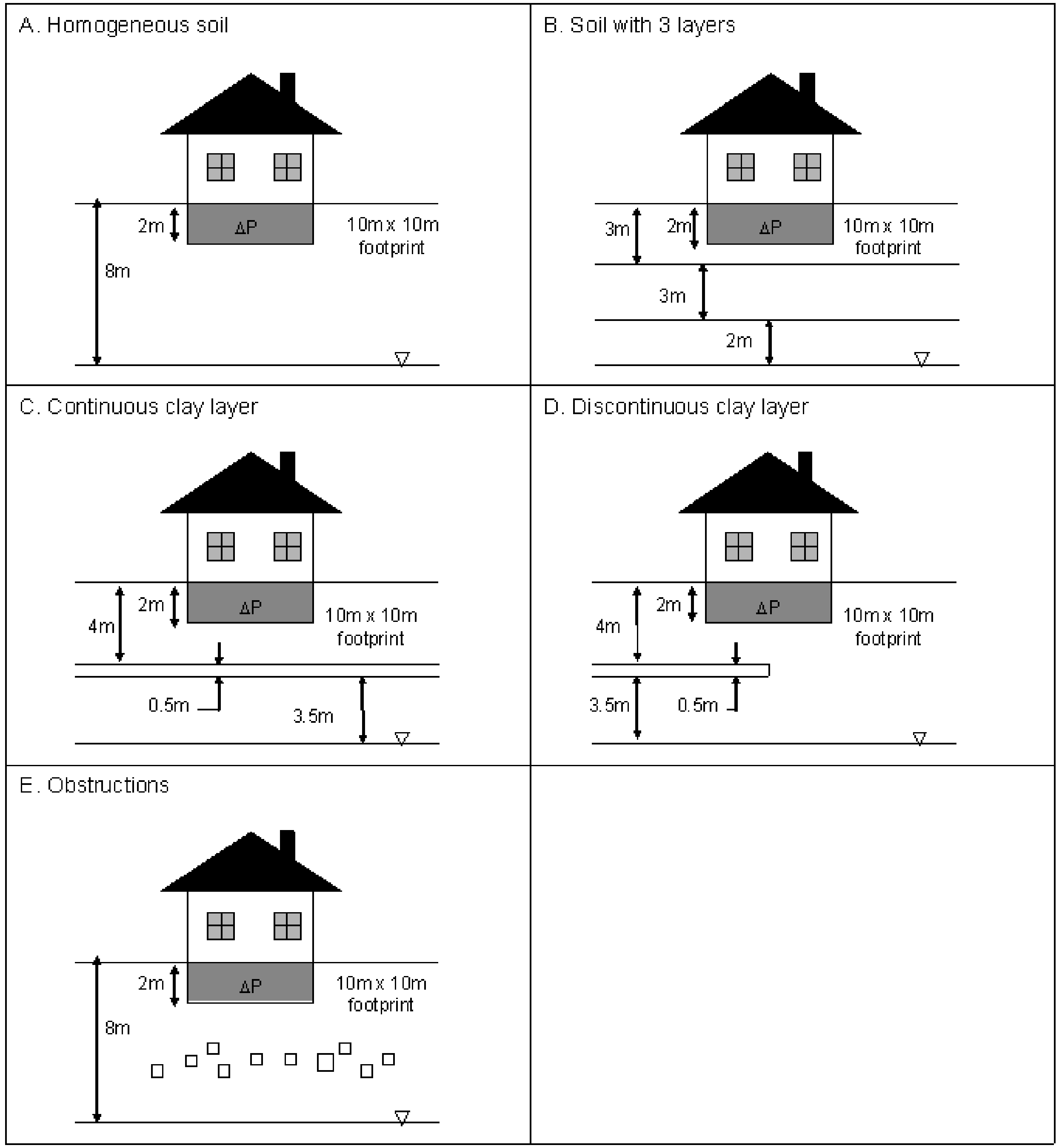
Sensitivity Analysis
(Permeability vs. Diffusivity)

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

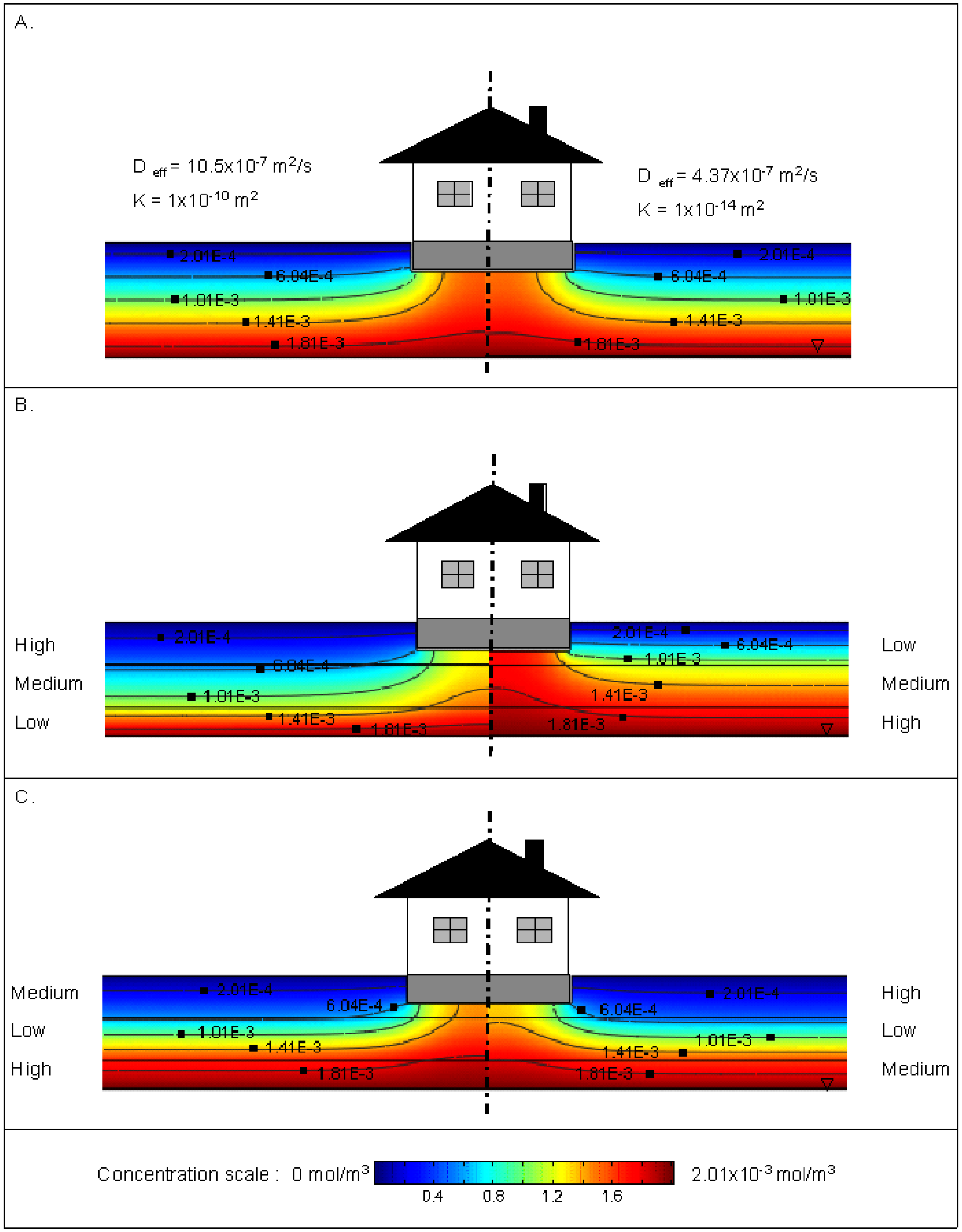
$$q = \frac{-\kappa\rho}{\mu} \frac{dP}{dx}$$



More Advanced Model Scenarios (Various Geologic Features)



Bozkurt et al.
(submitted GWMR, 2008)



No Pressurization

A. Homogenous

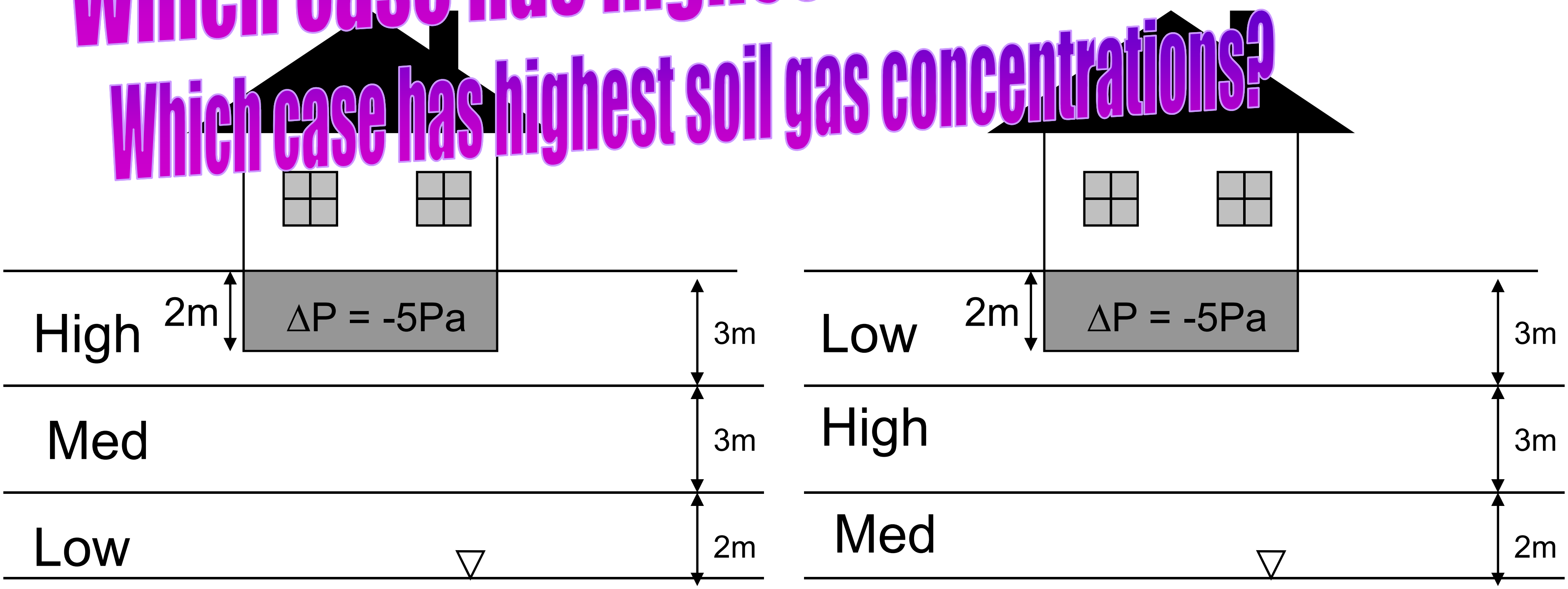
B. & C. Layered

Bozkurt et al.
(submitted GWMR, 2008)

Three Layers of Soil (Pressurized)

Which case has highest indoor air?

Which case has highest soil gas concentrations?

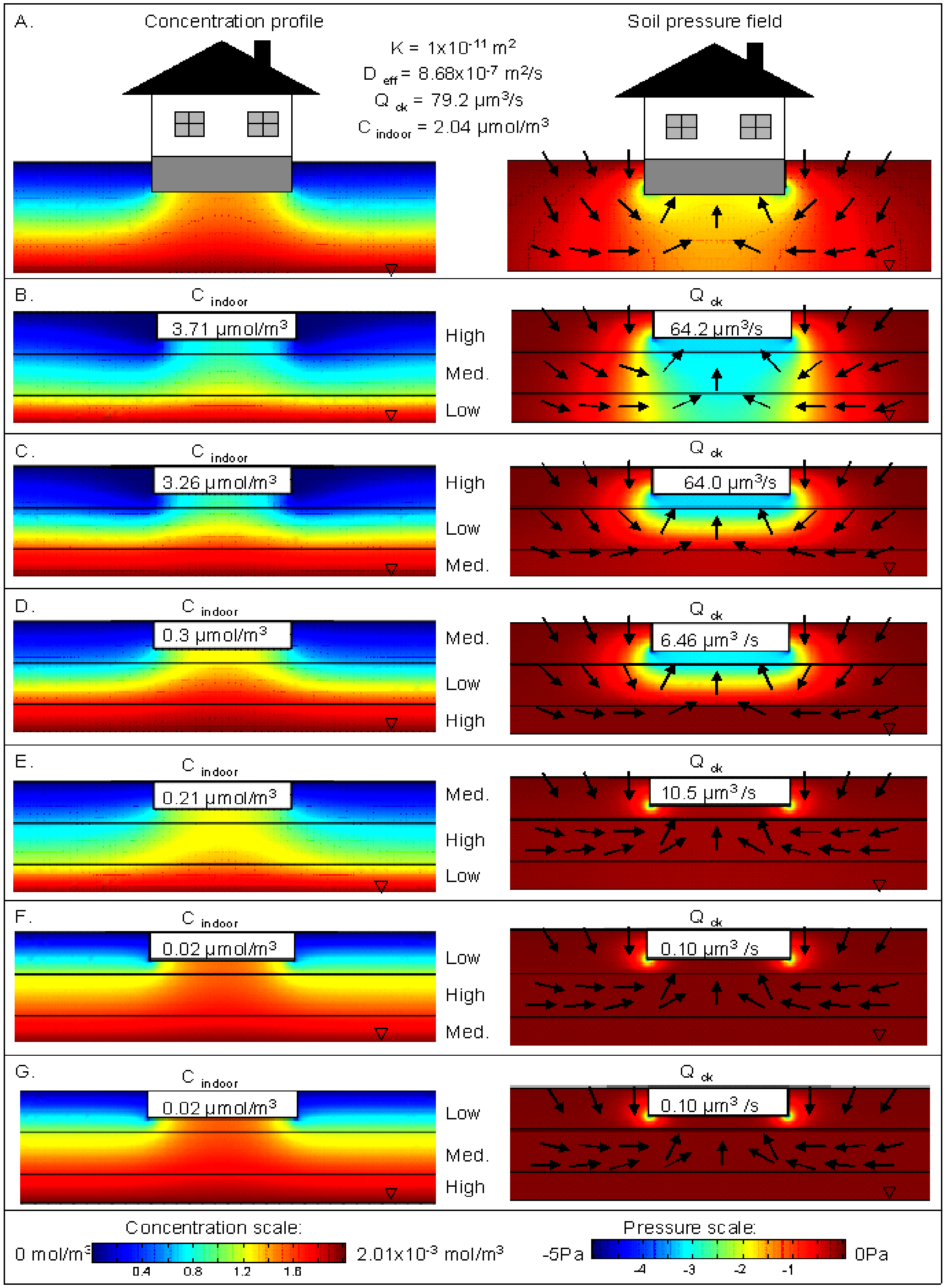


<u>High Permeability/Diffusivity</u>
$k_{High} = 10^{-10}\ m^2$, $D^{gas}_{eff,i\ High} = 1.05E\text{-}6\ m^2/s$

<u>Medium Permeability/Diffusivity</u>
$k_{Medium} = 10^{-12}\ m^2$, $D^{gas}_{eff,i\ Medium} = 8.68E\text{-}7\ m^2/s$

<u>Low Permeability/Diffusivity</u>
$k_{Low} = 10^{-14}\ m^2$, $D^{gas}_{eff,i\ Low} = 4.37E\text{-}7\ m^2/s$

Bozkurt et al.
(submitted GWMR, 2008)

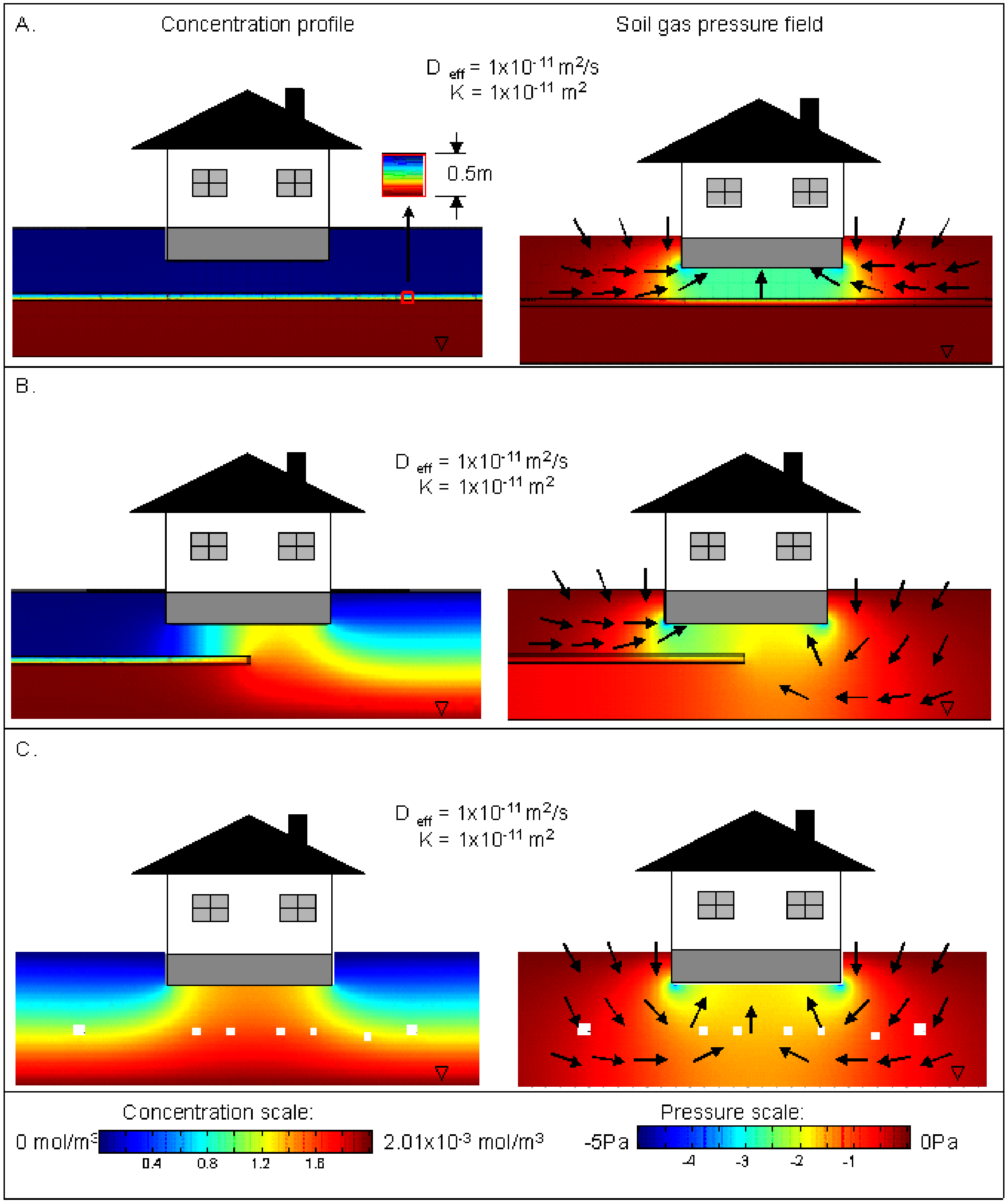


Layered Soil Results

High (top) highest indoor air

Low (top) highest soil gas concentrations

Bozkurt et al.
(submitted GWMR, 2008)



Other Geologic Features

Soil surrounding clay/obstructions, K=10^{-11} m^2	Indoor Air (mg/m^3)
Continuous Clay	0.0029
Discontinuous Clay	0.16
Obstructions (Plain)	0.27

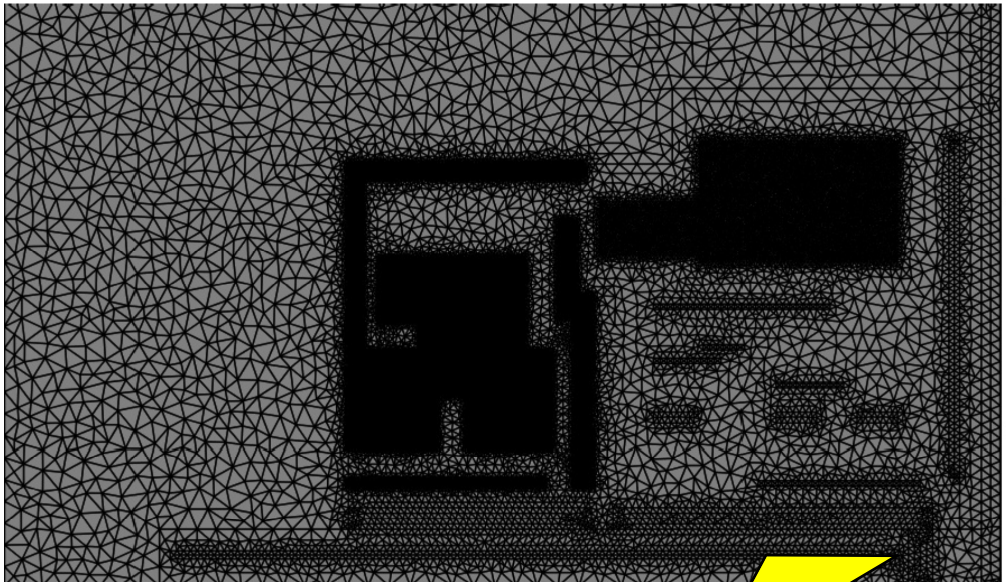
Bozkurt et al.
(submitted GWMR, 2008)

Conclusions

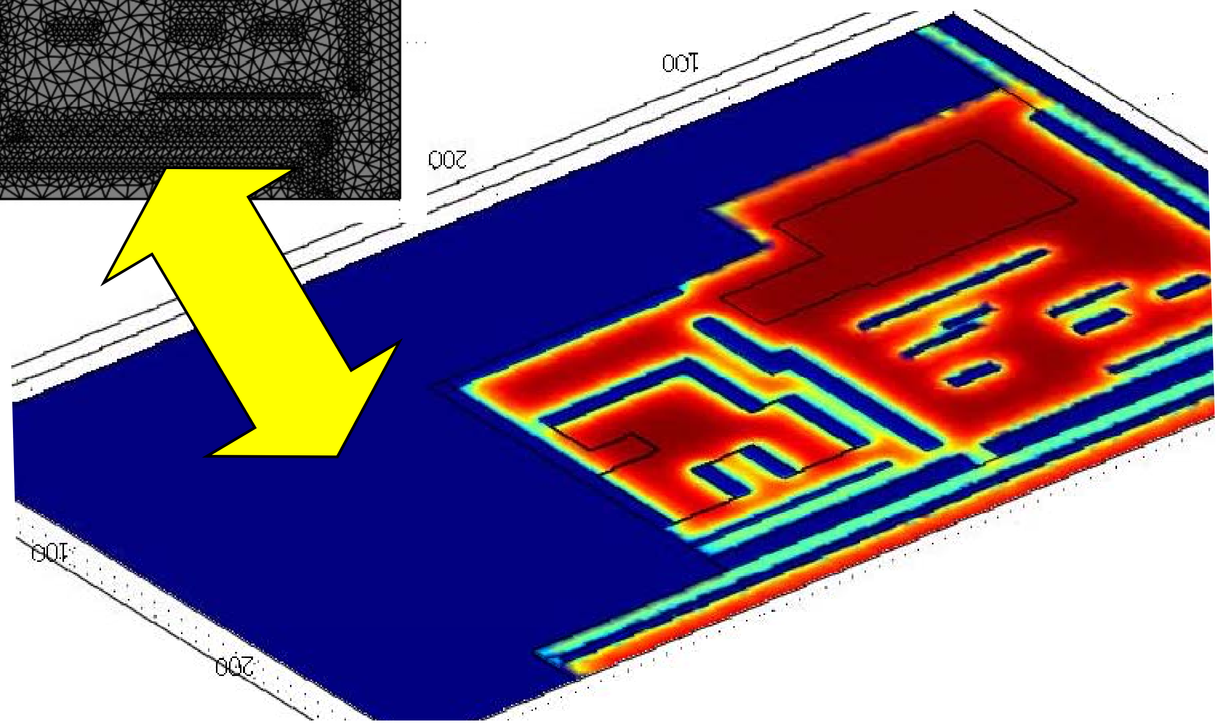
- Vapor intrusion potentials are difficult to predict if soil gas concentrations are used by themselves.
- Modeling can be used as tool to interpret field results.
- Field verification/calibration/validation are being conducted as a next step…

Current Efforts

Modeling Approach

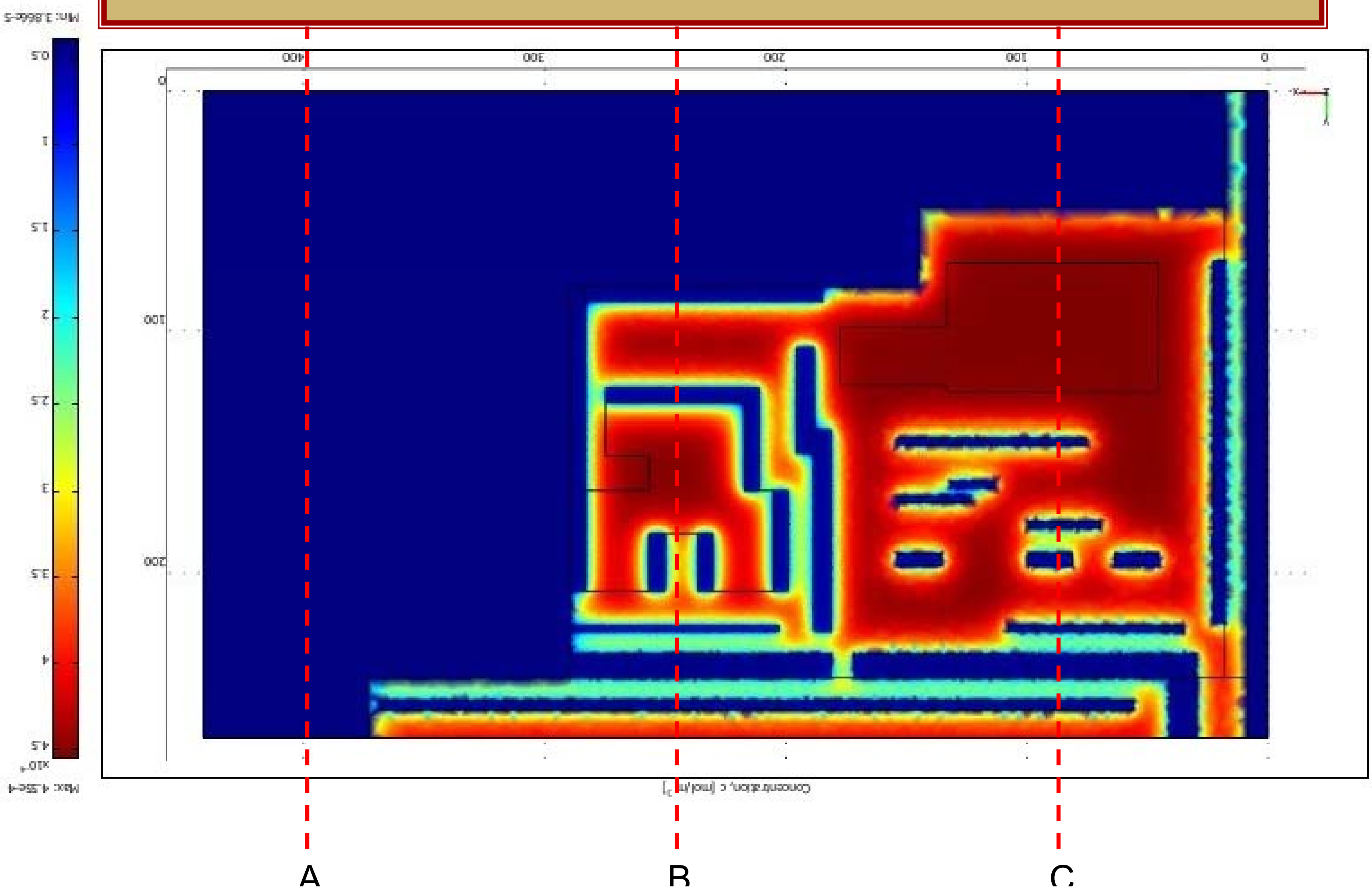


Mesh generation is complex. Proper mesh geometry is critical to accuracy of model results.

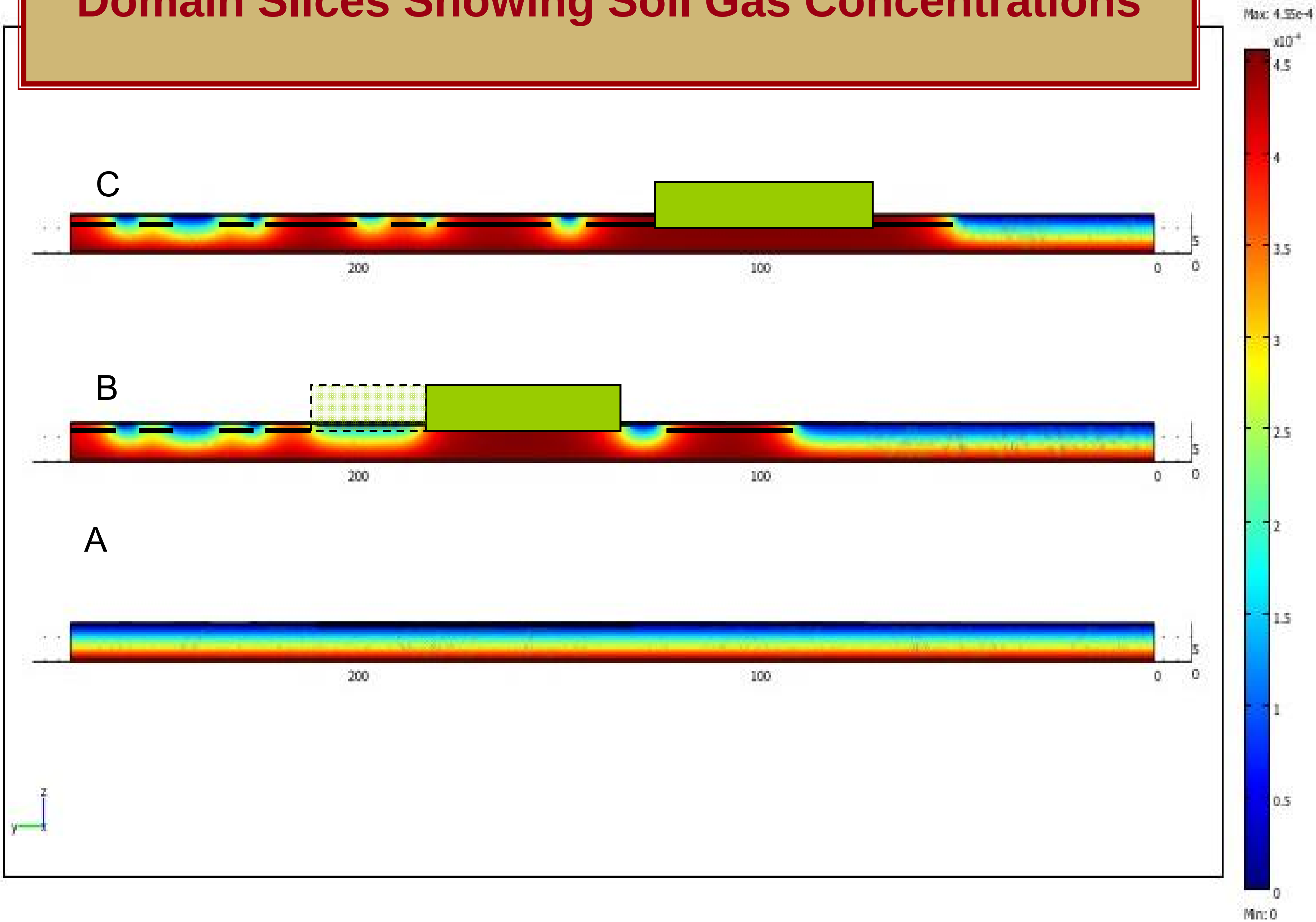


Iterative Process: Evaluate instabilities in concentration and re-mesh.

Soil Gas Concentrations (2m bgs)



Domain Slices Showing Soil Gas Concentrations



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

Contact Info:

- Have a site that might be a good candidate for model verification?
- Have questions about our research?

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