A Different Way of Looking at Soil Vapor Intrusion

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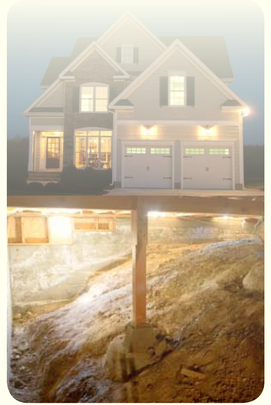
ABSTRACT

The objectives of this work were as follows:

- Develop a general multi-compartment mass transfer model incorporating advection, diffusion, and phase changes into a single equation in order to permit rapid and systematic calculation for a variety of circumstances
- Describe the analogies of the model with electrical circuit theory
- Demonstrate correspondence of the model with the Johnson and Ettinger soil vapor intrusion (SVI) model
- Apply the model to example SVI problems, namely:
  1. Application to a 3-phase (tar, water, air) system.
  2. Application to a two-compartment building model.
  3. Incorporation of groundwater (saturated and capillary zone) mass transfer into an SVI model.

Note: Derivations and other details are contained in the full text available from the authors.



MODEL

Multiple compartment model

Derivation of the Basic Equation

In one dimension, x-direction flux in the ith compartment (F_i) can be written as:

$$F_i = v_i A_i C_i - D_i \frac{\partial c_i}{\partial x} A_i = Q_i C_i + k_i \left(C_i - C_{i+1}\right) \quad (1)$$

where

C_i = concentration
D_i = diffusion coefficient
v_i = advection velocity
A_i = cross-sectional flux area in compartment i.

where we have defined:

$$Q_i = v_i A_i \quad (2)$$

$$k_i = \frac{D_i A_i}{L_i} \quad (3)$$

where

L_i = the gradient scale of the concentration in the ith compartment
Q_i = volume flux due to advection, multiplying by C_i gives the mass flux due to advection
k_i = has units of volume flux; however, it is multiplied by $(C_i - C_{i+1})$ to obtain the mass flux due to diffusion.

Assuming steady state conditions and conservation of flux between n+1 environmental compartments $i = 0$ (source), 1, 2,…n the overall mass transfer coefficient, K_n such that $C_n = K_n C_0$ is found:

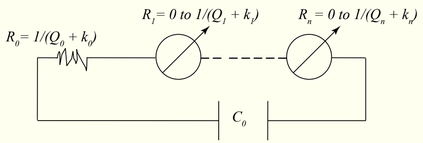
$$K_n = \left(\frac{1}{(Q_0 + k_o)} + \sum_{i=1}^{n} \frac{1}{(Q_i + k_i)} \prod_{j=0}^{i-1} \left(\frac{k_j}{(Q_j + k_j)} \right) \left(\frac{1}{(P_j)} \right) \right)^{-1} \quad (4)$$

where Π is the product function and P_j is the dimensionless partition coefficient between compartments j and $j+1$. Neither i nor j appears in the final result; they are "dummy" parameters for the product and summation functions.

Derivation of Equation (4) is subject to the truncation requirement that $D_n = 0$ or $C_n >> C_{n+1}$. (For SVI problems, the requirement is met if the concentration outdoors in compartment n+1 is much greater than the indoor air concentration in compartment n.)

Note that if the flux in any compartment is purely advective (i.e., $k_i = 0$), according to Equation (4), subsequent compartments make no further contribution to the overall mass transfer coefficient.

Equation (4) permits a variety of complex situations to be treated systematically.



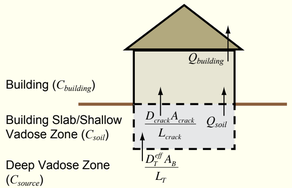
Circuit diagram with no phase changes

Equation (4) can be interpreted in terms of electric circuit theory as follows:

1. The resistances, R_i, in each compartment are in series.
2. The maximum possible resistance in each compartment is $((Q_i + k_i)P_i)^{-1}$, so that $1/(Q_iP_i)$ and $1/(k_iP_i)$ can be viewed as parallel resistances.
3. The actual resistance in each compartment is equal to the maximum possible resistance reduced by a) the fraction of the flux entering a compartment that is solely due to diffusion in all the preceding compartments, and b) the product of all the phase changes $(1/P_i)$. This is analogous to a potentiometer or rheostat element whose resistance R_i varies from 0 to a maximum value $((Q_i + k_i)P_i)^{-1}$.

Correspondence of Equation (4) with the Johnson and Ettinger (J&E) Model (J&E notation.)

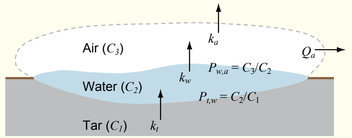
Region	n	Advection Volume Flux (Q_i)	Diffusion Volume Flux Parameter (k_i)	Partition Coefficient (P_i)
Deep Vadose Zone	0	0	$\left(D_T^{eff}/L_T\right) A_B$	1
Building Slab/ Shallow Vadose Zone	1	Q_{soil}	$(D_{crack}/L_{crack}) A_{crack}$	1
Living Space/ Building Envelope	2	$Q_{building}$	0	1
Result	$K_2 = \left(\frac{1}{\frac{D_T^{eff}}{L_T} A_B} + \frac{1}{Q_{soil} + \left(\frac{D_{crack}}{L_{crack}}\right) A_{crack}} + \frac{\left(\frac{D_{crack}}{L_{crack}}\right) A_{crack}}{Q_{soil} + \left(\frac{D_{crack}}{L_{crack}}\right) A_{crack}} \frac{1}{Q_{building}} \right)^{-1}$ J&E attenuation coefficient $\alpha = \frac{K}{Q_{building}}$. Reduces to J&E results for $\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}} \to 0, \infty$			



Mass fluxes in the Johnson and Ettinger model

Example: Three-Phase Tar (t)→Water (w)→Air (a)

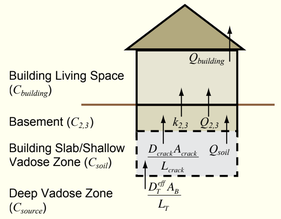
Region	n	Advection Volume Flux (Q_i)	Diffusion Volume Flux Parameter (k_i)	Partition Coefficient (P_i)
Tar	0	0	k_t	$P_{t,w}$
Water	1	0	k_w	$P_{w,a}$
Air	2	Q_a	k_a	1
	$K_2 = \left[\frac{1}{k_t} + \frac{1}{P_t k_w} + \frac{1}{P_t P_w (\ _a + Q_a)} \right]^{-1}$			
Result	Diffusion through tar can be the controlling resistance, particularly for a viscous tar.			



Schematic of a three-phase system

Example: Two-Compartment Building Model (J&E notation with addition of basement to living space advection and diffusion flux parameters $Q_{2,3}$ and $k_{2,3}$)

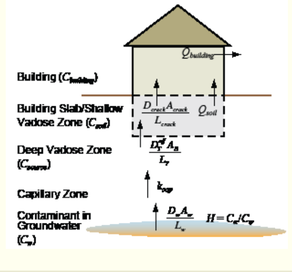
Region	n	Advection Volume Flux (Q_i)	Diffusion Volume Flux Parameter (k_i)
Deep Vadose Zone	0	0	$\left(D_T^{eff}/L_T\right) A_B$
Building Slab/ Shallow Vadose Zone	1	Q_{soil}	$(D_{crack}/L_{crack}) A_{crack}$
Basement	2	$Q_{2,3}$	$k_{2,3}$
Living Space/ Building Envelope	3	$Q_{building}$	0
	$K_3 = \left(\frac{1}{\frac{D_T^{eff} A_B}{L_T}} + \frac{1}{Q_{soil} + \frac{D_{crack}A_{crack}}{L_{crack}}} + \frac{1}{(Q_{2,3} + k_{2,3})} \left(\frac{\frac{D_{crack}A_{crack}}{L_{crack}}}{Q_{soil} + \frac{D_{crack}A_{crack}}{L_{crack}}} \right) + \frac{1}{Q_{building}} \left(\frac{\frac{D_{crack}A_{crack}}{L_{crack}}}{Q_{soil} + \frac{D_{crack}A_{crack}}{L_{crack}}} \right) \left(\frac{k_{2,3}}{Q_{2,3} + k_{2,3}} \right) \right)^{-1}$		
Result	1. Basement Concentration > Living Space Concentration 2. Living Space Concentration (2-compartments) < Living Space Concentration (1-compartment)		



Mass flux with a two-compartment building model

Example: Addition of Saturated and Capillary Zones (J&E notation with diffusion volume flux parameters k_w in groundwater and k_{cap} in air filled capillary zone, as in EPA's modification to J&E model)

Region	n	Advection Volume Flux (Q_i)	Diffusion Volume Flux Parameter (k_i)	Partition Coefficient (P_i)
Groundwater	0	0	k_w	H (Henry's Law Constant)
Capillary Zone	1	0	k_{cap}	1
Deep Vadose Zone	2	0	$\frac{D_T^{eff} A_B}{L_T}$	1
Building Slab/ Shallow Vadose Zone	3	Q_{soil}	$\frac{D_{crack}A_{crack}}{L_{crack}}$	1
Building Envelope	4	$Q_{building}$		1
	$K_4 = \left(\frac{1}{k_w} + \frac{1}{H} \left(\frac{1}{k_{cap}} + \frac{1}{\frac{D_T^{eff}A_B}{L_T}} + \frac{1}{Q_{soil} + \frac{D_{crack}A_{crack}}{L_{crack}}} + \frac{\frac{D_{crack}A_{crack}}{L_{crack}}}{Q_{soil} + \frac{D_{crack}A_{crack}}{L_{crack}}} + \frac{1}{Q_{building}} \right) \right)^{-1}$			
Conclusion: (based on incorporating mass conservation)	"If the water table did not fluctuate, diffusion in groundwater would generally constitute the dominant resistance. Any model that fails to account for this resistance or alternatively for water table fluctuations will be lacking."			



Mass fluxes including diffusion through capillary zone from contaminated groundwater

CONCLUSIONS

"All models are wrong. Some models are useful"…
George Box

The model embodied in Equation (4) is equivalent to the J&E model for the same physical situation. However, Equation (4) permits a variety of new and complex situations to be treated systematically and rapidly. It would be useful in any multi-compartment situation, including SVI problems. Furthermore, the model structure has an analogy in electrical circuit theory, which can be useful in understanding what the important parameters are and how different parameters interact.