Use of COMSOL as an Educational Tool through its Application to Ground Water Pollution

Presented at the COMSOL Conference 2009 Milan

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16 October - COMSOL 2009 Milan

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Description of the course

1. Transport and transfer of pollutants in the soil
2. Waste disposal and ground water protection
3. Curiculum
    - Undergraduate level in a generalist engineering school ,
        - 9/33 hours
    - MSc in Soil & Rock Mechanics
        - 12/21 hours

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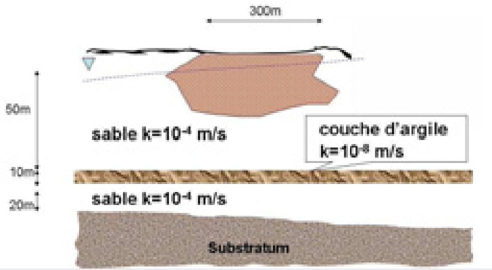
Statement of problem

Domestic waste disposal near a river

1. Physical mechanisms
   - Ground water flow
   - Transport & transfer of pollutant



2. Geohydrological configuration
   - medium sand
   - clay layer
   - hydraulic gradient

Contents

Ground water flow

Discover COMSOL through an example with analytical solution

Lowering of water table through excavation of a trench

Q1: Give the conceptual model including the governing equations and the corresponding boundary conditions

R1: Water mass balance through a porous media respecting Darcy's flow rule:

$$-\underline{\nabla} \cdot (\underline{\underline{k}} \underline{\nabla} h) = S \frac{\partial h}{\partial t} \quad \underline{x} \in \Omega \tag{1}$$

with:

- h: hydraulic head,
- S: storage capacity which can be neglected,
- $\underline{\underline{k}}$ the hydraulic conductivity tensor.

Questions & answers

R1 The boundary conditions are:

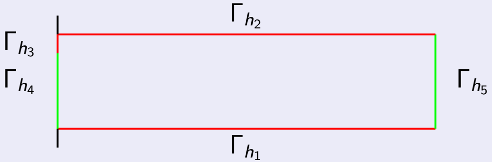
1. Neumann boundary condition:

$$\underline{n} \cdot (k_n \underline{\nabla}_n h) = 0 \quad \underline{x} \in \Gamma_{h_1}, \Gamma_{h_2}, \Gamma_{h_3} \tag{2}$$

2. Dirichlet conditions:

$$h = H_1 - 10 \quad \underline{x} \in \Gamma_{h_4} \tag{3}$$

$$h = H_1 m \quad \underline{x} \in \Gamma_{h_5} \tag{4}$$

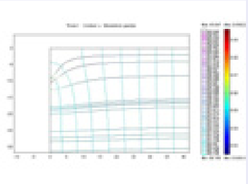


Questions & answers

Q2 Compute the flux of water to be pumped and discuss the precision. How can the difference be reduced?

R2 Dupuit assumption (flow is horizontal in each vertical section) gives the input and output flows on Γ_{h_5} and Γ_{h_4} boundaries:

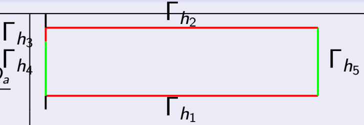
$$Q_{\Gamma_i} = \int_{\Gamma_i} k \frac{\partial h}{\partial n} dS \quad (5)$$



Flow lines & equipotential contours

Questions & answers

Flux error estimation / analytical solution Q_a

	$\frac{Q_{\Gamma_5}-Q_{\Gamma_4}}{Q_{\Gamma_5}}$ [%]	$\frac{Q_{\Gamma_4}-Q_a}{Q_a}$ [%]	$\frac{Q_{\Gamma_5}-Q_a}{Q_a}$ [%]	
mesh1	10.5	-1.1	10.5	
mesh2	7.5	2.2	10.5	
mesh3	5.2	4.6	10.4	
mesh_∞	2.7	7.5	10.4	

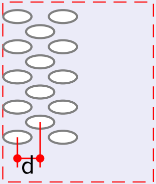
Questions & answers

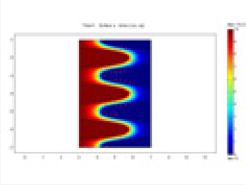
Sand lentils

- REV model
- Horizontal & vertical flow
- Computation of equivalent horizontal & vertical conductivity

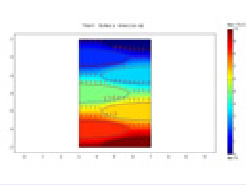
$$\int_{\Gamma_i} k \frac{\partial h}{\partial n} dS = K_{eq} \frac{\Delta h}{\Delta L} \quad (6)$$

- $k_h = 10k_v$





horizontal flow



vertical flow

Contents

Pollutant transfer and transport

Extension of the contamination plum

- A variety of pollutant origins with different physical characteristics can be studied
    - Miscible or immiscible,
    - Light or heavy,
    - bio-degradable,
    - etc
- Miscible one species pollutant (sake of simplicity)

Questions & answers

Q1: Give the conceptual model including the governing equations and the corresponding boundary conditions

R1: Mass balance of the species taking into account advection, diffusion, dispersion and possibly sorption:

$$r\frac{\partial c}{\partial t} - \underline{\nabla} \cdot (-\underline{\underline{D}} \cdot \underline{\nabla} c) + \underline{v} \cdot \underline{\nabla} c = 0 \quad (7)$$

with:

- c : concentration of the pollutant,
- $\underline{v}$: the advection transport velocity ($=\underline{V_r}/\theta$, $\underline{V_r} = -\underline{k}/\theta \cdot \underline{\nabla} h$, θ: porosity)
- $\underline{\underline{D}}$: hydrodynamic dispersion tensor given by:

$$\underline{\underline{D}} = \underline{\underline{D}}_0 + \alpha_L \underline{e}_L \otimes \underline{e}_L + \alpha_T \underline{e}_T \otimes \underline{e}_T \quad (8)$$

  - $\underline{\underline{D}}_0$: bulk diffusion of the medium,
  - α_L and α_T: longitudinal and transversal dispersivity coefficients,
  - $\underline{e}_A$: unit vector along the A direction
- r: retardation factor , equal to one when absence of adsorption.

Questions & answers

Boundary conditions

- Neumann condition with no diffusive flux:

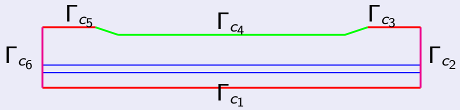
$$\underline{n} \cdot (D_n \underline{\nabla}_n c) = 0 \quad \underline{x} \in \Gamma_{c_1}, \Gamma_{c_3}, \Gamma_{c_5} \tag{9}$$

- Advective flux boundary:

$$\underline{n} \cdot (D_n \frac{\partial c}{\partial n}) + v_n \cdot c = v_n \cdot c \quad \underline{x} \in \Gamma_{c_2}, \Gamma_{c_6} \tag{10}$$

- Dirichlet condition:

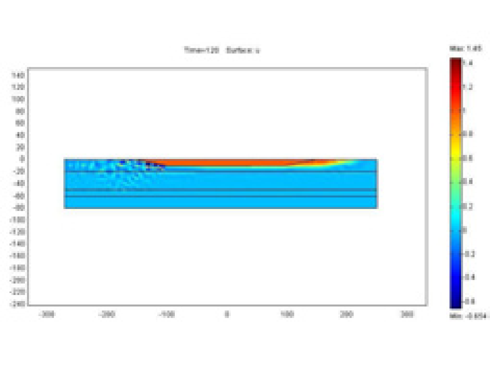
$$c(\underline{x}, t) = 1 \quad \underline{x} \in \Gamma_{c_4} \tag{11}$$



The domain and its boundaries for the solute transport problem

Questions & answers

Extension of pollution



Contours of concentration after 10 years

$$C* = 1$$

Questions & answers

Confinement walls

Q2 Give the flux of water to pump in order to prevent solute propagation and to keep the fill out of water

R2 Water flow patern modified after confinement and excavation.

Modification of hydraulic boundary conditions:

- Neumann boundary condition:

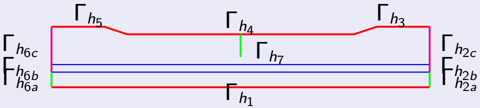
$$\underline{n} \cdot (k_n \underline{\nabla}_n h) = 0 \tag{12}$$

$\underline{x} \in \Gamma_{h_1}, \Gamma_{h_{2b}}, \Gamma_{h_{2c}}, \Gamma_{h_3}, \Gamma_{h_4}, \Gamma_{h_5}, \Gamma_{h_{6b}}, \Gamma_{h_{6c}}$

- Dirichlet conditions:

$$h = H_1 \quad \underline{x} \in \Gamma_{h_{2a}}, \Gamma_{h_{6a}} \tag{13}$$

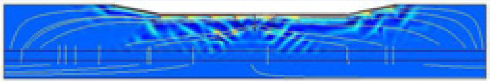
$$h = H_1 - 10m \quad \underline{x} \in \Gamma_{h_7} \tag{14}$$



R3 Sand lentils: multiplication of the flux to be pumped by 10

Questions & answers

Confinement walls



Contours of concentration after the construction of the confining wall (t=10 years)

Contents

Conclusion

1. Step by step approach using COMSOL
   - intuitive use
   - adequate default values
   - practical post-processing
   - automatic report
2. Other possibilities
   - Remediation techniques
     - reactive permeable barrier
     - bio-degradation
     - venting
     - ...
   - Physical models
     - transfert mechanisms: degradation
     - immiscible species: multiphase flow
     - multiple species & coupling between them
     - ...
   - Numerical point of view
     - streamline
     - regularisation
     - non linearities (isoterm, conductivity,...)
   - taking into account uncertainties
   - interpretation of hydrogeological data