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

Eric Suuberg
School of Engineering, Brown University
Providence, Rhode Island
With Kelly Pennell, Ozgur Bozkurt, Yijun Yao, Rui Shen, Niklas Novoa

Some Examples of Calculations Using 3-D Models

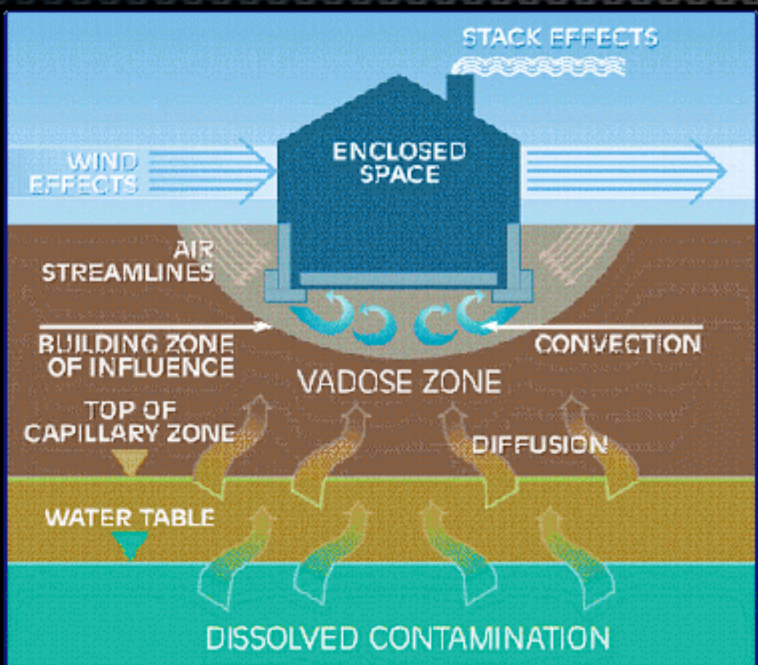
- There are many models out there...
- Full 3-D Models- different calculational approaches
- How does the assumed nature of foundation breaches affect results?
- Diffusion dominated profiles of COCs in soil vs. predicting actual contaminant entry rates
- The role of advection

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

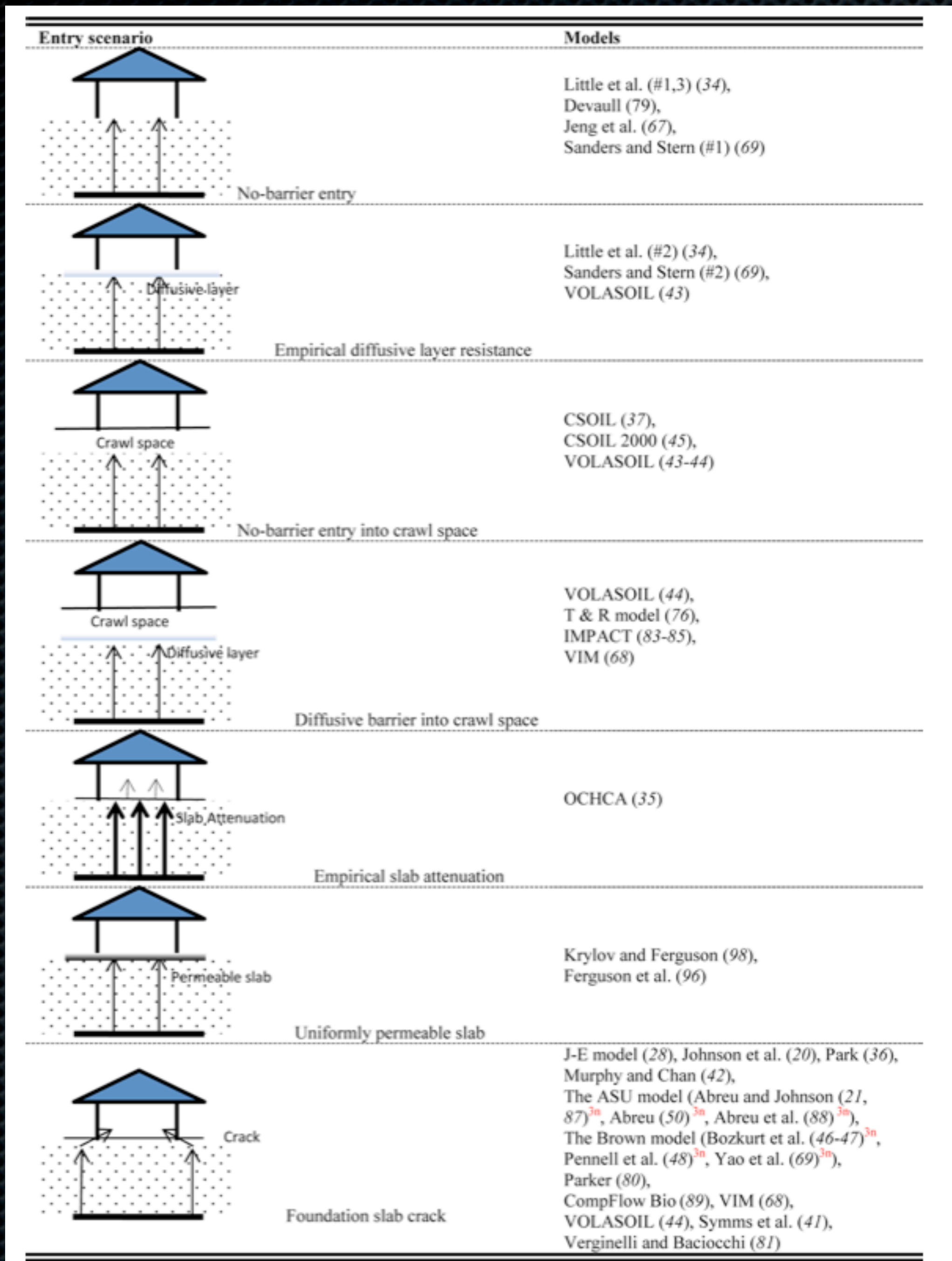
Modeling Approach

- A finite element computational package (Comsol) used to describe transport processes.



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

- 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.

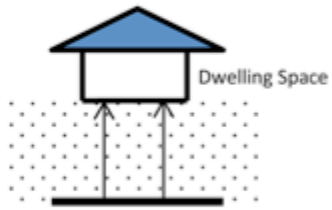
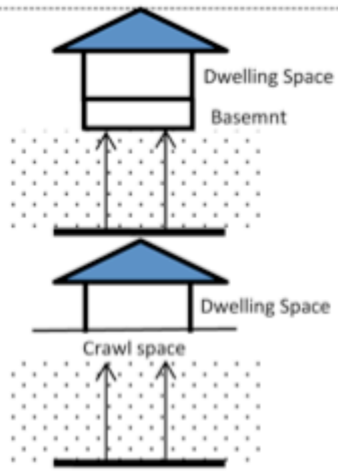
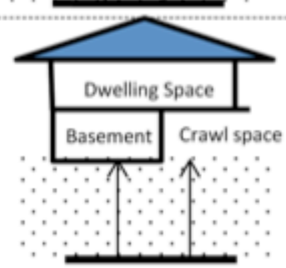


Entry scenario	Models
No-barrier entry	Little et al. (#1,3) (*34*), Devaull (79), Jeng et al. (*67*), Sanders and Stern (#1) (*69*)
Diffusive layer Empirical diffusive layer resistance	Little et al. (#2) (*34*), Sanders and Stern (#2) (*69*), VOLASOIL (*43*)
Crawl space No-barrier entry into crawl space	CSOIL (*37*), CSOIL 2000 (*45*), VOLASOIL (*43-44*)
Crawl space Diffusive layer Diffusive barrier into crawl space	VOLASOIL (*44*), T & R model (*76*), IMPACT (*83-85*), VIM (*68*)
Slab Attenuation Empirical slab attenuation	OCHCA (*35*)
Permeable slab Uniformly permeable slab	Krylov and Ferguson (*98*), Ferguson et al. (*96*)
Crack Foundation slab crack	J-E model (*28*), Johnson et al. (*20*), Park (*36*), Murphy and Chan (*42*), The ASU model (Abreu and Johnson (*21*, *87*)[3n], Abreu (*50*)[3n], Abreu et al. (*88*)[3n]), The Brown model (Bozkurt et al. (*46-47*)[3n], Pennell et al. (*48*)[3n], Yao et al. (*69*)[3n]), Parker (*80*), CompFlow Bio (*89*), VIM (*68*), VOLASOIL (*44*), Symms et al. (*41*), Verginelli and Baciocchi (*81*)

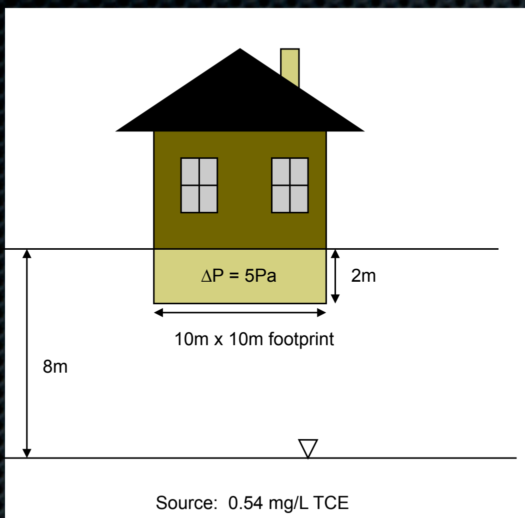
Lots of mathematical models of VI already in use worldwide

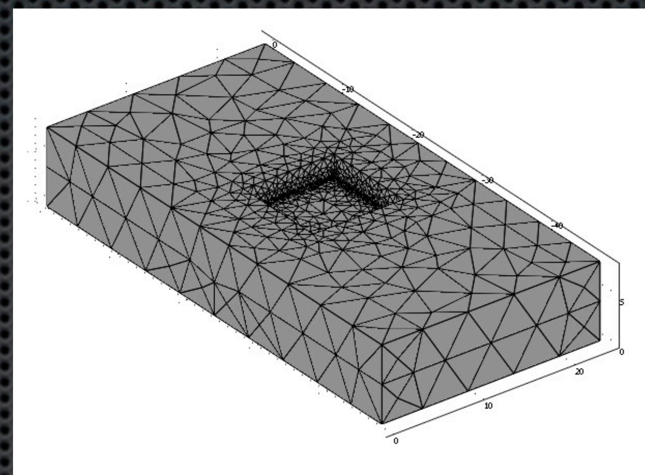
Source: Yao et al., *Env. Sci. Tech.*, *47*, 2457-2470 (2013).

Need to make important choices about how to handle above-ground effects.

Entry scenario		Models
	Single CST	Little et al. (34), OCHCA (35), Sanders and Stern (69), J-E model (28), Johnson et al. (20), Jeng et al. (67), Parker (80), Devaull (79), CompFlow Bio (89), Verginelli and Baciocchi (81), The ASU model (Abreu and Johnson (21, 87)[3n], Abreu (50)[3n], Abreu et al. (88)[3n]), The Brown model (Bozkurt et al. (46-47)[3n], Pennell et al. (48)[3n], Yao et al. (49)[3n]),
	Series CSTs	T & R model (76), CSOIL (37), VOLASOIL (43-44), CSOIL 2000 (45), IMPACT (83-85), Murphy and Chan (42), Olson and Corsi (103-104), Ferguson et al. (96), Krylov and Ferguson (98)
	Combined series and parallel CSTs	VIM (68)

3-D Modeling Approach- Finite Element Solver (COMSOL)





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.

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

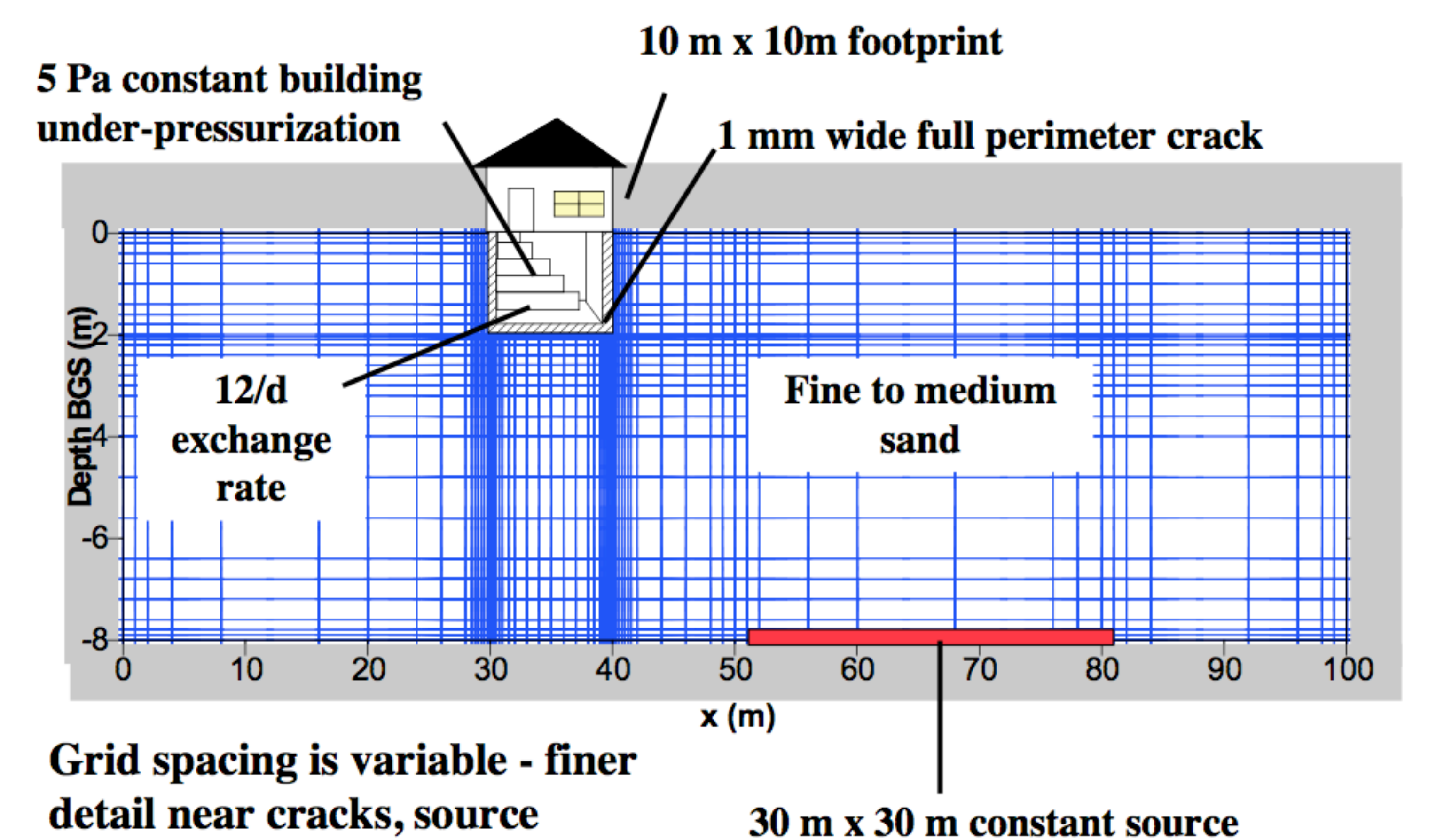
$$\phi = gz + \int_{Po}^{P}\frac{dP}{\rho}$$

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

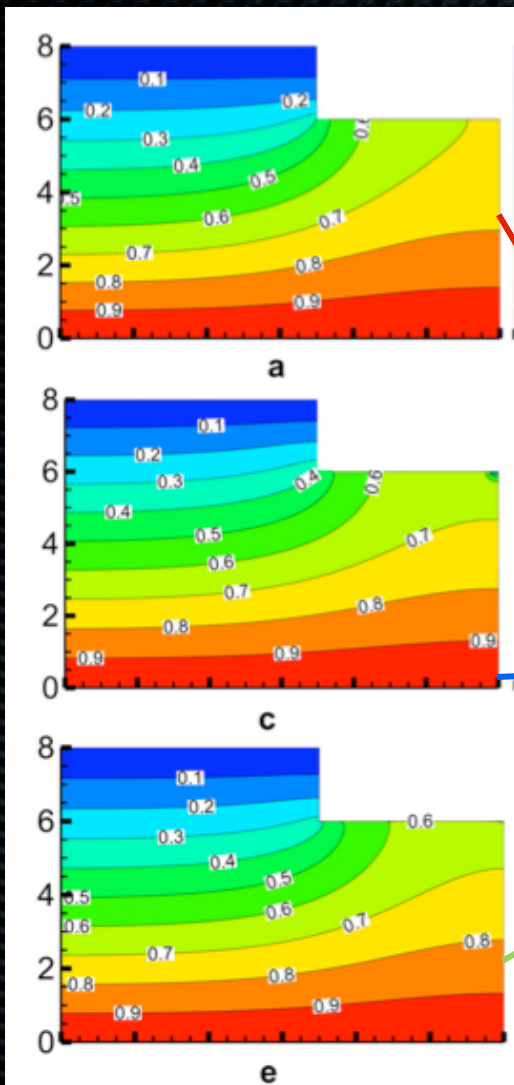
$$D_{ig} = d_i^{air} \cdot \frac{\eta_g^{10/3}}{\eta_T^{2}}$$

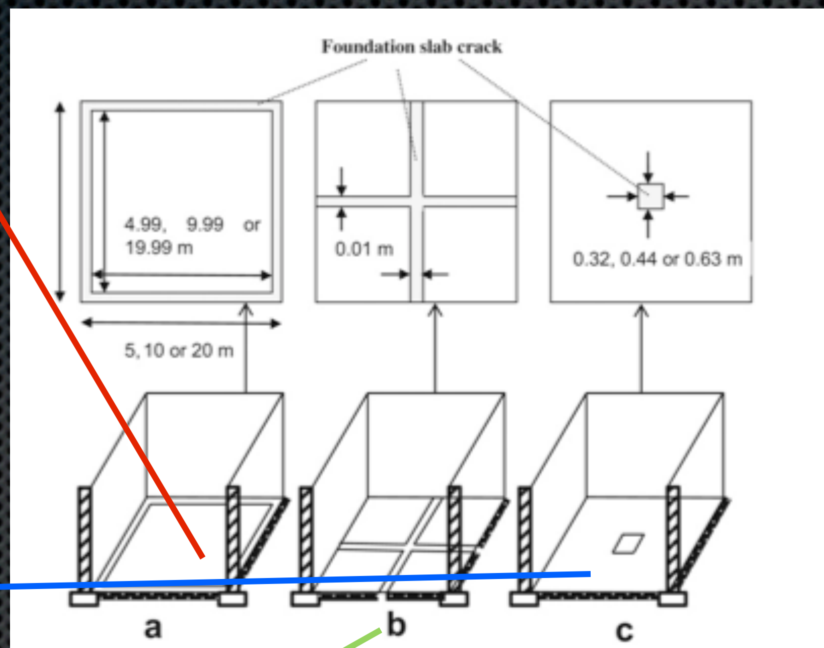
$$C_{indoor} = \frac{J_{T\,ck}}{A_e \cdot V_b + Q_{ck}}$$

Not the only 3-D model; Abreu and Johnson have developed a finite difference model



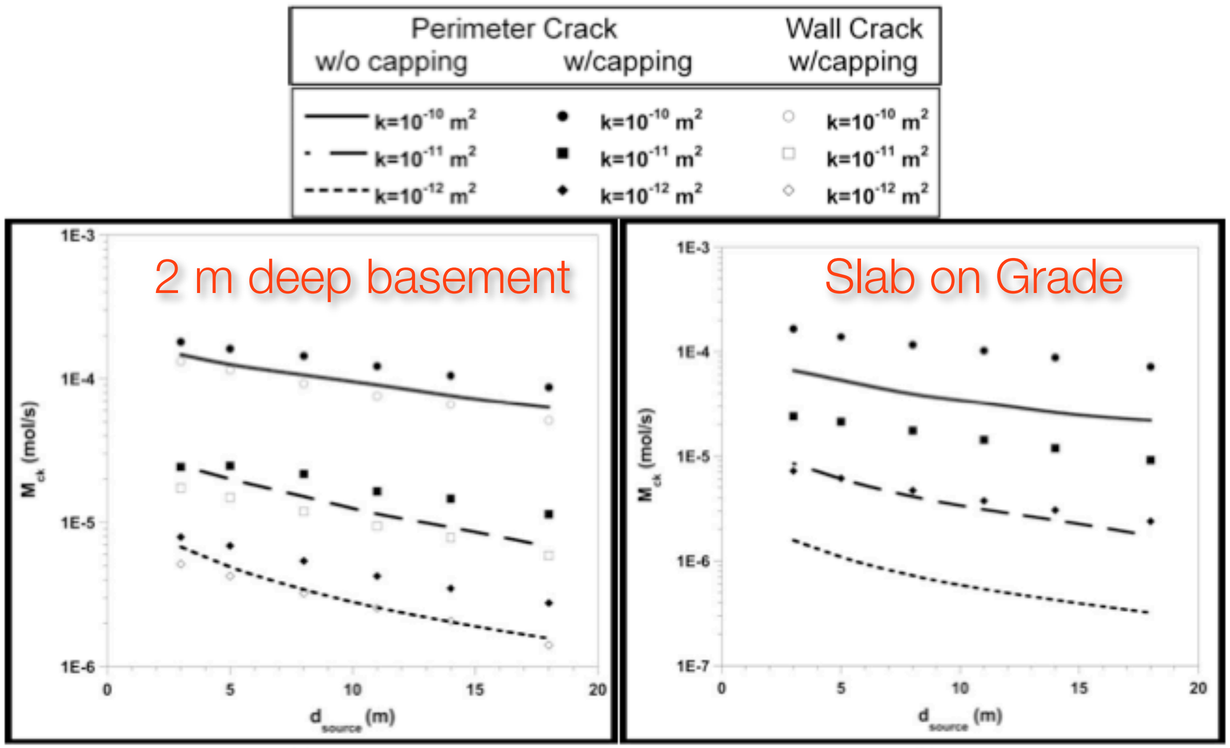
Grid spacing is variable - finer detail near cracks, source boundaries, and domain boundaries

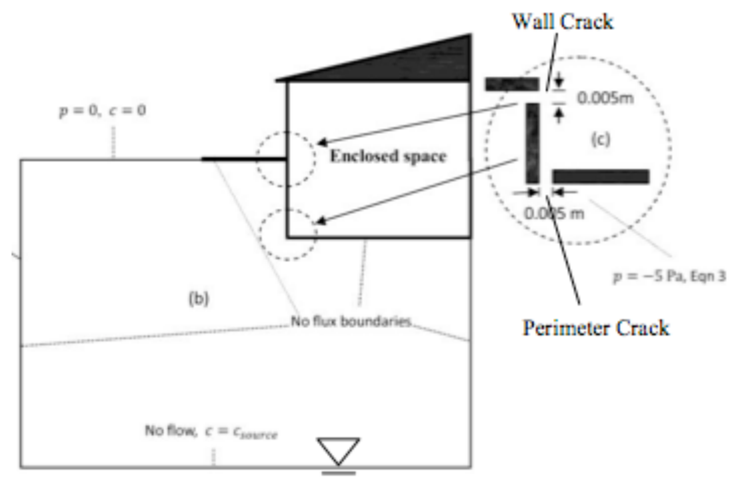




Really does not make much difference what sort of "cracks", i.e., foundation breaches, are selected.

Yao et al., *Building and Environment*, *59*, 417-425 (2013).





Yao et al., *Procedia Env. Sci.*, *4*, 245-250 (2011).

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)

First Scenario Modeled: Homogeneous Soil Properties Throughout the Domain

Groundwater at 8 m bgs

Basement depth 2m

GW TCE Concentration 54 µg/L

Effect of Geology on Vapor Concentration Profiles:

Permeability	Soil Gas Entry Rate, Q (L/min)	P crack (Pa)	C crack (mg/m^3)	Mass flow rate (mg/sec)	C indoor air (µg/m^3)
High (10^{-10} m^2)	47.5	-5	75	5.89×10^{-2}	1800
Moderate (10^{-11} m^2)	4.75	-5	110	8.70×10^{-3}	268
Low (10^{-14} m^2)	0.0048	-5	174	6.01×10^{-4}	18.6

IN action level 1.2µg/m^3

Sand and Gravel

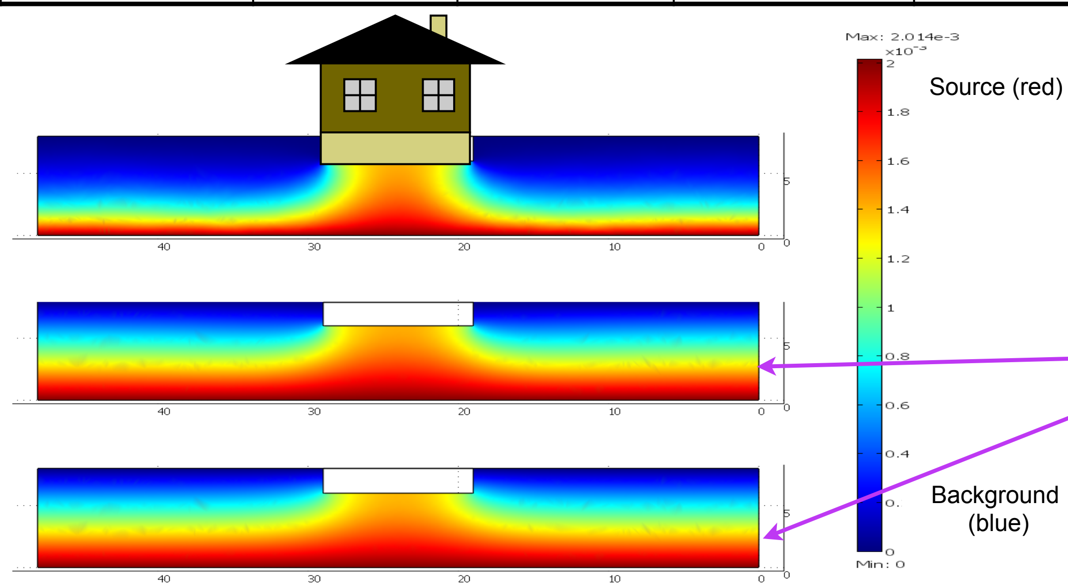
(High permeability)

Silty Sand

(Moderate permeability)

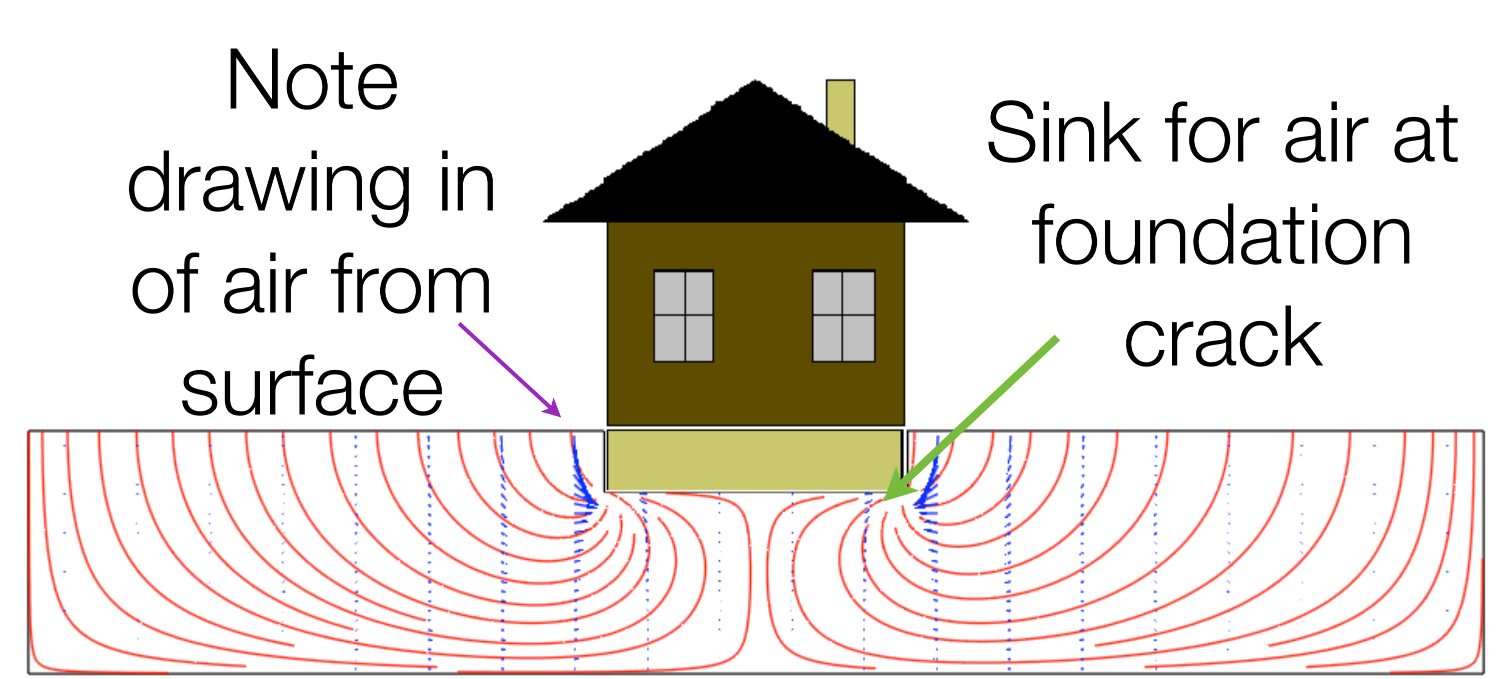
Silty Clay

(Low permeability)



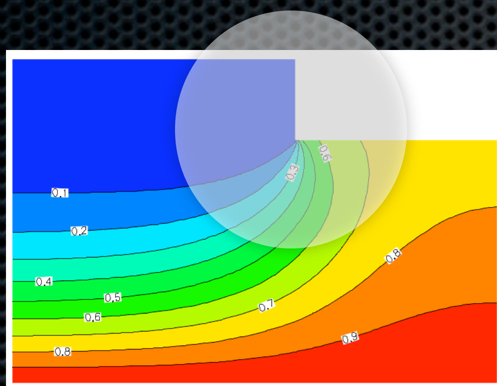
Diffusion Controlled Gradients

Steady state contaminant concentration gradient in soil mainly determined by diffusion



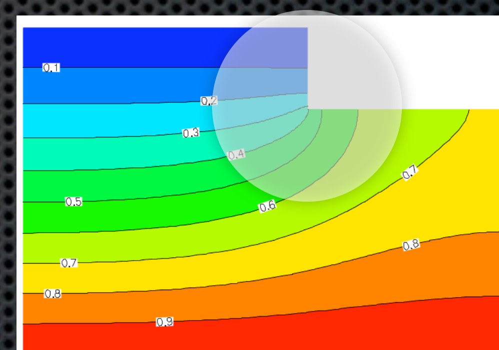
Blue Arrows indicate magnitude of air flow
Red Lines are streamlines

Interplay of advection and diffusion critical



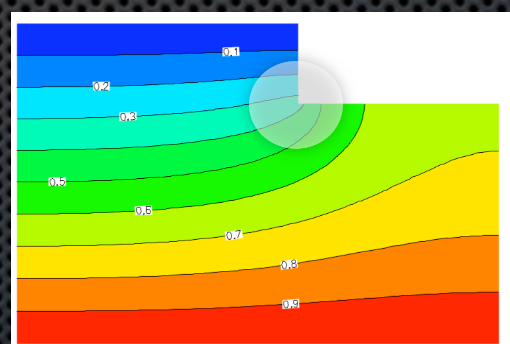
$k=10^{-10}\ m^2$

Draws in lots of air



$k=10^{-11}\ m^2$

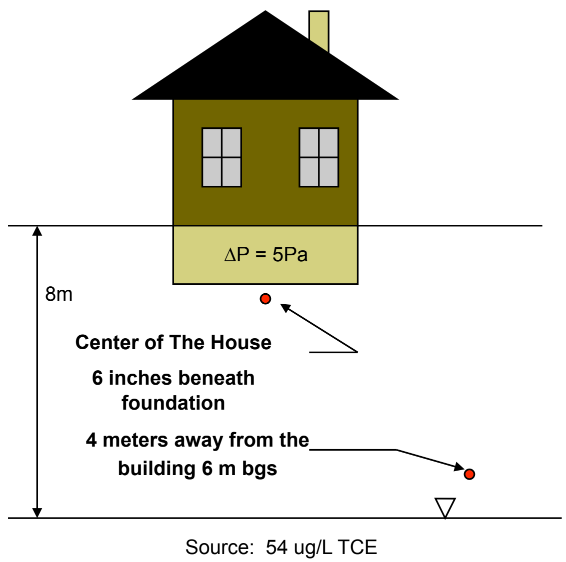
Draws in some air, but most of "circle of influence" is contaminated soil

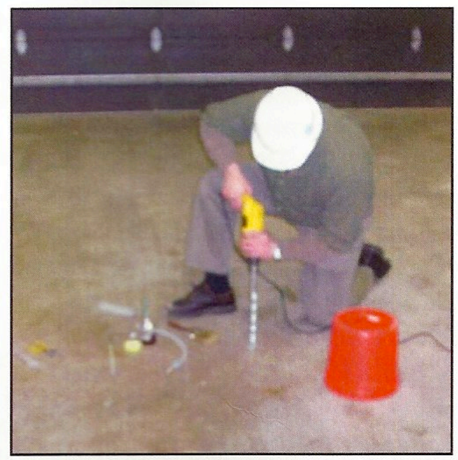


$k=10^{-12}\ m^2$

less of the "circle of influence" is in contaminated soil

Second Scenario Modeled: Active Sampling and Different Sampling Locations





We simulated various sampling points at different depths and locations using a sampling rate of 6L/8hr.

Photos from O'Brien and Gere

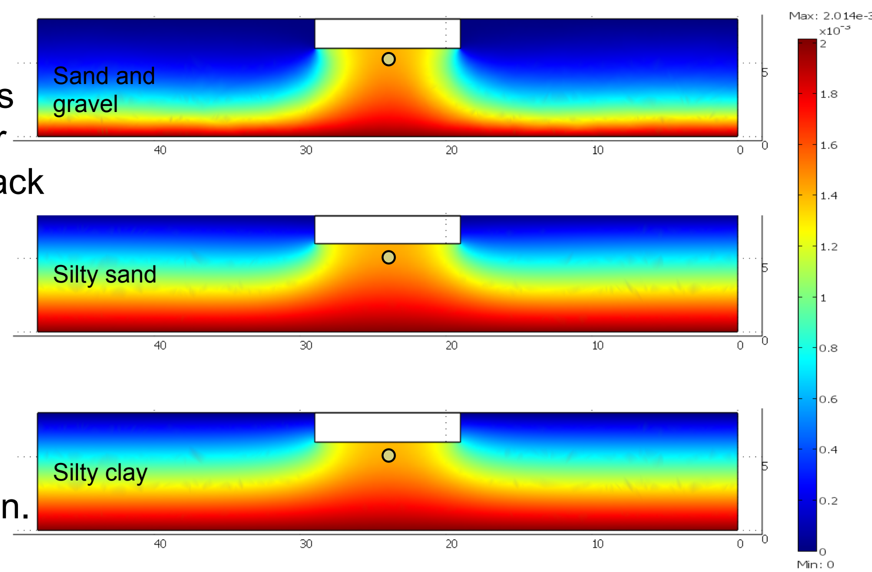
Second Scenario Modeled: Active Sampling and Different Sampling Locations

Where should samples be collected?

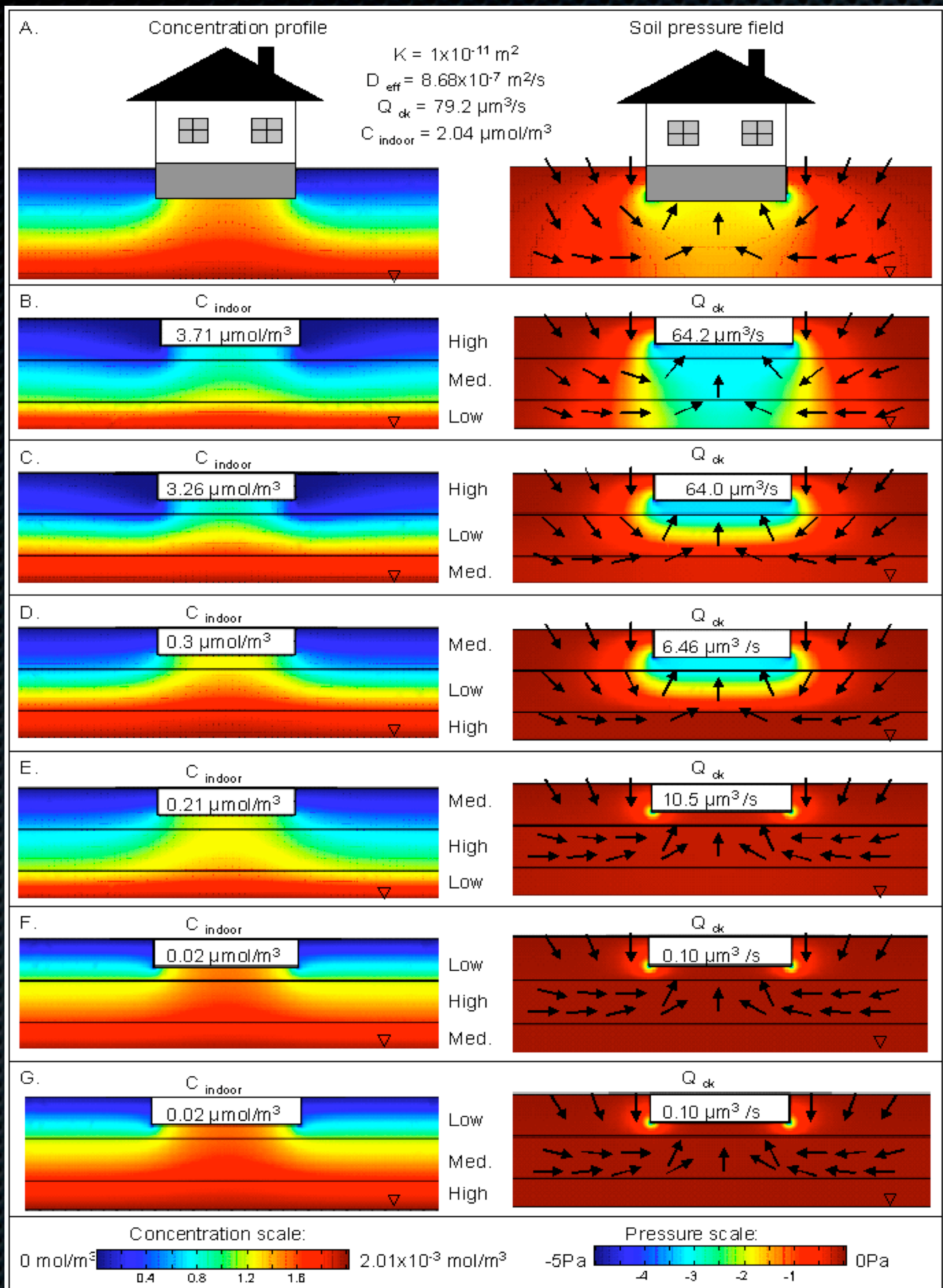
	Permeability	C sampling location (mg/m^3)	C indoor Air (mg/m^3)	Soil Gas Entry Rate (L/min)	$C_{indoor}/C_{sampling}$
Center of The House Immediately beneath foundation	High (10^{-10} m^2)	217	1.78	47.5	8.20×10^{-3}
	Moderate (10^{-11} m^2)	190	0.27	4.75	1.41×10^{-3}
	Low (10^{-14} m^2)	174	1.86×10^{-2}	0.0048	1.07×10^{-4}

The concentration values at the sampling point for all three cases are very similar; however, higher soil gas flow rate through the crack carries more contaminant vapor into the building, causing higher indoor air concentration for high permeability cases.

Sub slab sampling may lead to incorrect conclusions about the indoor contaminant concentration.



Third Scenario: Effect of Different Soil Layers

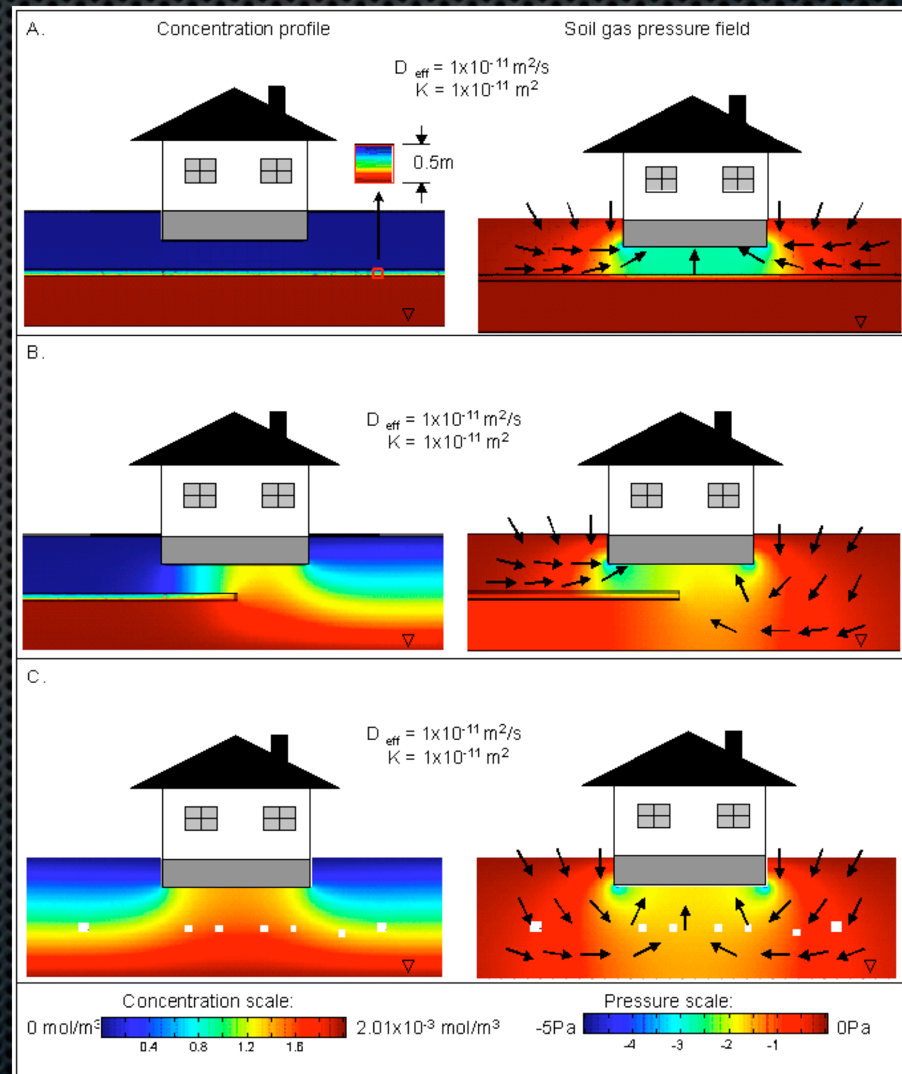


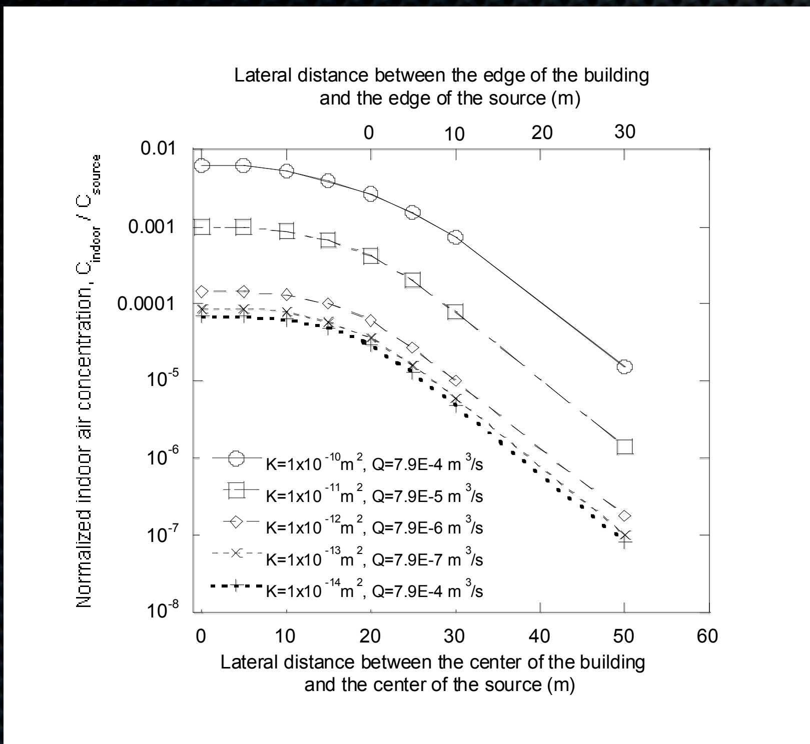
Complexity of different permeability soil layers.

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.

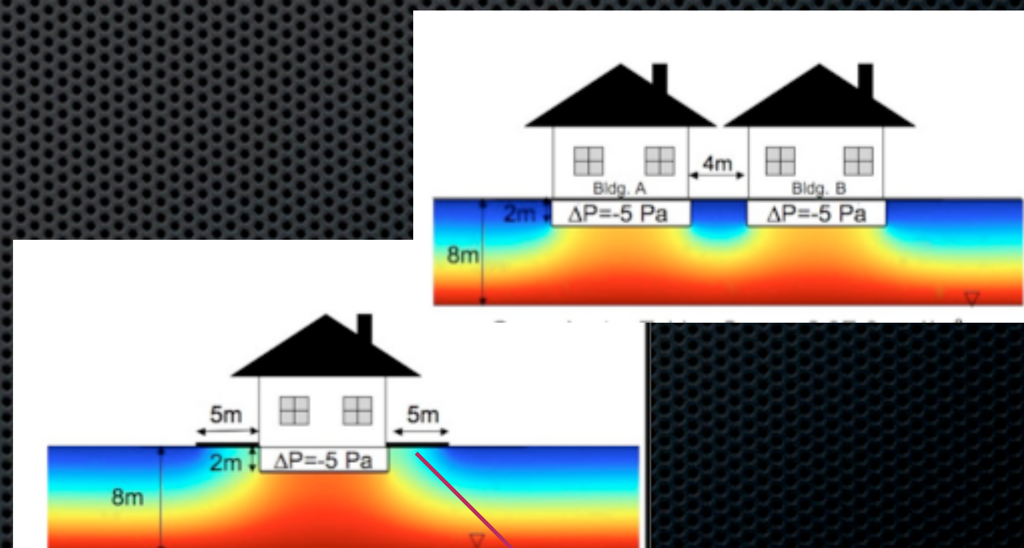
Lots of empirical data that "defy explanation"- need a good quantitative modeling analysis/good CSM.





Structure on an open field is fine...

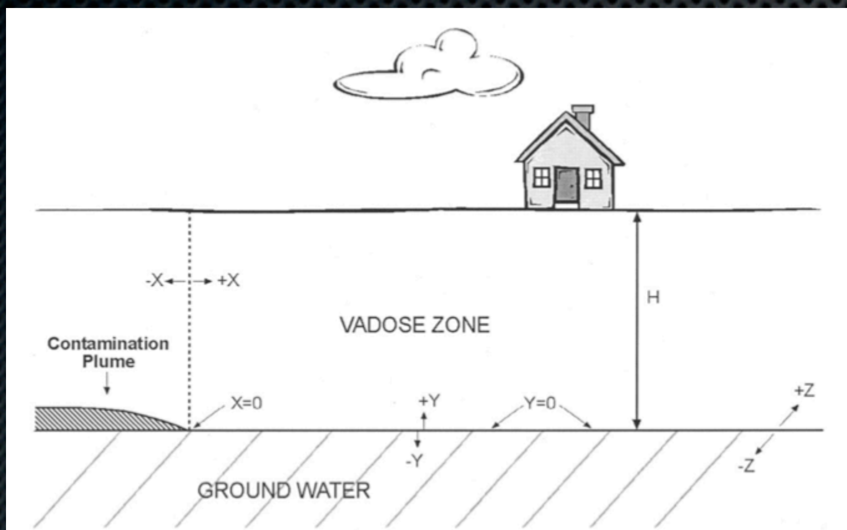
But what about urban environments?



Adjacent capping and structures
$k = 10^{-11}\ m^2$
5 m driveway increases C_{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??



$$D_e\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial C^2}{\partial y^2}\right) = 0$$

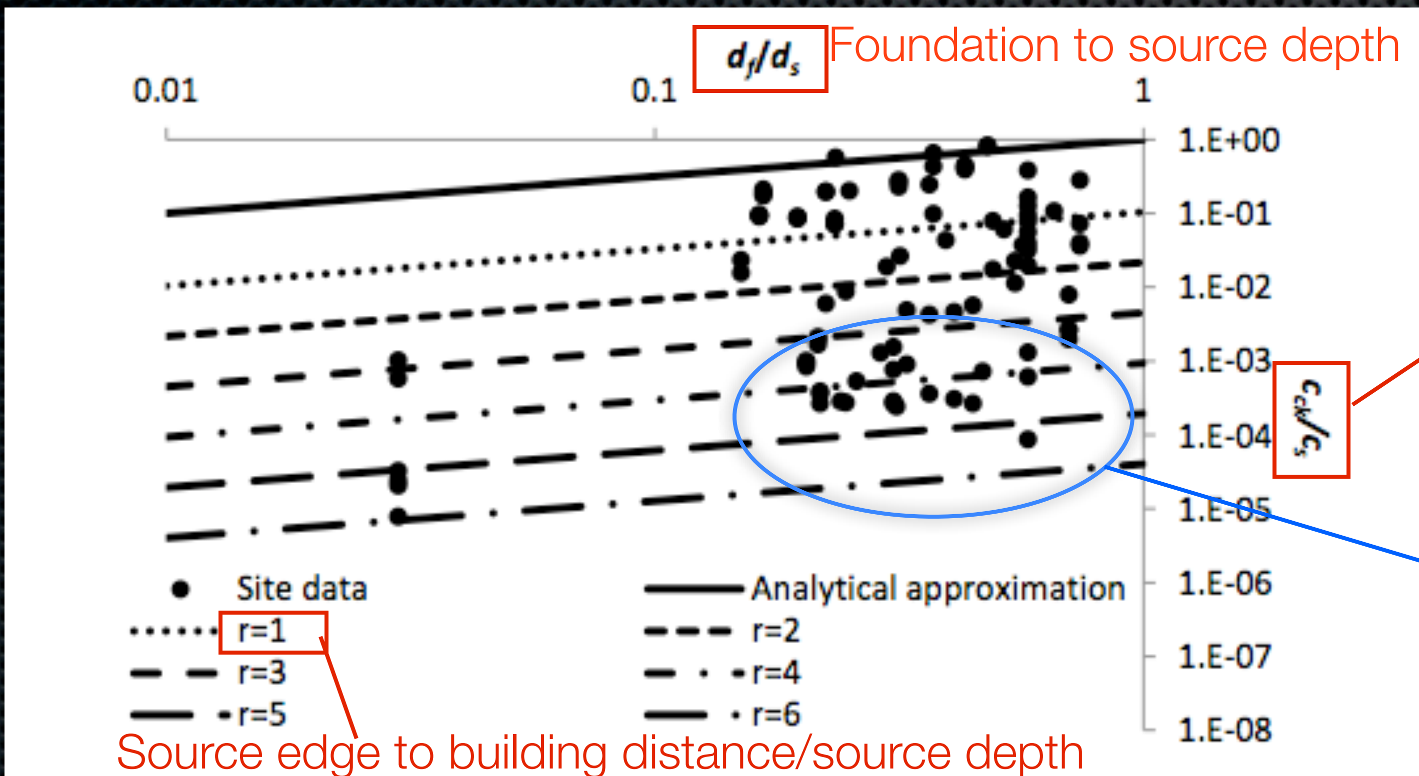
Solved simple 2-D Laplace Equation

insignificant at lateral distances of only η = 5. The value of 100 ft given in the U.S. EPA guidance is a conservative upper limit for sites with groundwater shallower than 10 ft and diffusion-limited vapor transport. Our work suggests that the risk from breathing contaminated indoor air from subsurface contamination need only be investigated for buildings within a relatively short distance (e.g., within one or two residential sized lots) from the edge of the contamination plume.

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?

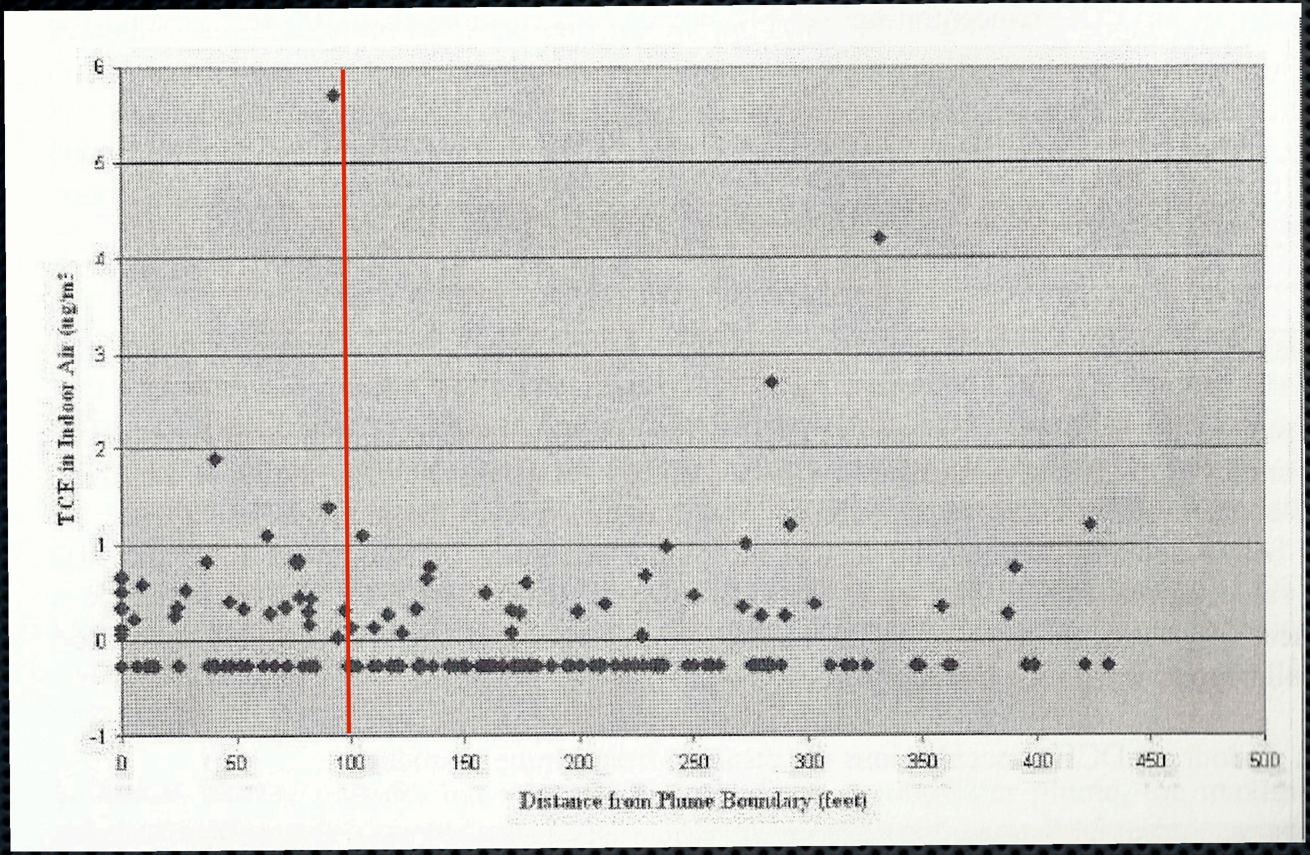


Yao et al. *Vadose Zone Journal*,2013

Subslab to Source Concentration

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

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



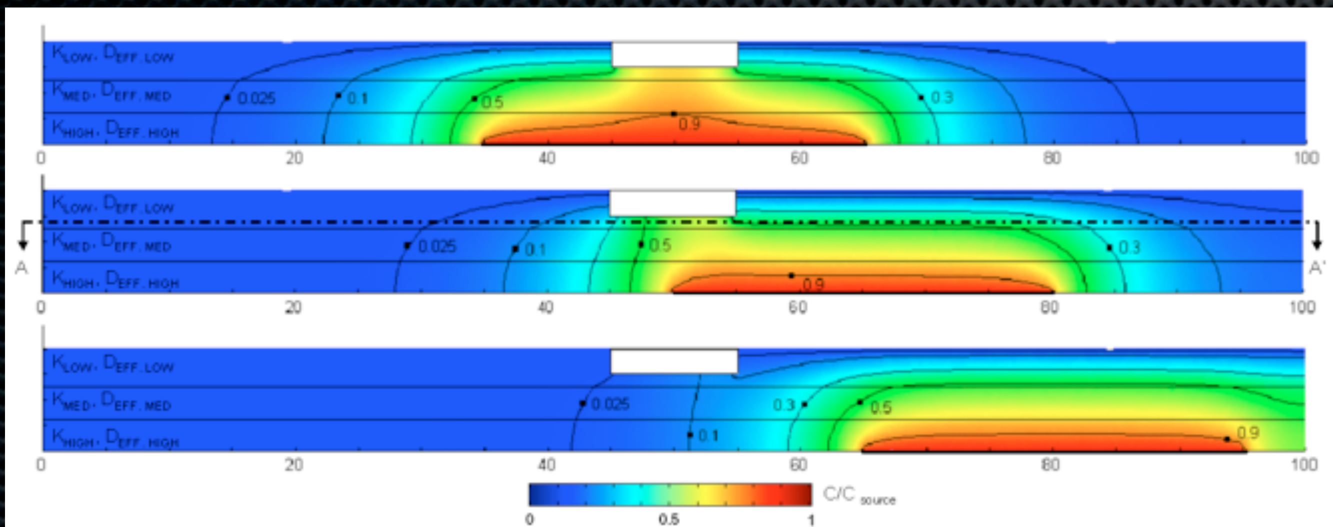
Redfield (Denver) Site

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

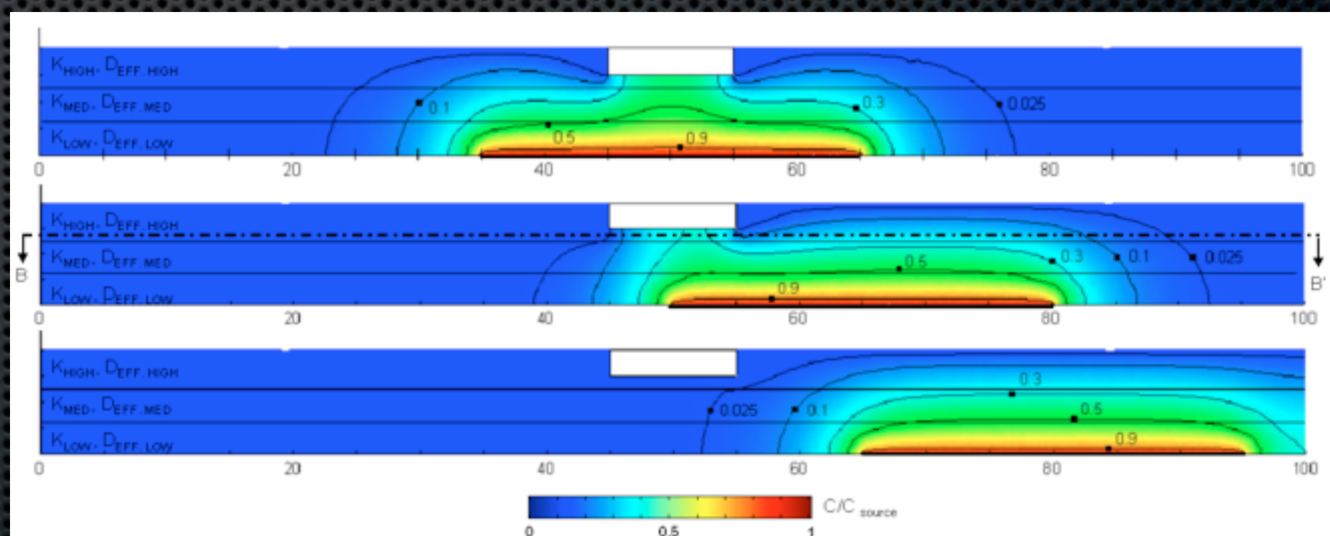
Data from Folkes et al., AWMA Vapor Intrusion Conference, 2007

Depending upon action level, 100 ft may or may not be enough.

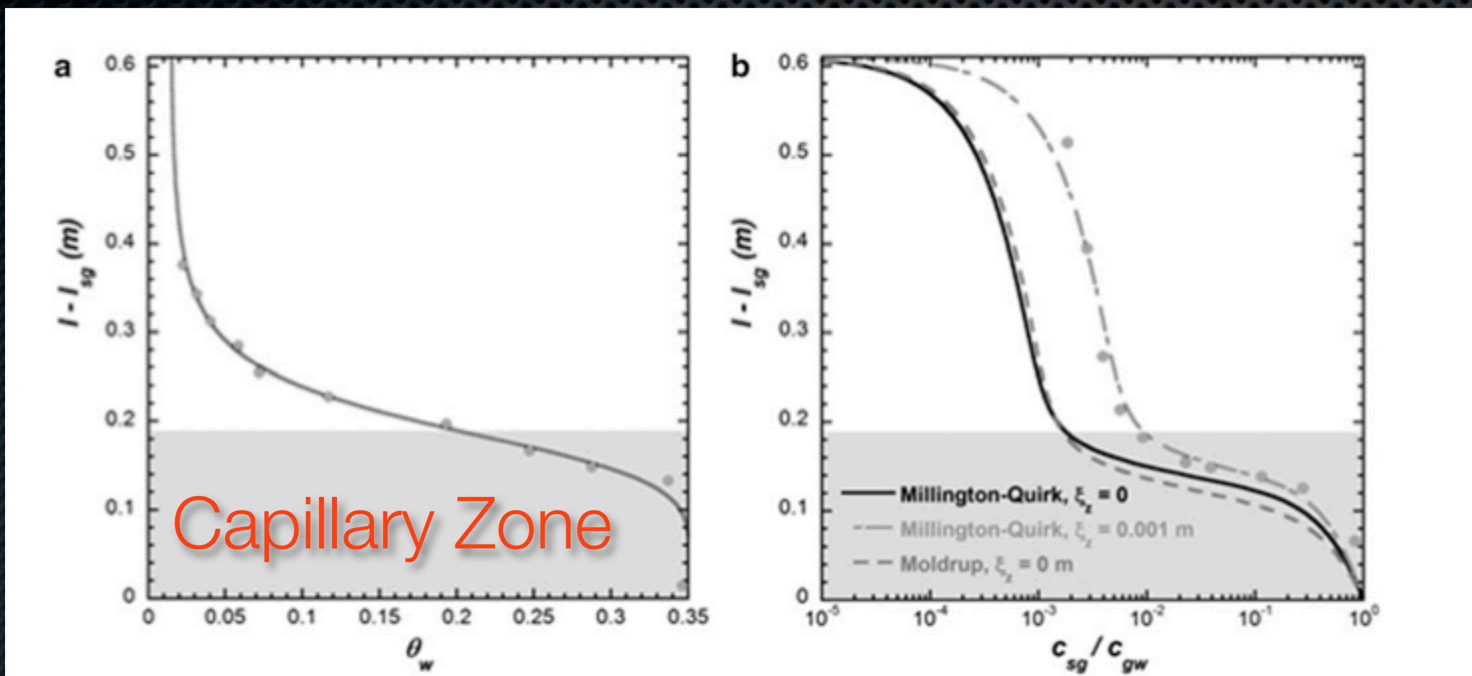
Low permeability top layer
C_{indoor}/C_{source} = 0.0185



High permeability top layer
C_{indoor}/C_{source} = 0.29



Capillary zone resistance is very important



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

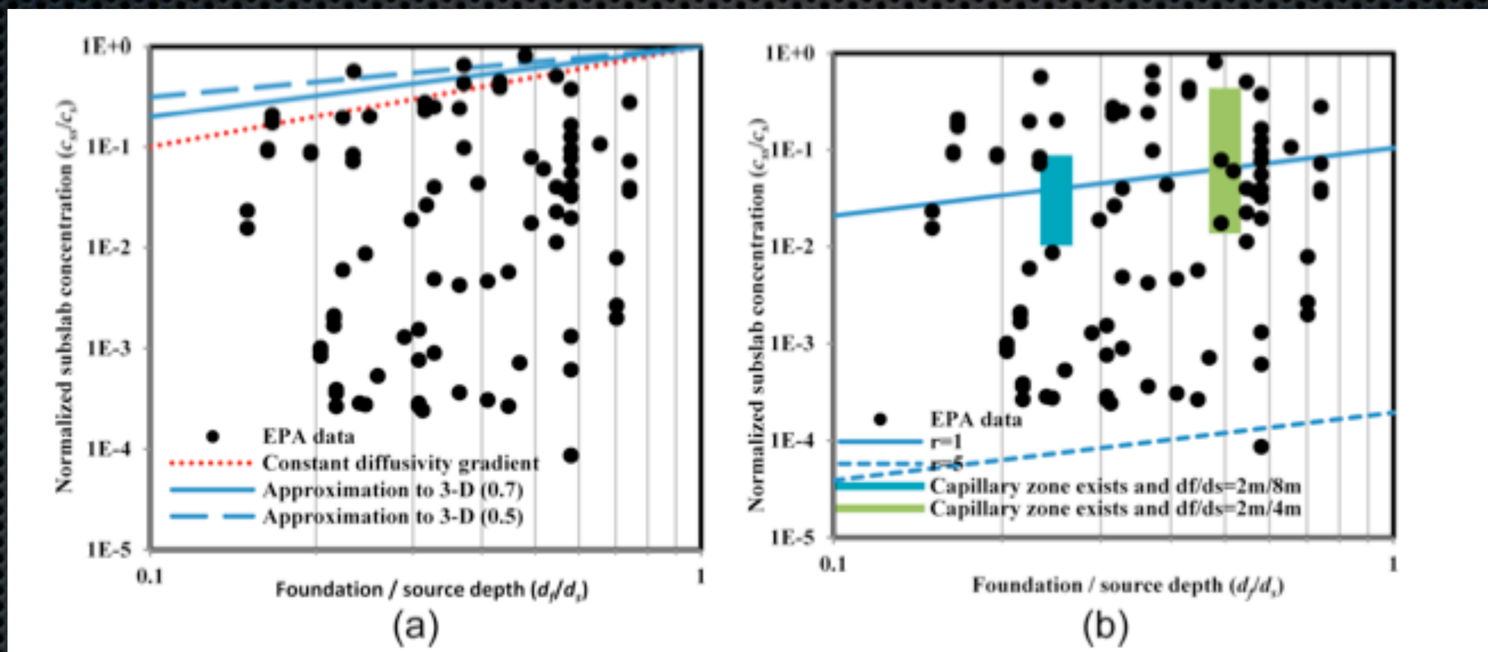
Shows extent to which open porosity filled with water; diffusion through water layer slow

Shows how dramatically COC concentration drops through capillary zone- big part of AF_{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)

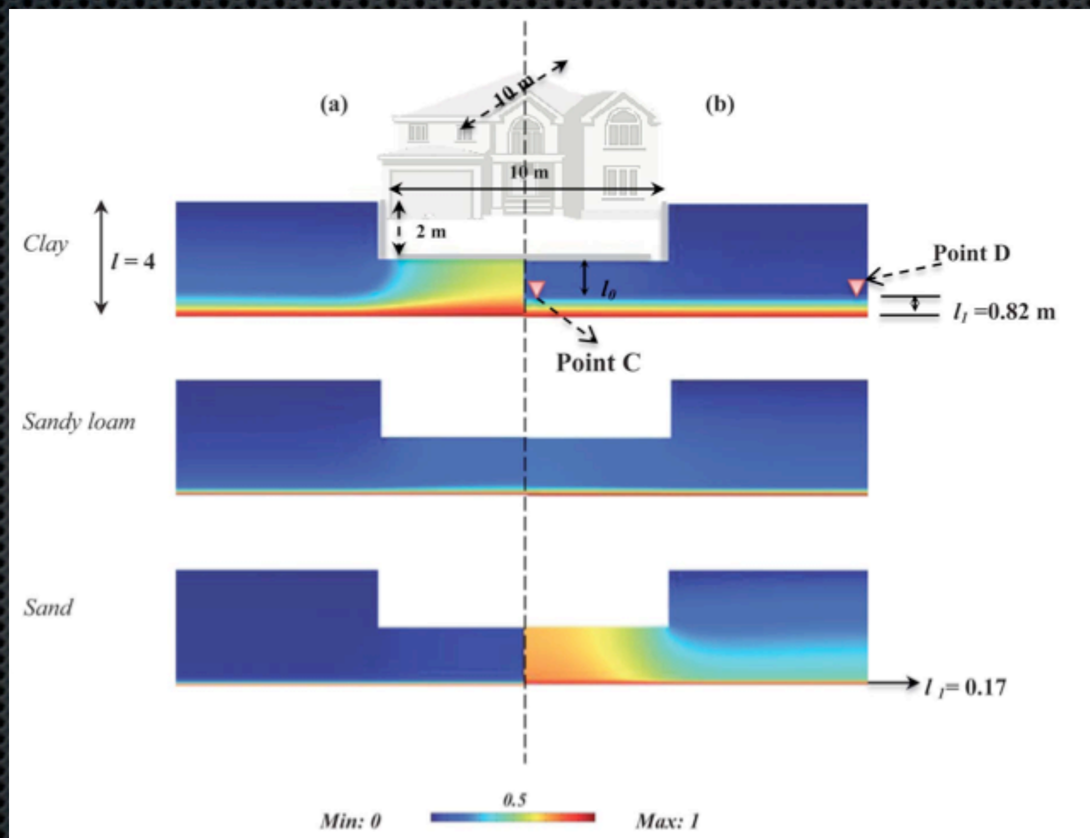
Predictions with capillary fringe (blue/green bars)

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

Shen et al., *Env. Sci. Proc. Impacts*, *15*, 1444 (2013).

In clay, moisture profile smooth, looks like uniform soil

In clay, high resistance forced in capillary layer

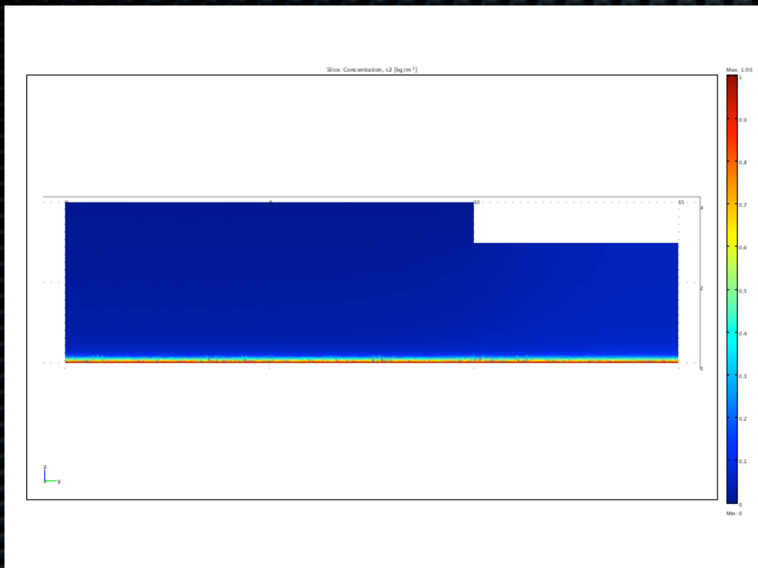


In sand, narrow high resistance capillary layer

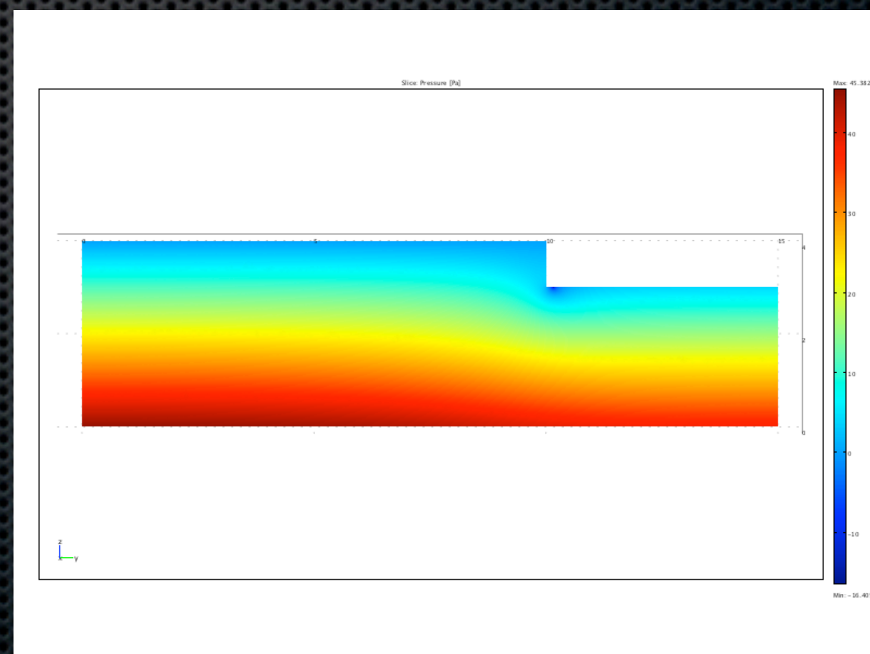
In sand, more uniform resistance forced

Results using true soil moisture profile

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



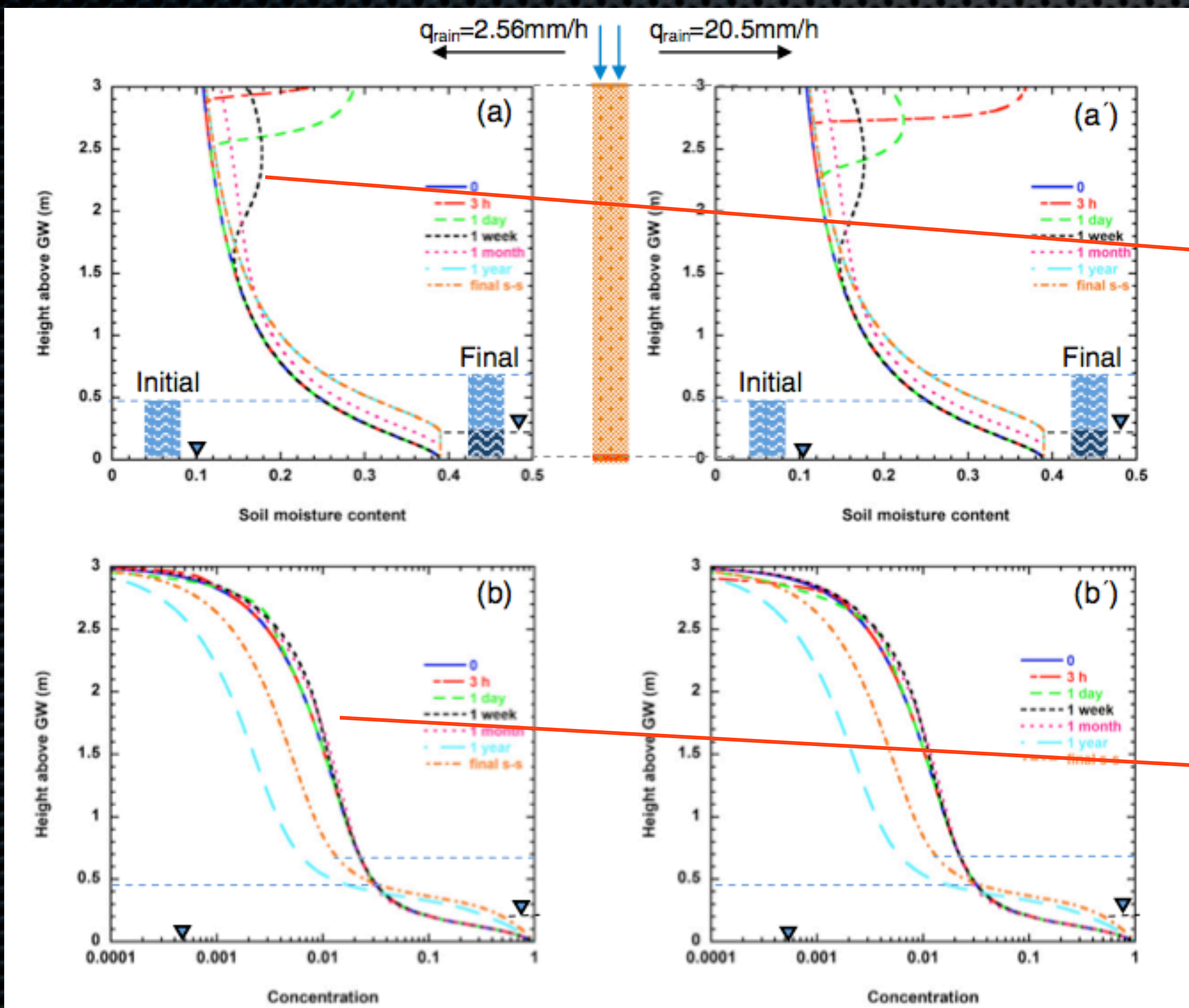
AF = 1.58×10^{-5} for actual capillary zone calculation



AF=1×10^{-3} (uniform loamy sand)

Rainfall Events

Shen et al., *Sci. Total Env.*, *437*, 110 (2012)



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?

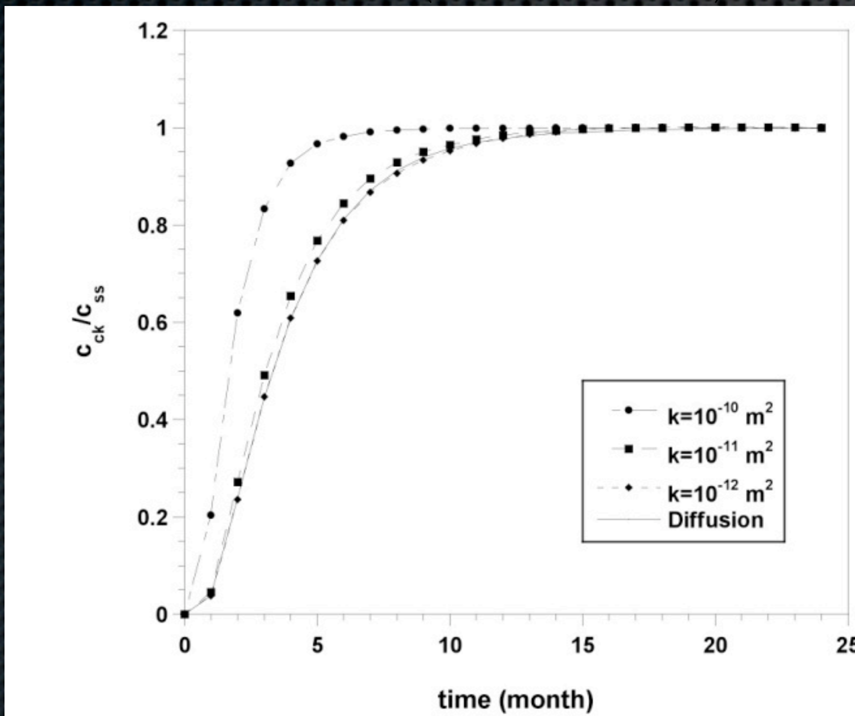
Transient Situations

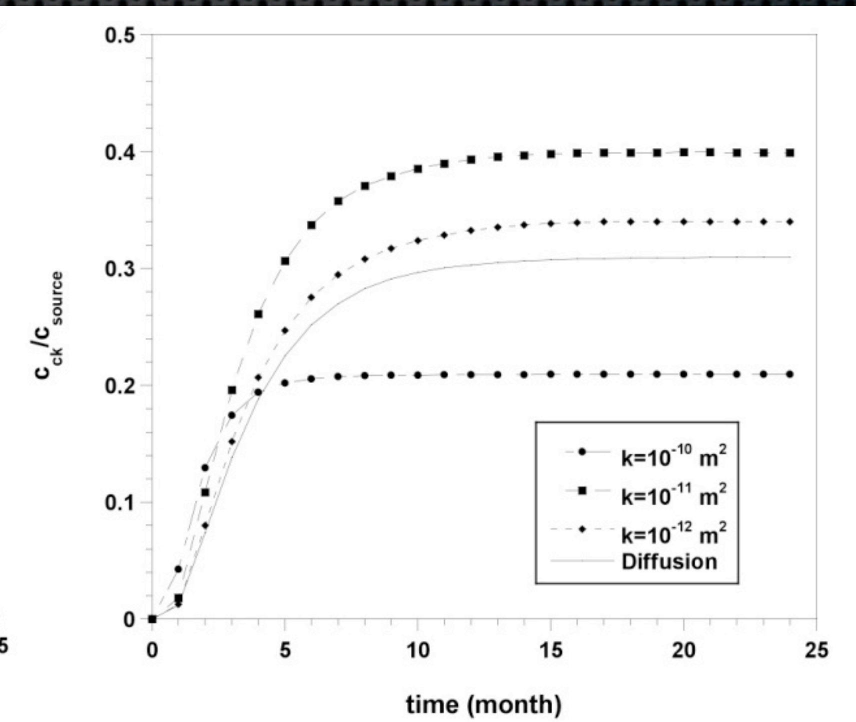
Darcy's Law

$$\left(x_p\left(1-\eta_g\right)+x_f\eta_g\right)\frac{\partial p}{\partial t}=\nabla\left(\frac{k}{\mu_g}\left(\rho_g g\nabla z+\nabla p\right)\right)$$

Advection and Diffusion

$$\frac{\partial C_{ig}}{\partial t}+\nabla(q_g C_{ig}-D_{ig}\nabla C_{ig})+R_{ig}=0$$





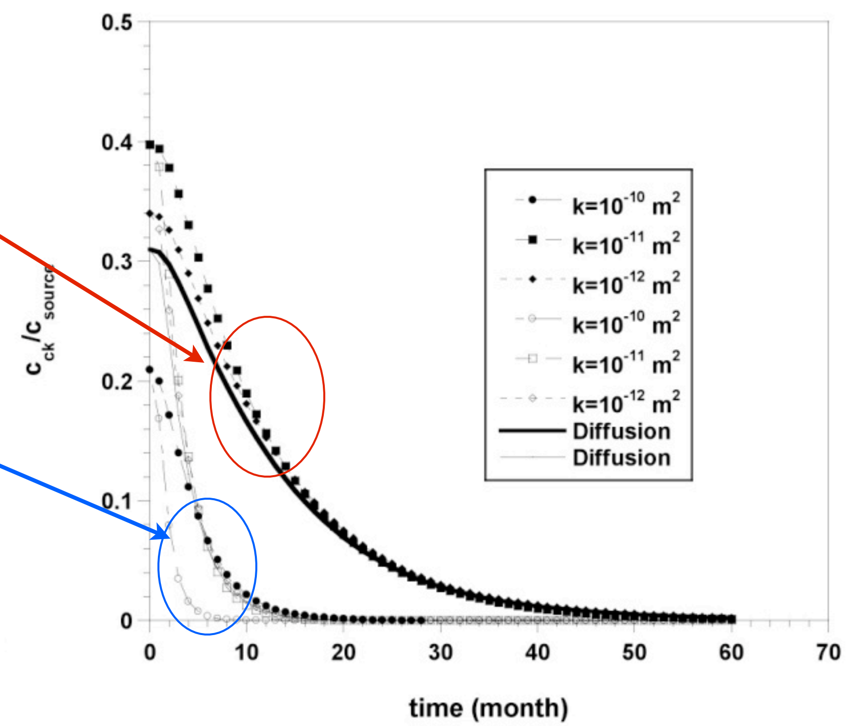
With sudden appearance of a source at 8 m-shows typical response is diffusion rate determined

Note subslab profiles take months/years to develop.

Time response of subslab concentration if the groundwater is "clean"at t=0 and

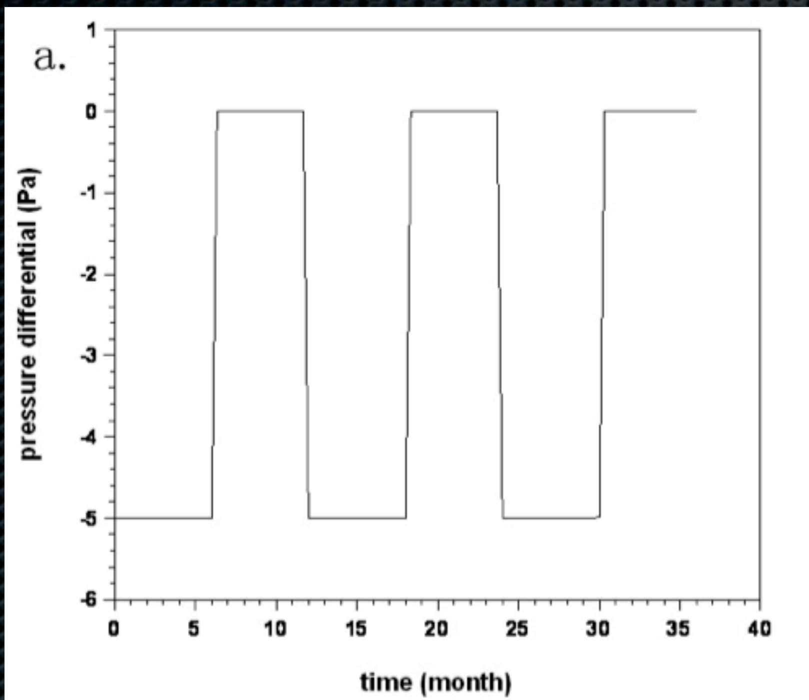
the groundwater does not act as a sink

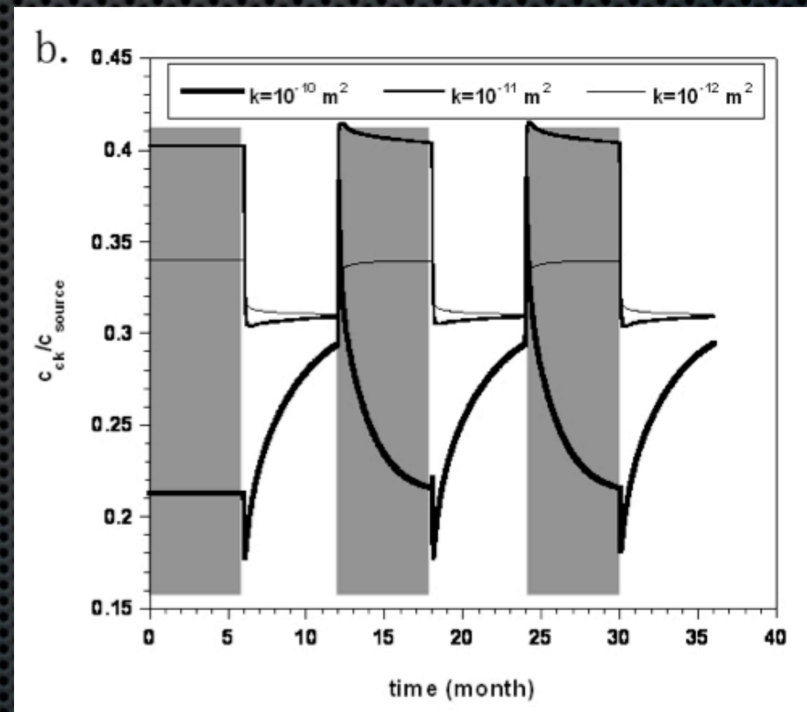
the groundwater acts as a sink



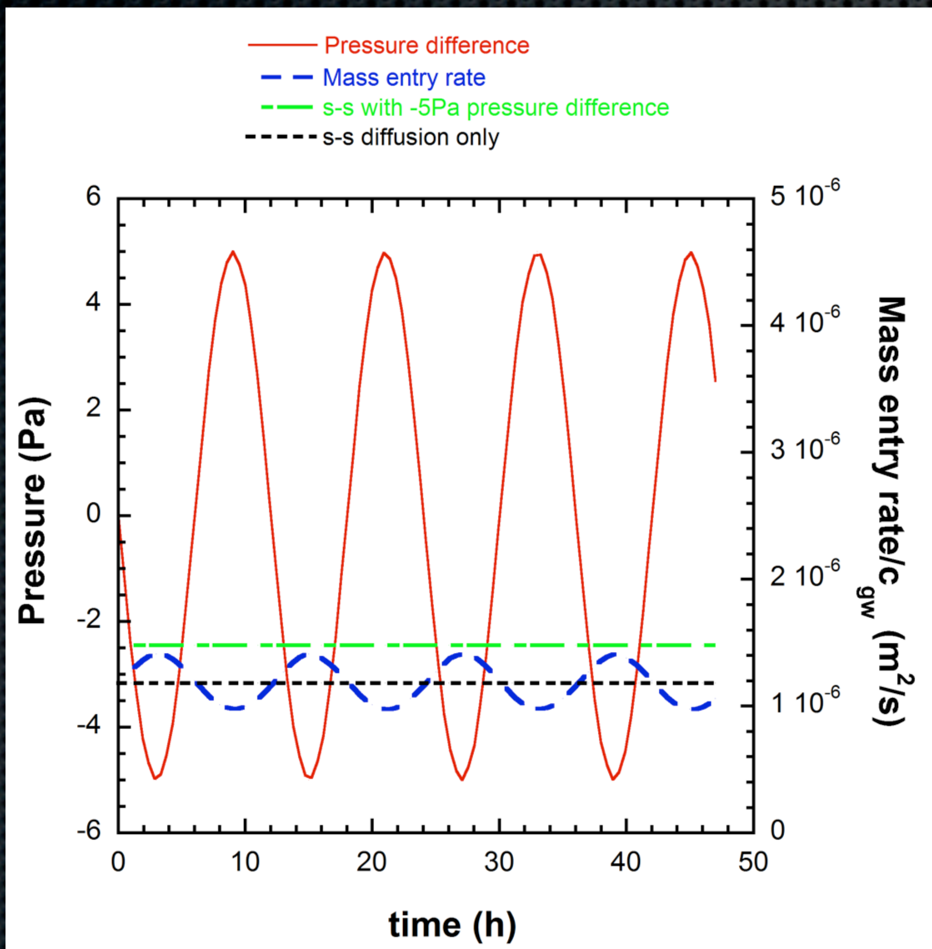
Note the very long timescales of response to "remediation"

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.

$$\frac{D_{eff}*A_B}{L_T}(c_{source}-c_{ck}) = Q_{ck} * \frac{\exp\left(\frac{Q_{ck}d_{ck}}{A_{ck}D^{ck}}\right)C_{ck}-C_{indoor}}{\exp\left(\frac{Q_{ck}d_{ck}}{A_{ck}D^{ck}}\right)-1}$$

$$Q_{ck} * \frac{\exp\left(\frac{Q_{ck}d_{ck}}{A_{ck}D^{ck}}\right)C_{ck}-C_{indoor}}{\exp\left(\frac{Q_{ck}d_{ck}}{A_{ck}D^{ck}}\right)-1} = Q_{building} * c_{indoor}$$

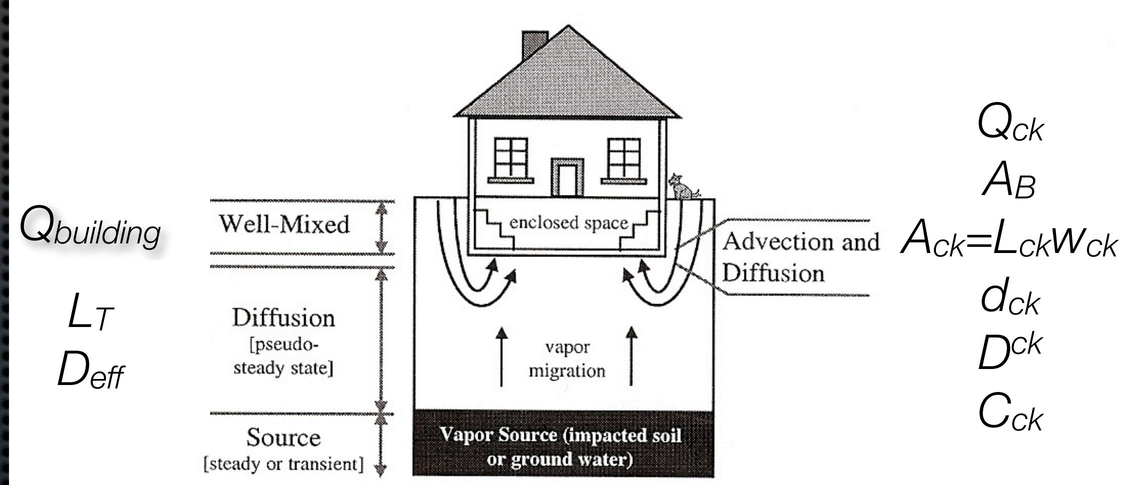
$$\alpha = \frac{c_{indoor}}{c_{source}} = \frac{\frac{D_{eff}*A_B}{Q_{building}L_T}\exp\left(\frac{Q_{ck}d_{ck}}{A_{ck}D^{ck}}\right)}{\exp\left(\frac{Q_{ck}d_{ck}}{A_{ck}D^{ck}}\right)+\frac{D_{eff}*A_B}{Q_{ck}L_T}\left(\exp\left(\frac{Q_{ck}d_{ck}}{A_{ck}D^{ck}}\right)-1\right)+\frac{D_{eff}*A_B}{Q_{building}L_T}}$$

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

Environ. Sci. Technol. 1991, 25, 1445–1452

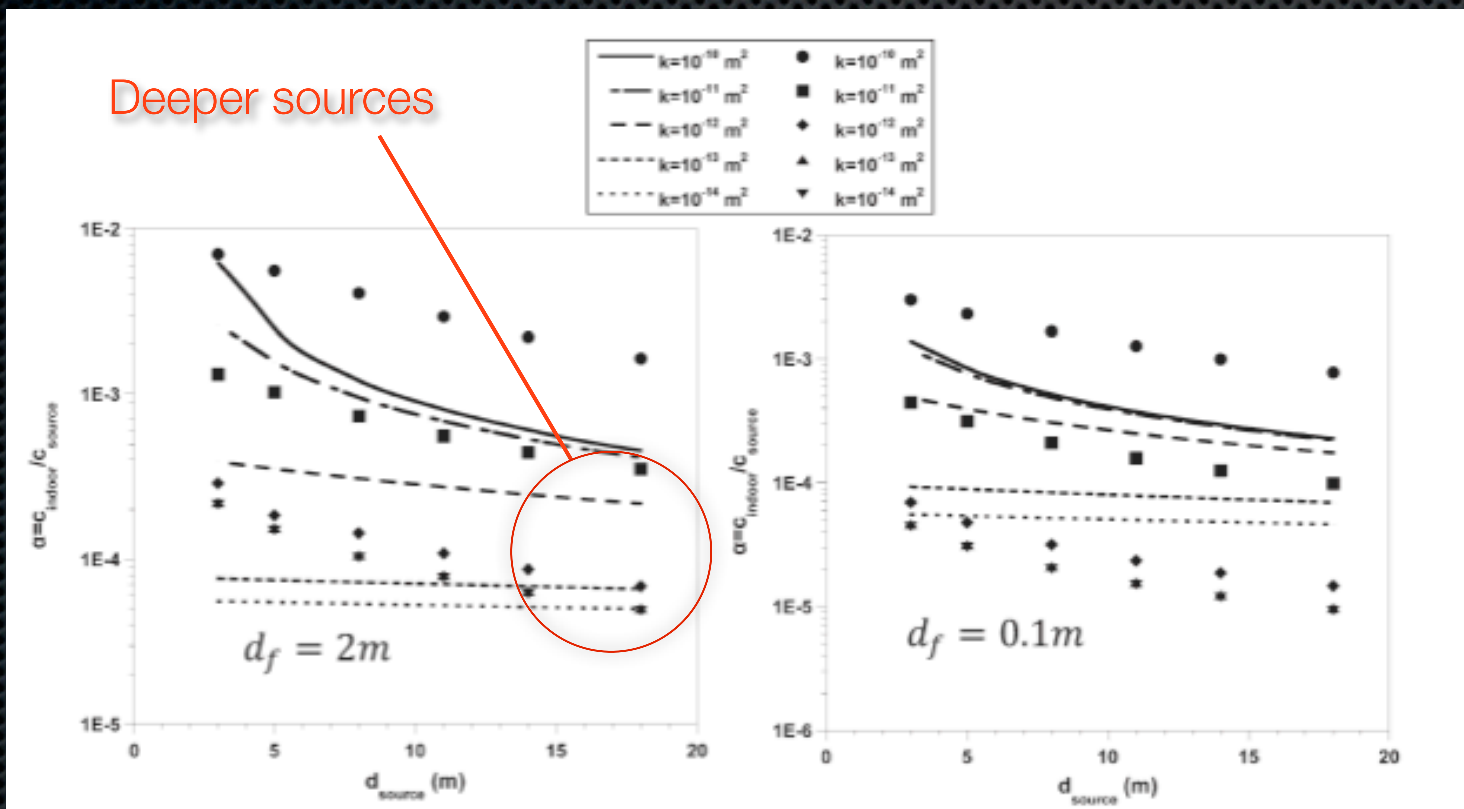
Heuristic Model for Predicting the Intrusion Rate of Contaminant Vapors into Buildings

Paul C. Johnson* and Robert A. Ettinger
Shell Development, Westhollow Research Center, Houston, Texas 77251



Attenuation factor depends upon $Q_{building}$

Comparison of EPA JE results with full 3D



Basement cases

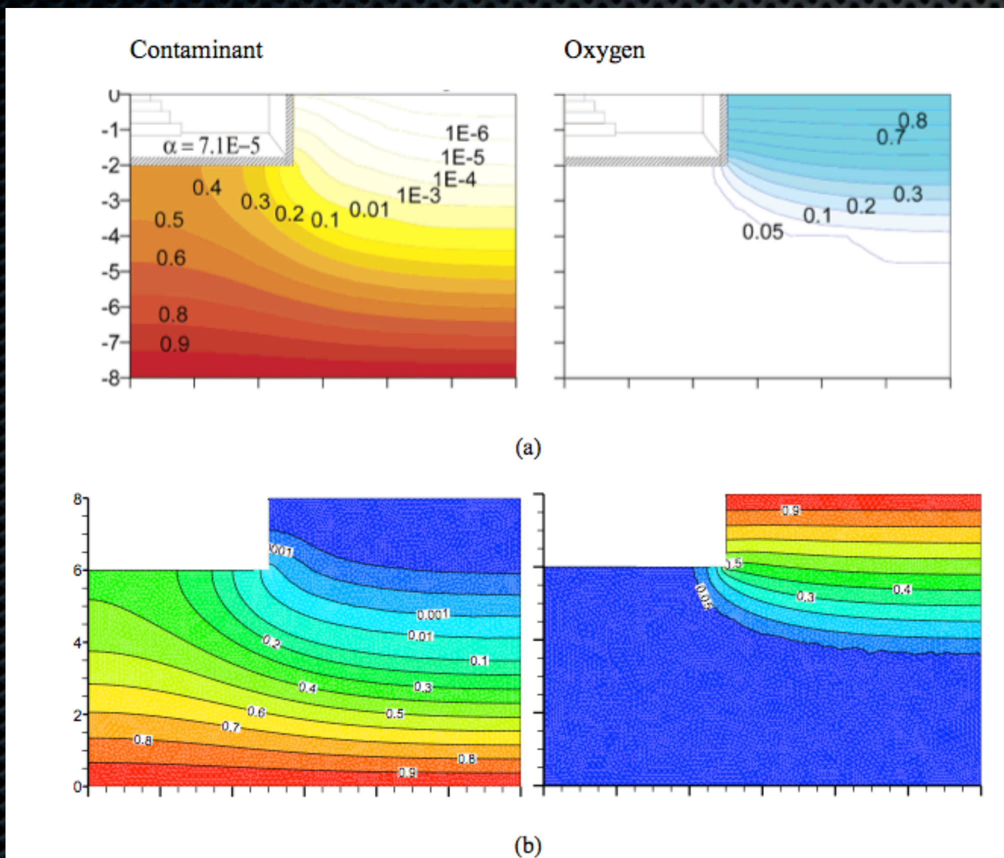
Slab-on-grade cases

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...

Biodegradation Can be Handled



Abreu and Johnson, *EST*, *40*, 2304-2315 (2006)

$$0 = -\nabla \cdot (q_g c_{ig}) + \nabla \cdot (D_i \nabla c_{ig}) - R_i$$

$$R_c = \frac{\lambda_2 \phi_w}{H_c} c_c c_o$$

Yao, 2012

$$\frac{dc_c}{dt} = -\frac{\lambda_2 \phi_w}{H_c \phi_g} c_c c_o$$

No agreement on if c_o should be explicit in models