Modeling of Vapor Intrusion and Volatile Organic Compounds Transport in the Soil

– Review and Implementation

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1 Conceptual model

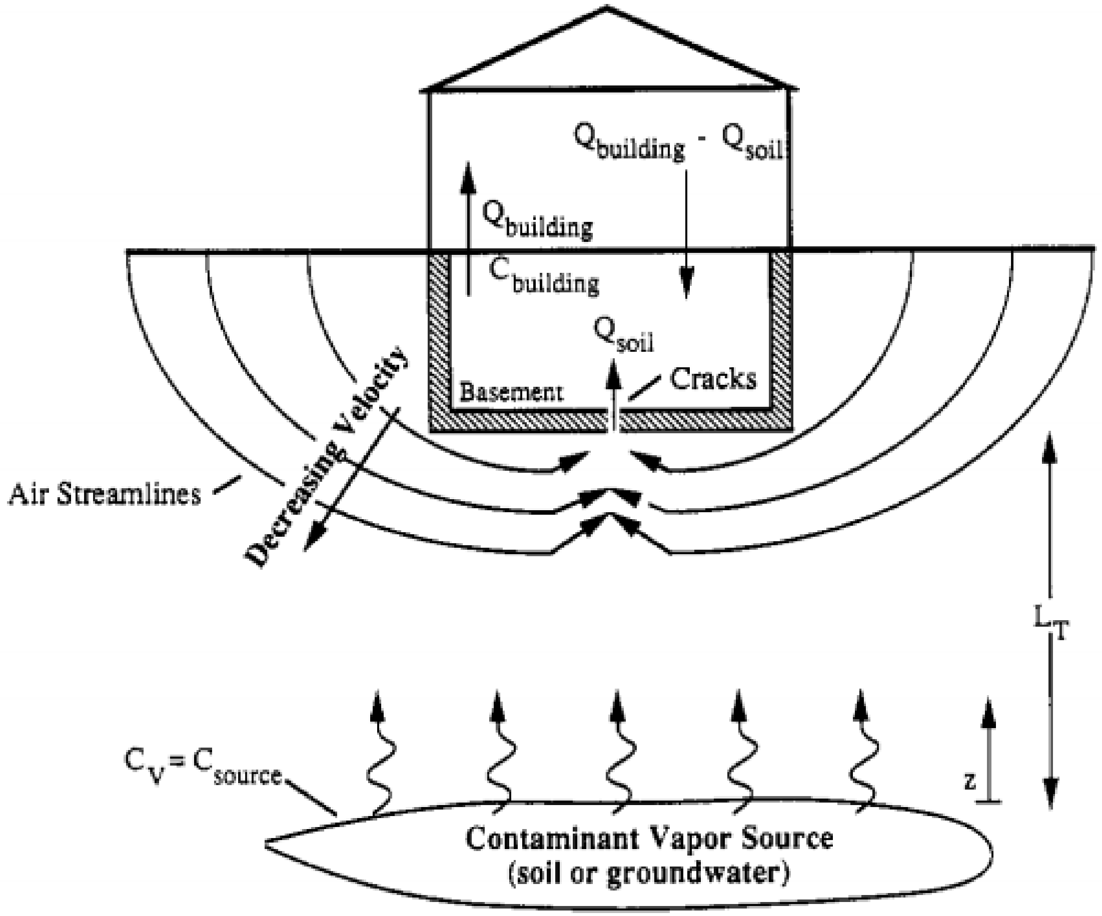


Figure 1. Vapor intrusion scenario.

Vapor intrusion

Some of the volatile organic compounds, contained in contaminants of interest from the subsurface, can enter the building through soil gas transportation.

Johnson, P. C., & Ettinger, R. A. (1991). Heuristic model for predicting the intrusion rate of contaminant vapors into buildings.

1 Conceptual model

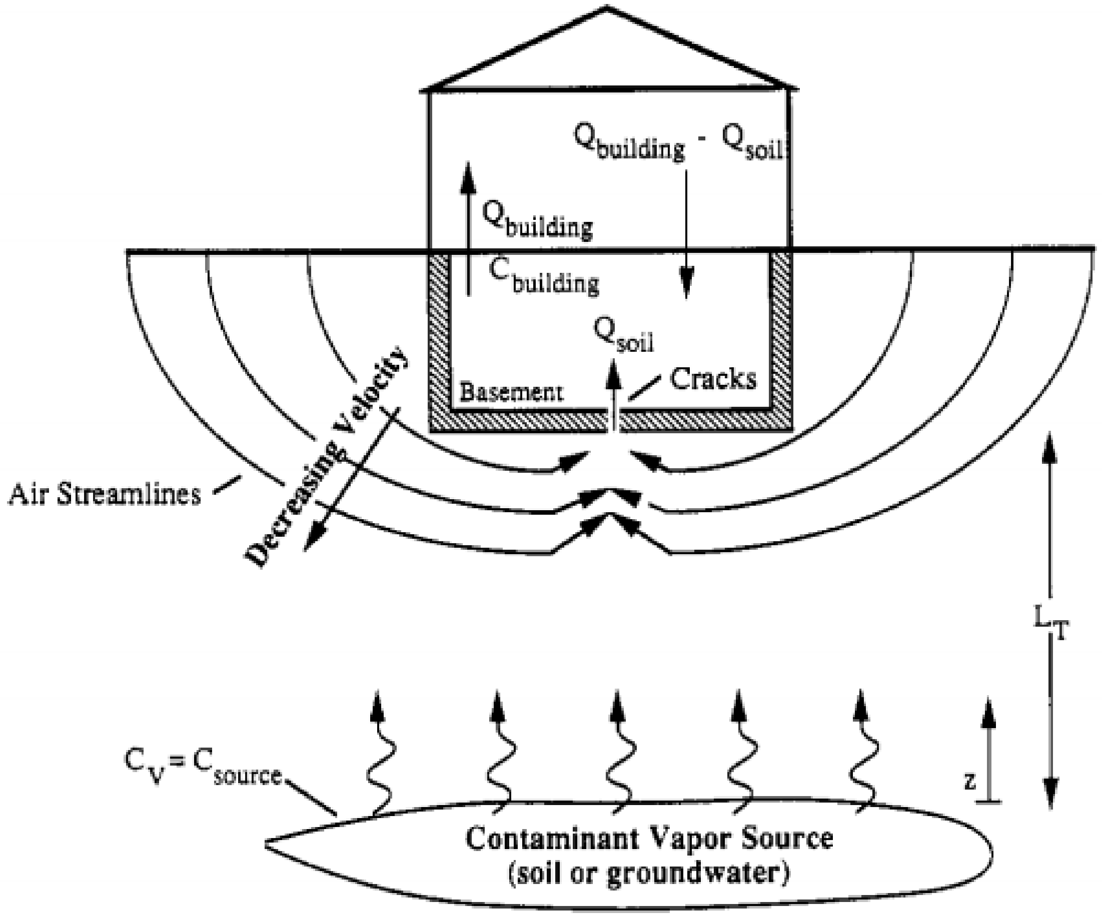


Figure 1. Vapor intrusion scenario.

VOC contaminants

- Sources: gas station, improper disposal, accidental spillage, or leaking landfill liners
- Forms: can become bound to the soil matrix, dissolved in groundwater (or soil water) and/or exist as a separate, residual phase known as a non-aqueous phase liquid (NAPL)
- Two broad categories: chlorinated solvents and petroleum hydrocarbons.

Johnson, P. C., & Ettinger, R. A. (1991). Heuristic model for predicting the intrusion rate of contaminant vapors into buildings.

1 Conceptual model

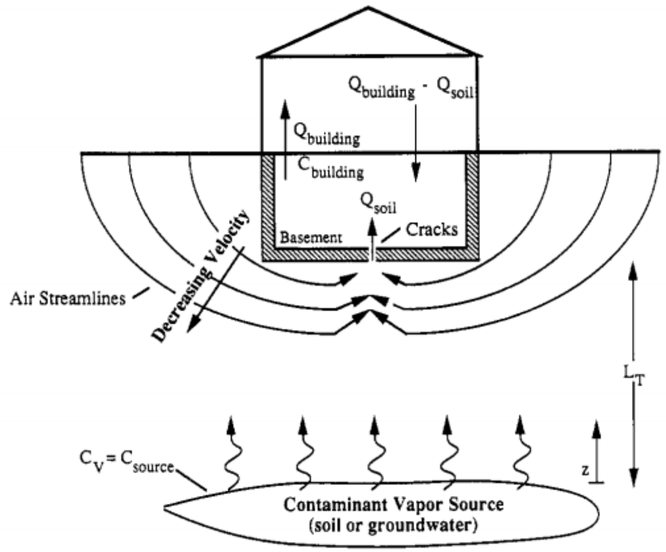
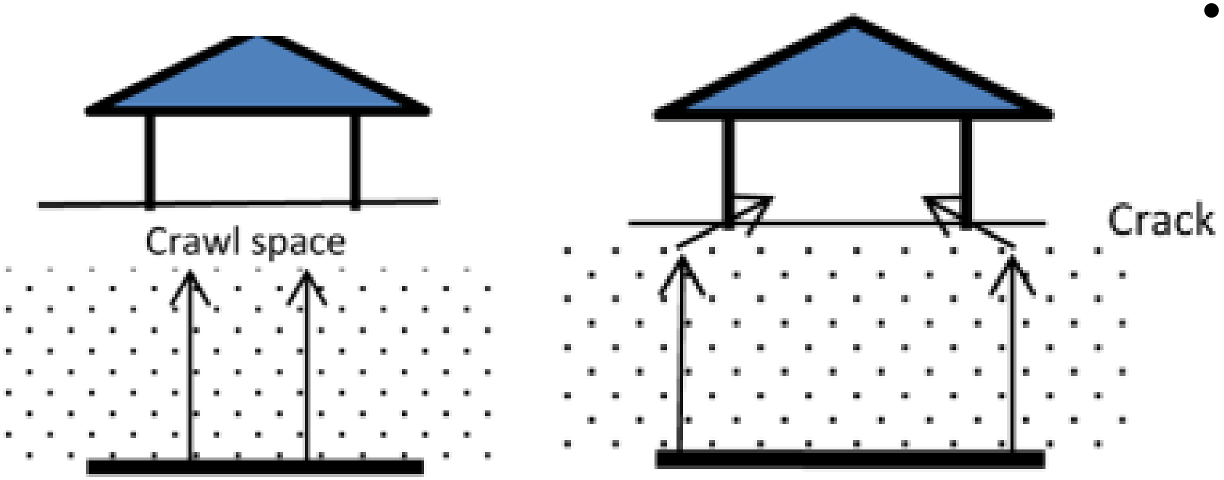


Figure 1. Vapor intrusion scenario.



Buildings

- Slab
- Crawl space
- Basement

Yao, Y., Shen, R., Pennell, K. G., & Suuberg, E. M. (2013). A Review of Vapor Intrusion Models.

2 Mathematical model

Governing equations

1. Darcy's law:

$$\frac{\partial p}{\partial t} - \frac{p_{atm} k_g}{\phi_g \mu_g} \nabla \cdot (\nabla p) = 0 \quad (1)$$

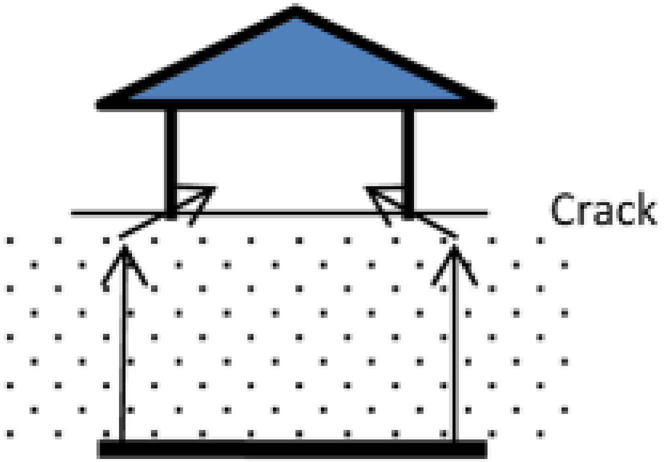
$$q_g = \frac{k_g}{\mu_g} \nabla p \quad (2)$$

2. Convection-diffusion equation:

$$\phi_{g,w,s} \frac{\partial c_{ig}}{\partial t} = -\nabla \cdot (q_g c_{ig}) - \nabla \cdot \left(\frac{c_{ig}}{H_i} q_w \right) + \nabla \cdot (D_i \nabla c_{ig}) - R_i \quad (3)$$

where

$$\phi_{g,w,s} = \phi_g + \frac{\phi_w}{H_i} + \frac{k_{oc,i} f_{oc} \rho_b}{H_i} \quad (4)$$



3. Millington and Quirk equation:

$$D_i = D_i^g \frac{\phi_g^{10/3}}{\phi_t^2} + D_i^w \frac{\phi_w^{10/3}}{\phi_t^2} \quad (5)$$

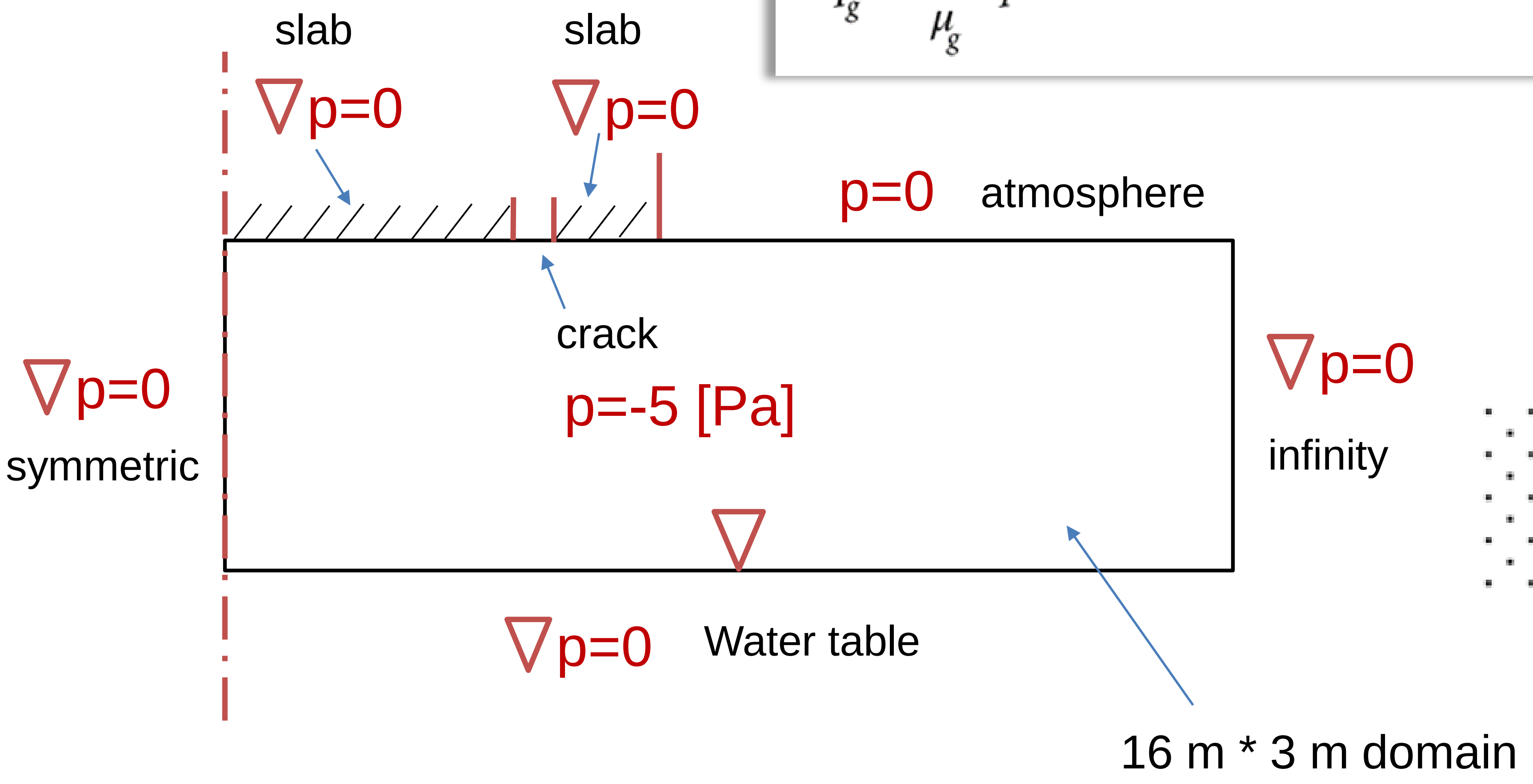
2 Mathematical model

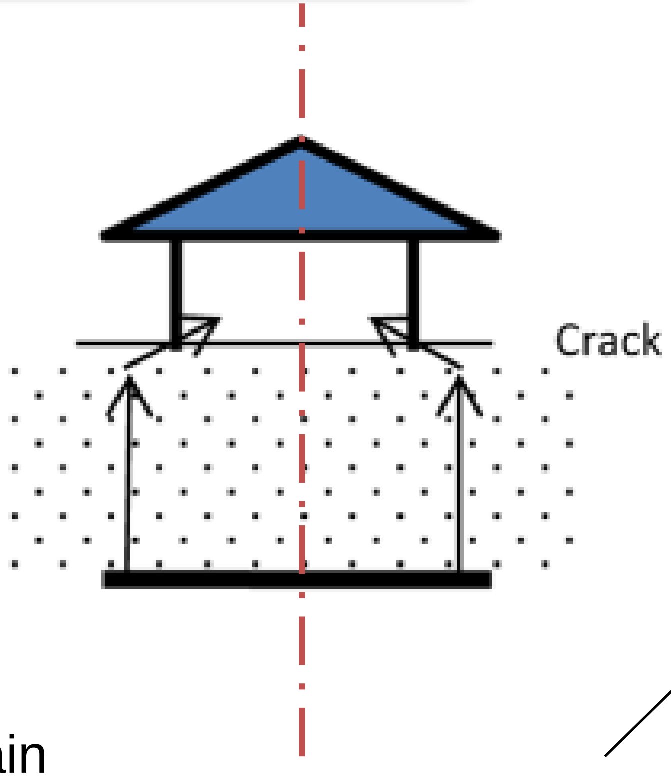
Boundary conditions

1. Darcy's law:

$$\frac{\partial p}{\partial t} - \frac{p_{atm} k_g}{\phi_g \mu_g} \nabla \cdot (\nabla p) = 0 \quad (1)$$

$$q_g = \frac{k_g}{\mu_g} \nabla p \quad (2)$$





3 Numerical model

- Comsol:

  Simulation software;

  especially for Multiphysics problems

- 229 codes:

  Created by MIT Course 229 Staffs

- parameters:

  ϕg (air filled porosity) = 0.38

  Kg (permeability) = 1e-12 [m^2]

1. Darcy's law:

$$\frac{\partial p}{\partial t} - \frac{p_{atm} k_g}{\phi_g \mu_g} \nabla \cdot (\nabla p) = 0 \qquad (1)$$

$$q_g = \frac{k_g}{\mu_g} \nabla p \qquad (2)$$

where p is the soil gas pressure $[M/L/T^2]$, t is time $[T]$, p_{atm} is atmospheric pressure $[M/L/T^2]$, k_g is the soil permeability to gas flow $[L^2]$, ϕ_g is the air filled porosity $[L^3_{gas}/L^3_{soil}]$, μ_g is the soil gas viscosity $[M/L/T]$, and q_g is the soil gas flow per unit area $[L^3_{gas}/L^2_{soil}/T]$. This equation neglects density-driven flow effects and gravity, which are expected to be insignificant for the problems of interest here.

3 Numerical model

1. Darcy's law:

$$\frac{\partial p}{\partial t} - \frac{p_{atm} k_g}{\phi_g \mu_g} \nabla \cdot (\nabla p) = 0 \qquad (1)$$

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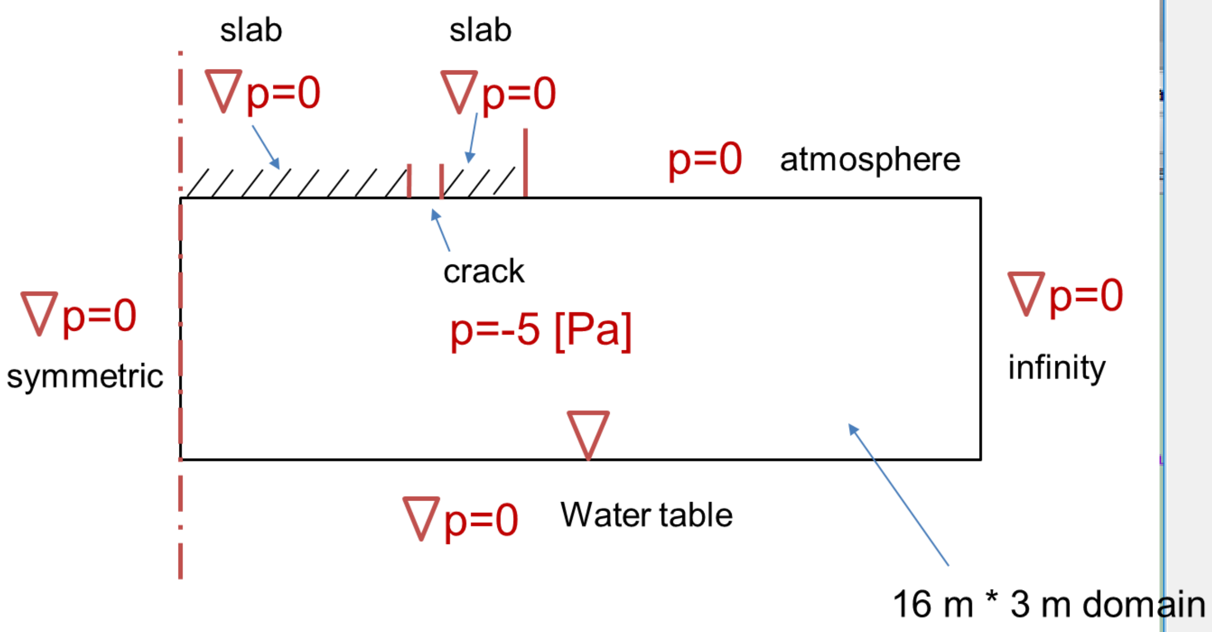
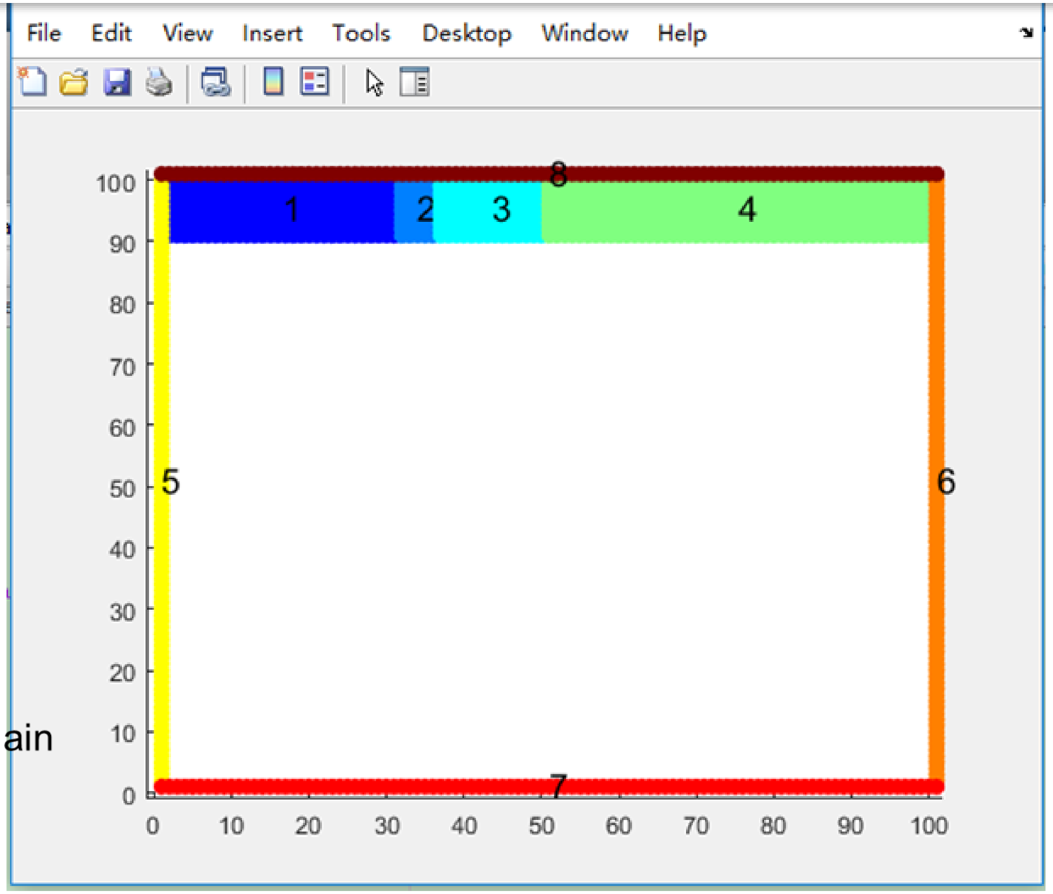
- 229 codes:





3 Numerical model

- 229 codes:
- Finite volume method

$$\frac{\partial p}{\partial t} - c\nabla(\nabla p) = 0$$

$$\Delta x \Delta y \frac{\partial \overline{p}}{\partial t} - c\int (\nabla p)\cdot \vec{n}\, dA = 0$$

CDS approximation

$$\Delta x \Delta y \frac{\partial \overline{p}}{\partial t} - c\sum_{faces} (\nabla p)\cdot (\vec{n}) A_{face} = 0$$

$$\frac{d\underline{\overline{p}}}{dt} = \underline{\underline{A}}\,\underline{\overline{p}}$$

FV discretization of Laplace operator

$$\underline{\overline{p}} = \begin{bmatrix} \overline{p}_1 \\ . \\ . \\ \overline{p}_{Nx*Ny} \end{bmatrix}$$

1. Darcy's law:

$$\frac{\partial p}{\partial t} - \frac{p_{atm} k_g}{\phi_g \mu_g}\nabla\cdot(\nabla p) = 0 \qquad (1)$$

$$q_g = \frac{k_g}{\mu_g}\nabla p \qquad (2)$$

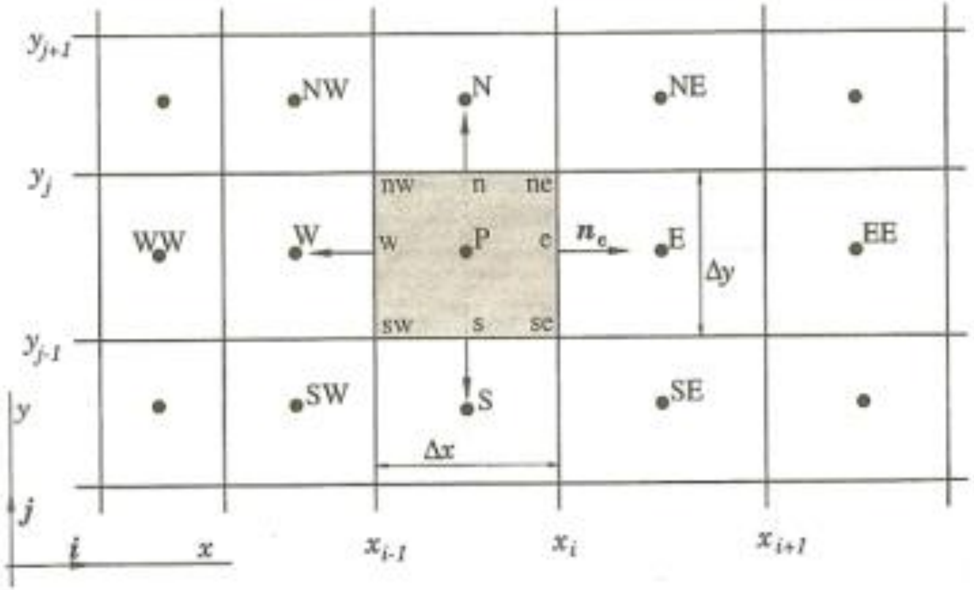


Fig. 4.2. A typical CV and the notation used for a Cartesian 2D grid

Pierre F.J Lermusiaux. Lecture 15 notes

3 Numerical model

- 229 codes:
- Finite volume method

$$\frac{d\overline{p}}{dt} = \underline{\underline{A}}\,\overline{p}$$

FV discretization of Laplace operator - Dfs

$$\frac{3\overline{p^{n}} - 4\overline{p^{n-1}} + \overline{p^{n-2}}}{2\Delta t} = Dfs\,\overline{p^{n}} + Dfs\_bcs$$

First Derivative	Error
$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$	$O(h^2)$

1. Darcy's law:

$$\frac{\partial p}{\partial t} - \frac{p_{atm} k_g}{\phi_g \mu_g} \nabla\cdot(\nabla p) = 0 \qquad (1)$$

$$q_g = \frac{k_g}{\mu_g} \nabla p \qquad (2)$$

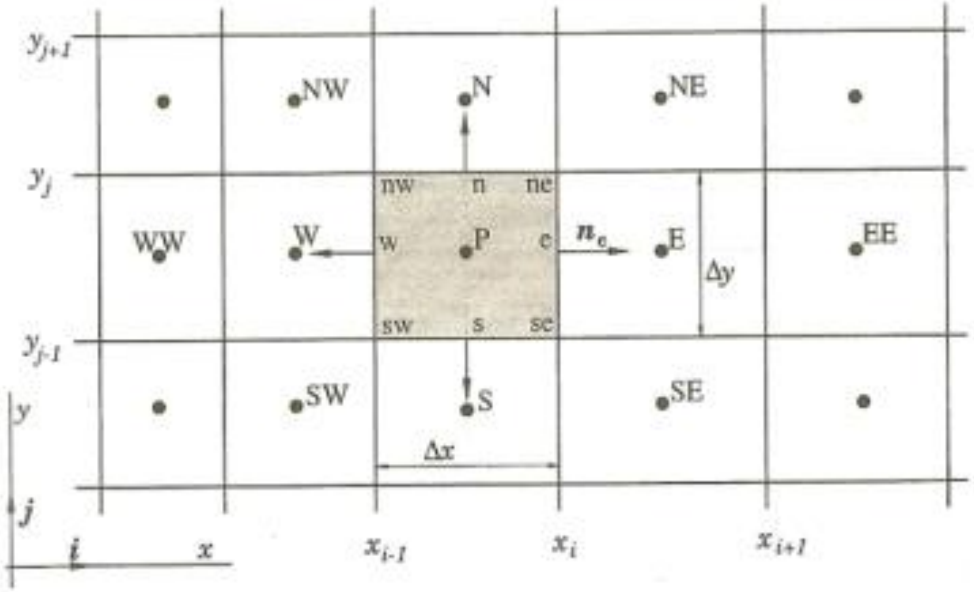


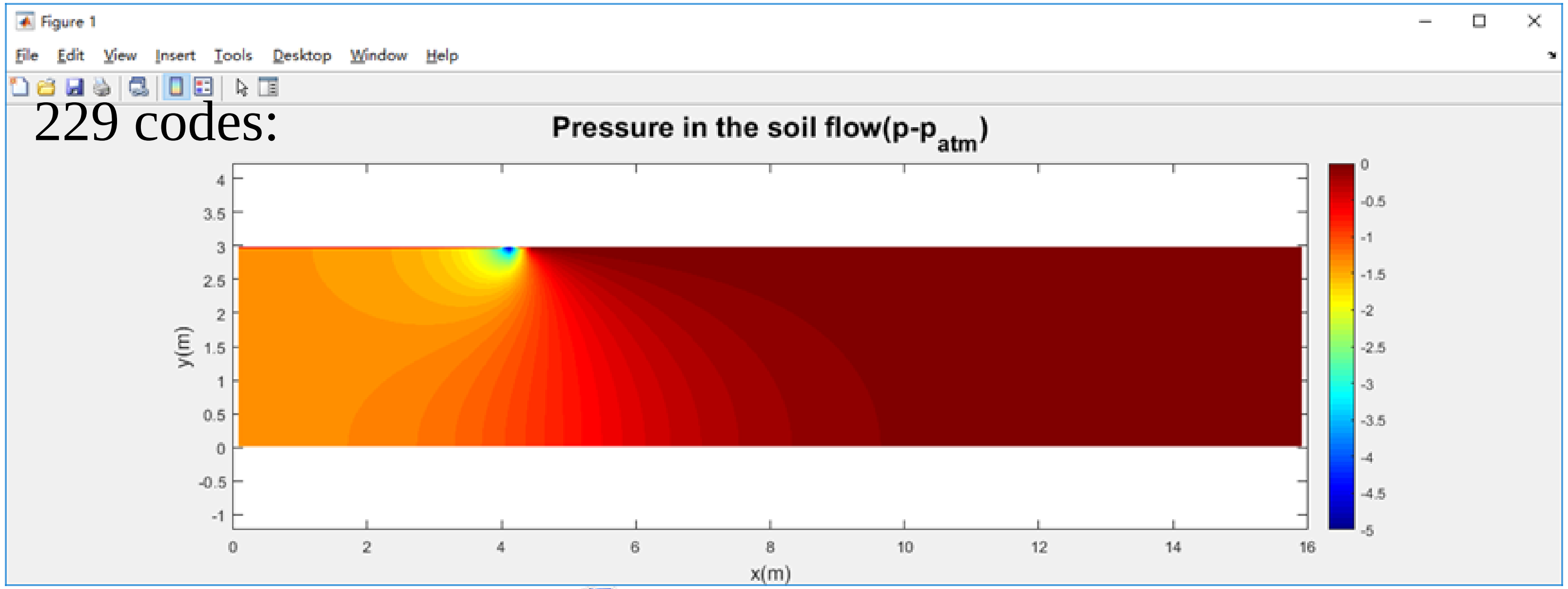
Fig. 4.2. A typical CV and the notation used for a Cartesian 2D grid

Pierre F.J Lermusiaux. Lecture 15 notes

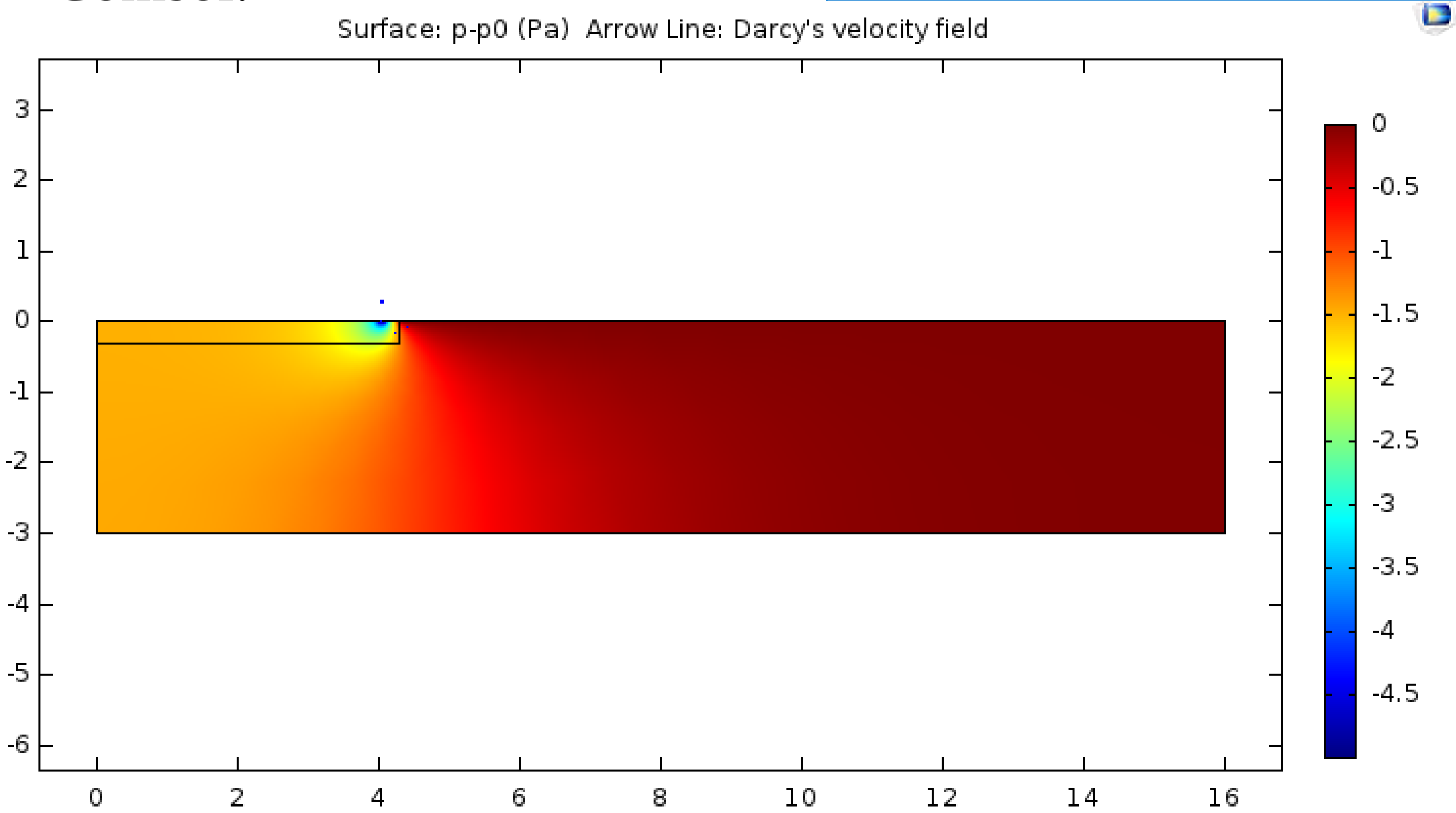
4 Results and discussion

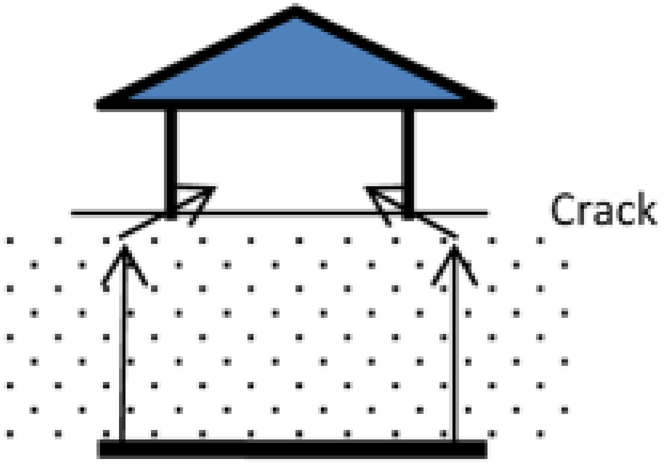
- Pressure field:
- Time = 20 h

- 229 codes:



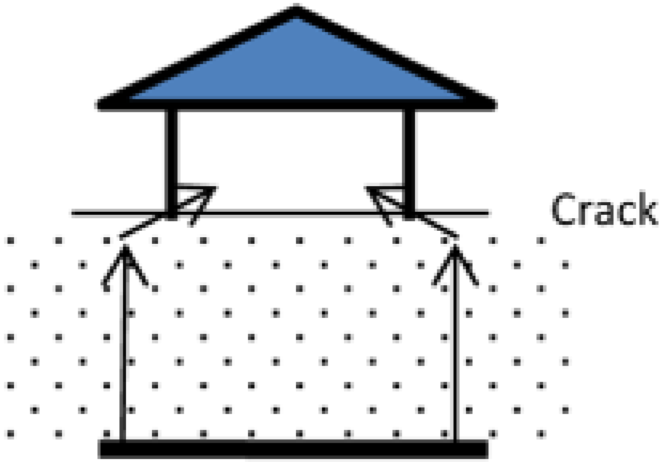
- Comsol:

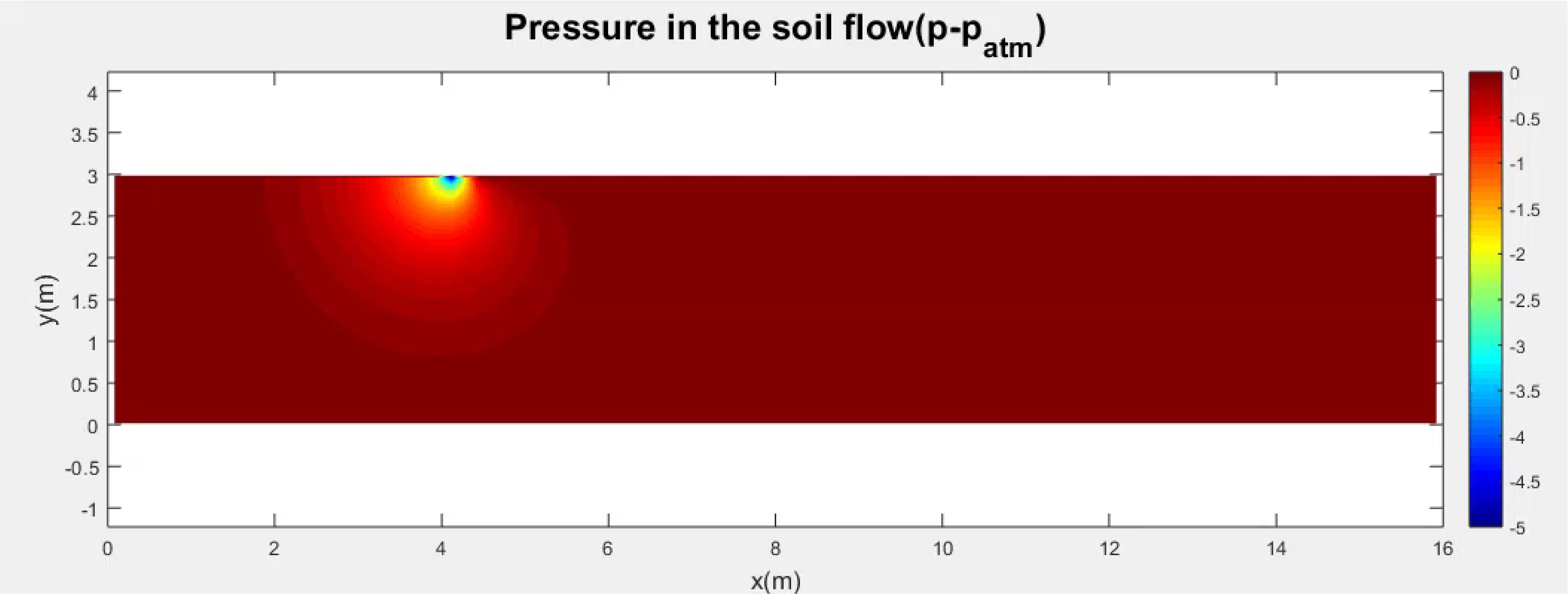




4 Results and discussion

- Pressure field:





3 Numerical model

2. Convection-diffusion equation:

chlorinated solvents

$$\phi_{g,w,s}\frac{\partial c_{ig}}{\partial t} = -\nabla\cdot(q_g c_{ig}) - \nabla\cdot\left(\frac{c_{ig}}{H_i}q_w\right) + \nabla\cdot(D_i\nabla c_{ig}) - R_i \quad (3)$$

Advection of gas — Advection of water — Diffusion — Reaction

where

Effective transport porosity

$$\phi_{g,w,s} = \phi_g + \frac{\phi_w}{H_i} + \frac{k_{oc,i}f_{oc}\rho_b}{H_i} \quad (4)$$

Gas phase — Liquid phase — Solid phase

Porosity n = 0.38

Diffusion coefficient Di<0.01cm^2/s

3. Millington and Quirk equation:

Effective diffusion coefficient

$$D_i = D_i^g\frac{\phi_g^{10/3}}{\phi_t^2} + D_i^w\frac{\phi_w^{10/3}}{\phi_t^2} \quad (5)$$

Gas phase — Liquid phase

3 Numerical model

- Comsol:

∇^2 Convection-Diffusion Equation *(cdeq)*

Δu Coefficient Form PDE *(c)*

Equation

Show equation assuming:

Study 1, Time Dependent

$$e_a\frac{\partial^2 c_v2}{\partial t^2} + d_a\frac{\partial c_v2}{\partial t} + \nabla\cdot(-c\nabla c_v2 - \alpha c_v2 + \gamma) + \beta\cdot\nabla c_v2 + a c_v2 = f$$

$$\nabla = [\frac{\partial}{\partial x},\frac{\partial}{\partial y}]$$

2. Convection-diffusion equation:

$$\phi_{g,w,s}\frac{\partial c_{ig}}{\partial t} = -\nabla\cdot(q_g c_{ig}) - \nabla\cdot\left(\frac{c_{ig}}{H_i}q_w\right) + \nabla\cdot(D_i\nabla c_{ig}) - R_i \qquad (3)$$

Advection of gas; Advection of water; Diffusion; Reaction

where

$$\phi_{g,w,s} = \phi_g + \frac{\phi_w}{H_i} + \frac{k_{oc,i}f_{oc}\rho_b}{H_i} \qquad (4)$$

Gas phase; Liquid phase; Solid phase

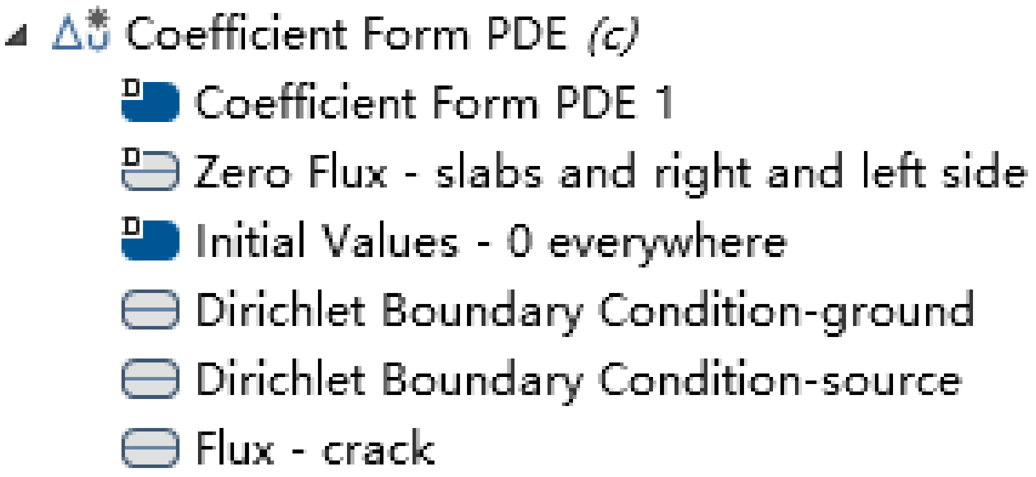
3. Millington and Quirk equation:

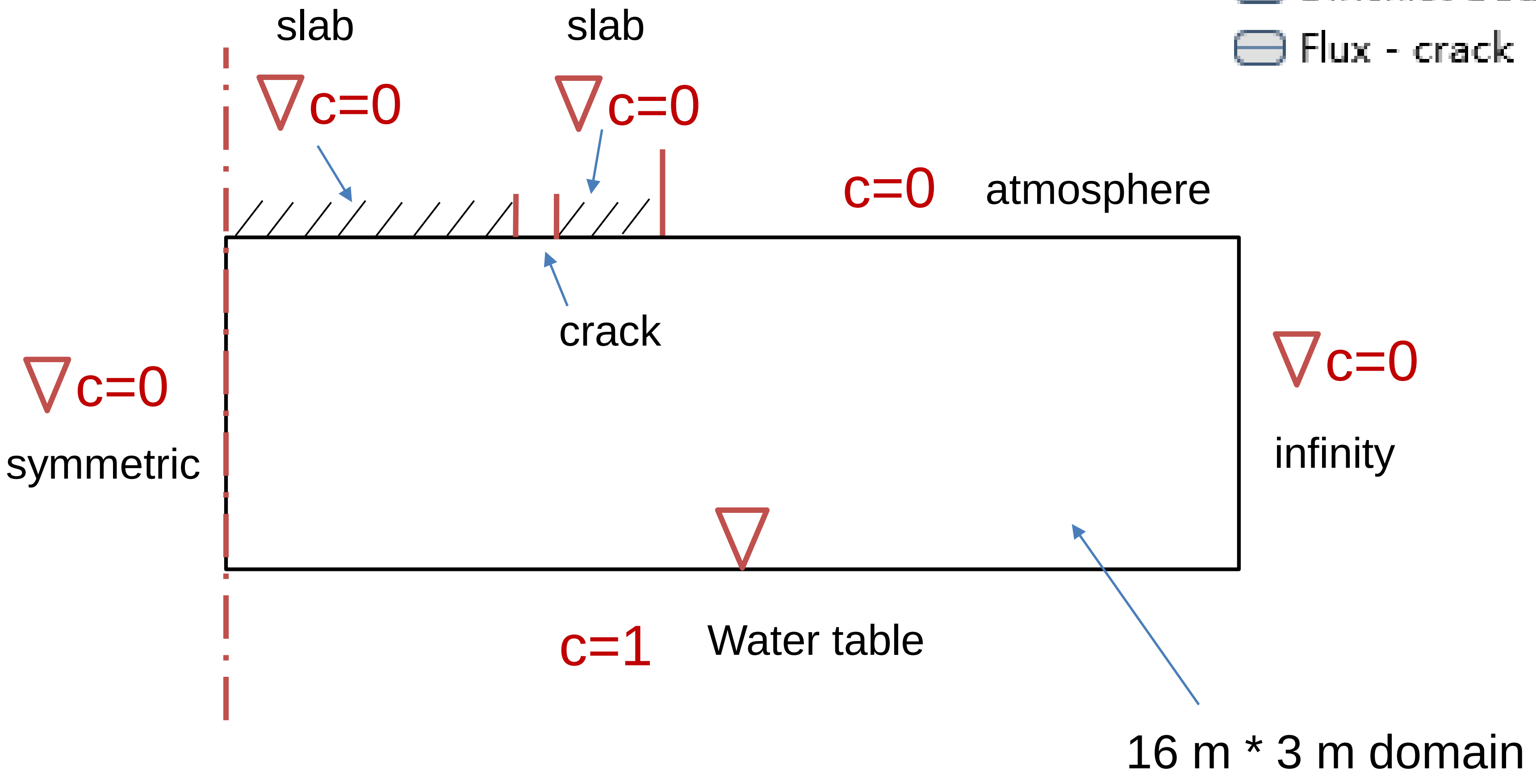
$$D_i = D_i^g\frac{\phi_g^{10/3}}{\phi_t^2} + D_i^w\frac{\phi_w^{10/3}}{\phi_t^2} \qquad (5)$$

Gas phase; Liquid phase

3 Numerical model

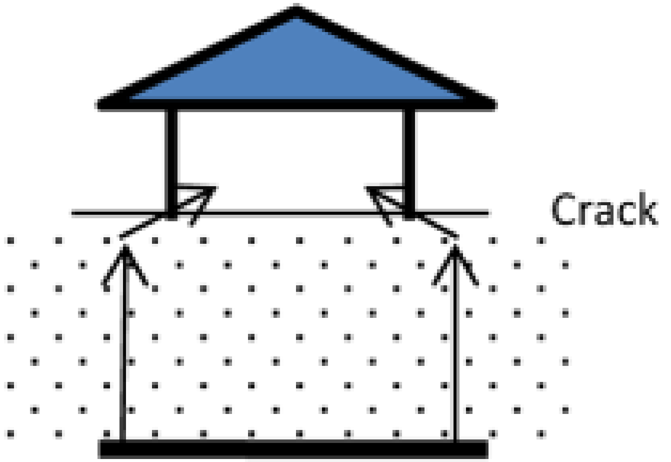
- Comsol: Boundary conditions

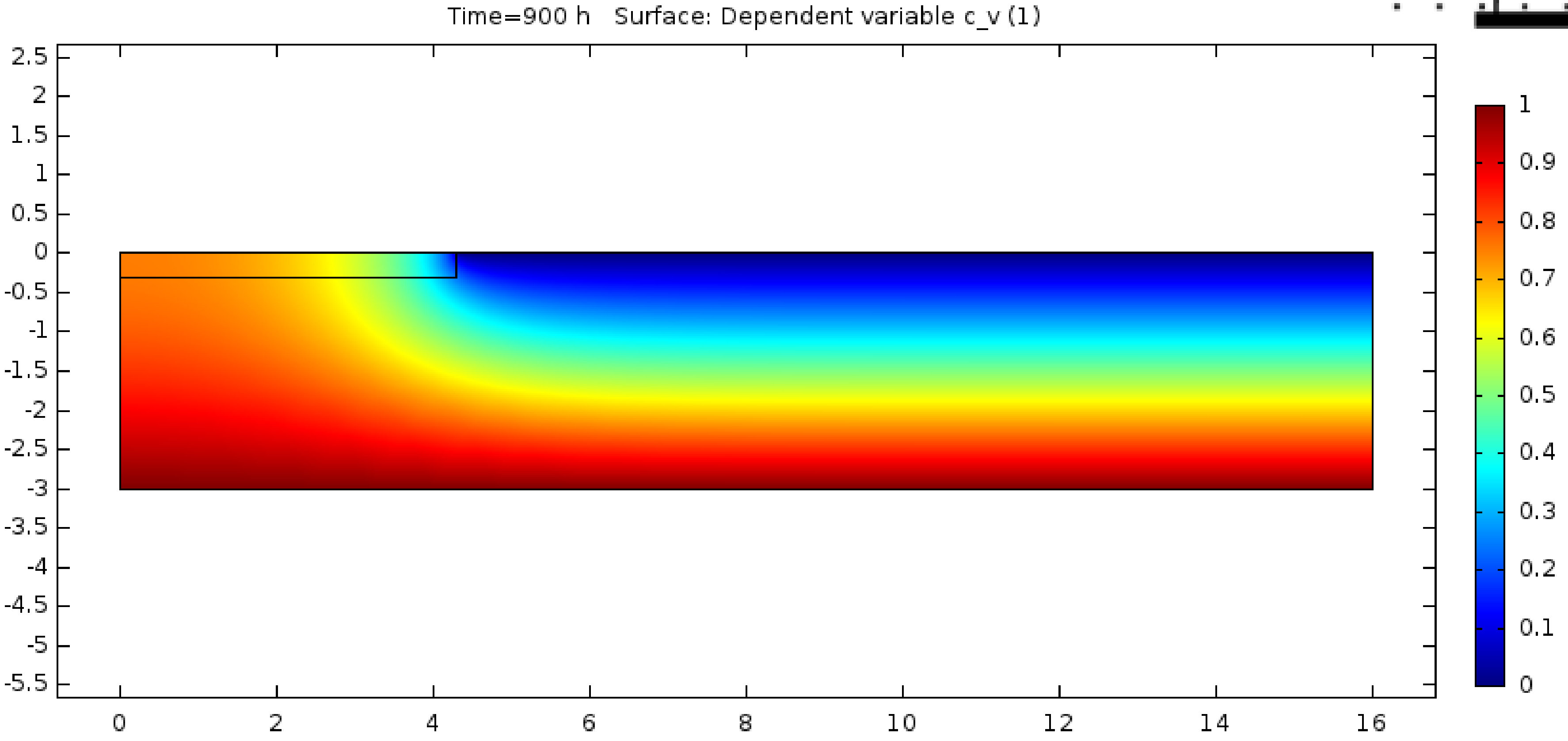




4 Results and discussion

- Comsol:

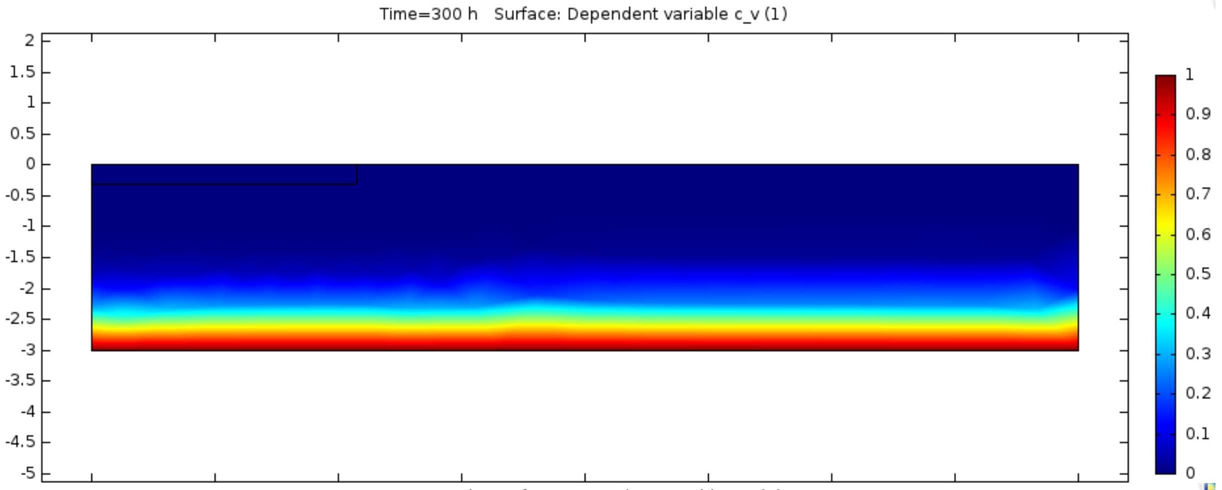




4 Results and discussion

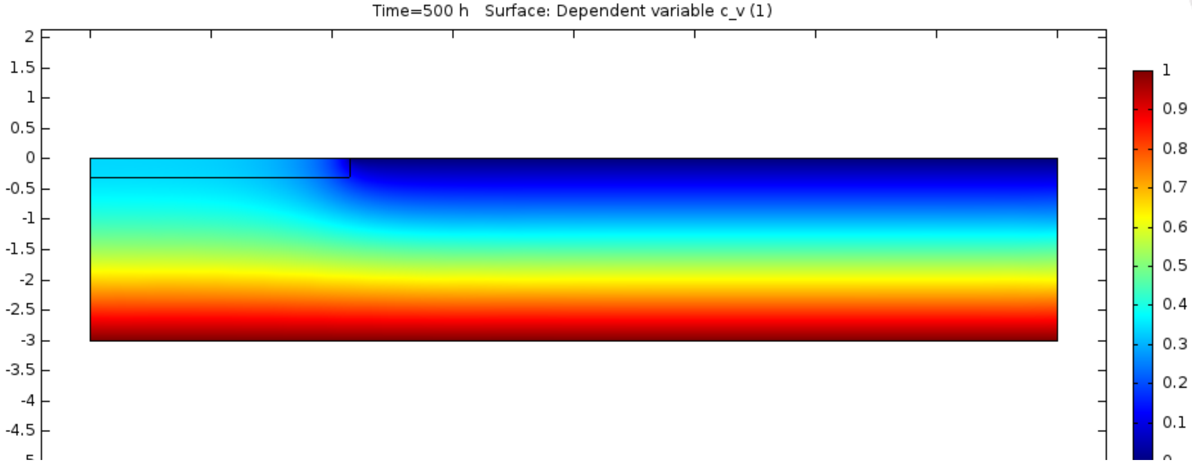
- Comsol:

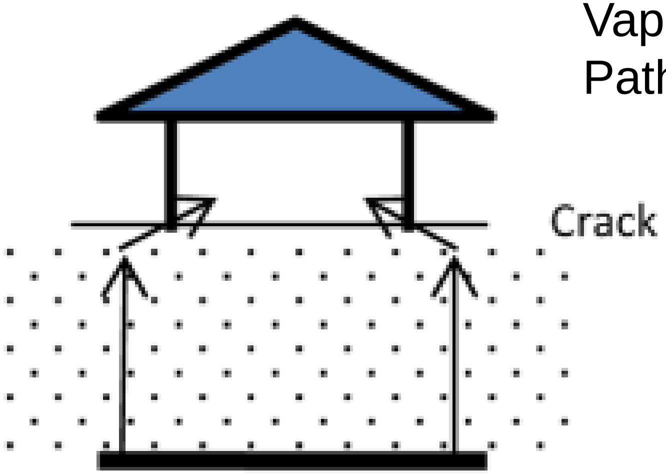
T = 300h



T = 500h

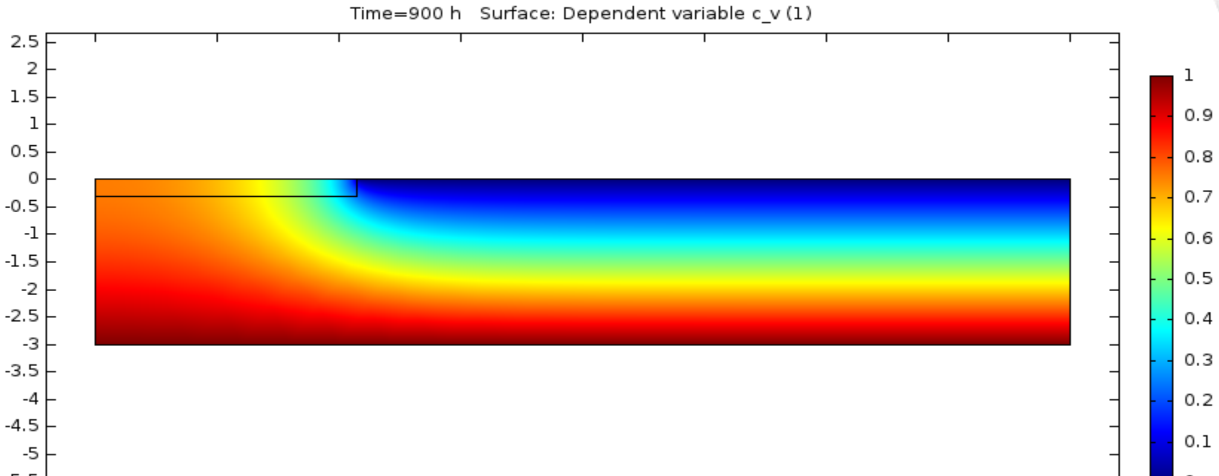
Vapor intrusion
Path way is complete





T = 900h

Vapor intrusion becomes steady;
Risk maximum



References

[1] Pierre F.J Lermusiaux. 229 Lecture notes
[2] Johnson, P. C., & Ettinger, R. A. (1991). Heuristic model for predicting the intrusion rate of contaminant vapors into buildings. Environmental Science & Technology, 25(8), 1445-1452
[3] Yao, Y., Shen, R., Pennell, K. G., & Suuberg, E. M. (2013). A Review of Vapor Intrusion Models. Environmental Science & Technology, 47(6), 2457-2470.
[4] Yao, Y., Shen, R., Pennell, K. G., & Suuberg, E. M. (2013). A Review of Vapor Intrusion Models. Environmental Science & Technology, 47(6), 2457-2470. doi: 10.1021/es302714g
[5] Illangasekare, T.; Petri, B.; Fučik, R.; Sauck, C.; Shannon, L.; Smits, K.; Cihan, A.; Christ, J.; Schulte, P.;Putman, B.; Li, Y. Vapor Intrusion from Entrapped NAPL Sources and Groundwater Plumes: Process Understanding and Improved Modeling Tools for Pathway Assessment, SERDP Project ER-1687 Final Report 2014.

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Q&A?