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

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Abstract: Ensuring the quality of underground water and controlling its quantity is of major concern for the population. Therefore, this subject attracts many students from different specialties at different levels of their curriculum. In fact, the pedagogic objectives of the course mat be different according to the level or/and interest of the students and COMSOL is used due to its versatility. In this paper, a case study related to a waste disposal is presented. Through a step by step approach the students get familiar with the software, the water flow problem, the solute transport, the soil properties and rehabilitation techniques.

Keywords: water flow, solute transport, contamination, confinement, education.

1 Introduction

Ground water is not only a source for drinking water but if contaminated it is a threat for the environnement. Many students are interested in this subject at different levels and thus, a versatile modeling tool can be a good means to acquire a better understanding of the problem. In fact, the pedagogic objectives of a course differ according to the level or/and interest of the students. Several aspects, such as the mathematical formulation, numerical discretization and the relative accuracy and precision are addressed at graduate level or in the framework of numerical modeling courses, while parametric studies on pre-prepared cases help to better understand the physical issues of the problem in more applied courses. Independantly from the background of the students and the level of their studies, the same case study may be used but with different degrees of complexity. In this paper, a case study elaborated for undergraduate students is presented. Many textbooks or courses can be consulted for deepening the subject adressed in this paper(see [1], [2],[3],[4] among others).

2 Statement of the problem

Consider a city using a site near a river for its domestic waste disposal since several years. The configuration of the site is given in Figure 1.

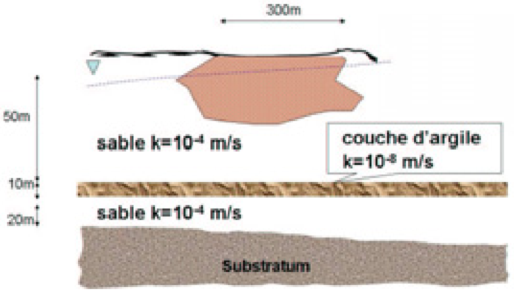


Figure 1: The geological cross-section of the site along the primary water flow direction.

The soil at the site is composed mainly of a medium sand including a 10m clay layer at the depth of 50 m. The substratum is about 80m depth. The piezometric data shows the presence of a hydraulic gradient of about 0.002. Other data can be found in the Appendix. The students are invited to look for complementary data if needed from the litterature.

Different types of questions have to be answered depending on the pedagogic objectives of the course. In all cases the description of the conceptual model is required. That includes the physical phenomena to be studied, the governing equations as well as the corresponding boundary and initial conditions. In general, for sake of simplicity, only 2D or 1D models are preferred.

2.1 Ground water flow

This elementary case study for which an analytical solution is available, will let the students get familiar with the software and its different menus.

Question 1:
In order to prevent rapidly the pollution propagation, it was decided to excavate a trench in which water would be pumped. This would lower the water table and generate an advective flow which would opse to the pollution diffusion.

Neglecting the transport and transfer of the pollutants and considering only the ground water flow, give the conceptual model including the governing equations and the corresponding boundary and initial conditions.

Question 2:
Compute the flux of the water to be pumped and compare it with the analytical expression obtained using the Dupuit assumption. How can the difference be reduced?

2.2 Pollutant transfer and transport

A variety of pollutant origins with different physical characteristics can be studied (Miscible, immiscible, light, heavy, bio-degradable, etc.). For the sake of simplicity, we opt for a miscible one species pollutant.

Question 1:
If the site is exploited since 10 years, give an approximate extension of the contamination plum.

Question 2:
In order to reduce the propagation of the contamination during the rehabilitation of the site, confinement walls embedded in the clay layer were constructed. Capturing trenches were excavated too to evacuate the existing and infiltered water. Give the flux of water to pump in order to prevent solute propagation and to keep the fill out of water.

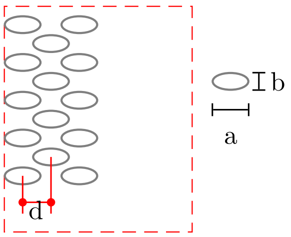


Figure 2: The geometrical configuration of the sand lenses.

Question 3:
The geotechnical investigation showed that the clay layer contains sand lenses. Considering the geometrical configuration given in Figure 2, give an estimation of the hydraulic conductivity of a homogeneous material which can represent this mixed layer when $a = 2.75m$, $b = 0.5m$ and $d = 2m$.

In order to treat the initial and boundary conditions and stress out their differences two cases can be studied. Firstly, the waste disposal is continuously supplied and secondly, the case where the site is no more exploited.

3 Use of COMSOL

The coefficient equation system form of COMSOL is very well adapted to this problem. It will let the students choose the adapted coefficients with respect to the phenomenon to be studied.

3.1 Ground water flow

Response 1:
In the first case, the steady state flow of water through a porous media is to be considered. The mass balance of water can be written as:

$$\underline{\nabla} \cdot \underline{V_r} = S\frac{\partial h}{\partial t} \tag{1}$$

where V_r is the infiltration velocity, h the hydraulic head. S is the storage capacity which can be neglected. Moreover, if the steady state is to be adressed it has no effect. Darcy's law which governs the flow of water in the porous media can be written as:

$$\underline{V_r} = -\underline{\underline{k}} \cdot \underline{\nabla} h \tag{2}$$

where $\underline{\underline{k}}$ is the hydraulic conductivity tensor. The governing equation is thus the mass balance of the water given as :

$$-\underline{\nabla} \cdot (\underline{\underline{k}}\underline{\nabla} h) = S\frac{\partial h}{\partial t} \quad \underline{x} \in \Omega \tag{3}$$

Due to the symmetry of the problem, only half of the domain may be modelled (Figure 3). The boundary conditions are:

Neumann boundary condition:

$$\underline{n} \cdot (k_n \underline{\nabla}_n h) = 0 \quad \underline{x} \in \Gamma_{h_1}, \Gamma_{h_2}, \Gamma_{h_3} \tag{4}$$

Dirichlet conditions:

$$h = H_1 \quad \underline{x} \in \Gamma_{h_4} \tag{5}$$

$$h = H_1 - 10m \quad \underline{x} \in \Gamma_{h_5} \tag{6}$$

In fact, H_1 can be any arbitrary value. As the stationary solution is calculated, no initial value is necessary. The obtained streamlines and the hydraulic head contours are given in Figure 4.

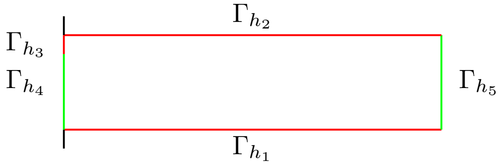


Figure 3: The domain and its boundaries for the flow problem.

The precision of the computation is studied using the flux obtained analytically applying the Dupuit assumption (the flow is horizontal in each vertical section). The input and output flows on Γ_{h_5} and Γ_{h_4} boundaries given by:

$$Q_{\Gamma_i} = \int_{\Gamma_i} k \frac{\partial h}{\partial n} dS \tag{7}$$

are computed using the boundary integration option in the postprocessing menu. Table 1 shows the obtained values for different meshes (Figure 5). mesh$_\infty$ corresponds to a very refined mesh with 90821 degrees of freedom, not illustrated here.

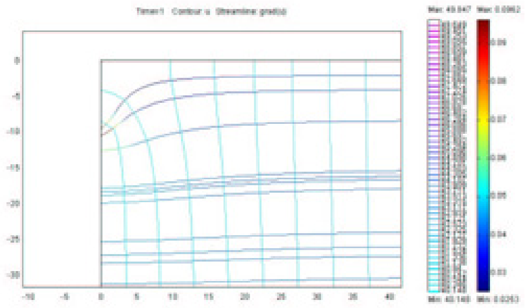
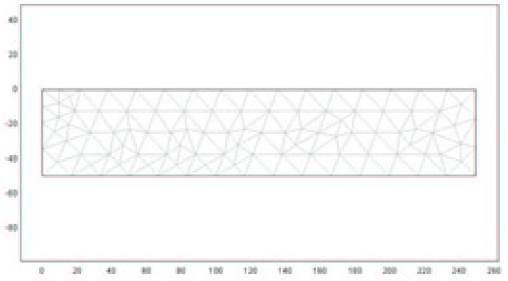


Figure 4: Streamlines and hydraulic head contours obtained for Q1.

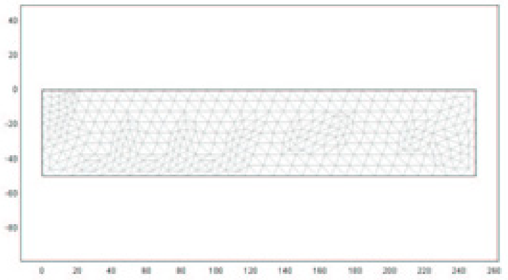
	$\frac{Q_{\Gamma_5}-Q_{\Gamma_4}}{Q_{\Gamma_5}}$ [%]	$\frac{Q_{\Gamma_4}-Q_a}{Q_a}$ [%]	$\frac{Q_{\Gamma_5}-Q_a}{Q_a}$ [%]
mesh1	10.5	-1.1	10.5
mesh2	7.5	2.2	10.5
mesh3	5.2	4.6	10.4
mesh$_\infty$	2.7	7.5	10.4

Table 1: Error estimations of the flux with respect to the analytical solution Q_a.

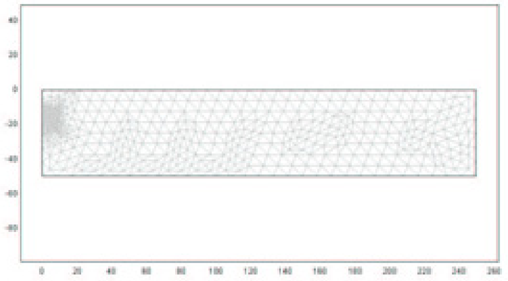
We note that the difference between the in-going and out-going flux reduces when the mesh is refined. The refinement in the vicinity of the singularity has more effect (mesh3). However, the error on the in-going flux is constant. This is due to the non validity of the Dupuit assumption in this case.



mesh1



mesh2



mesh3

Figure 5: Different meshes used in the computation of the water to be pumped

Response 2:
In order to obtain the hydraulic conductivity of the clay layer including the sand lenses, a representative elementary volume (REV) subjected to horizontal and vertical flow conditions can be studied. The same equation as above is applied with appropriate boundary conditions. Knowing the gradient head and the water flux in each direction, the hydraulic conductivity of the equivalent material is computed. For the configuration given in Figures 6 and 7, the following values are obtained: $k_x = 10^{-6} m/s$ and $k_y = 10^{-7} m/s$.

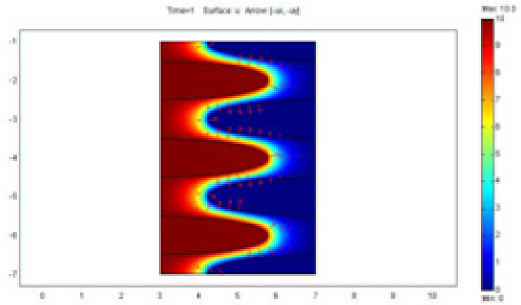


Figure 6: Head contours in the REV under horizontal flow.

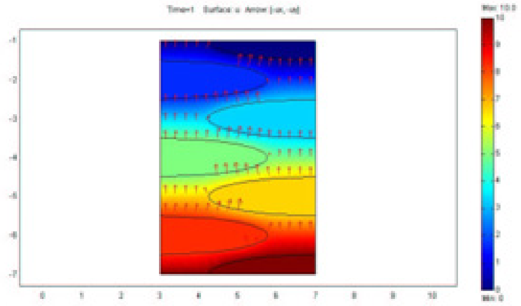


Figure 7: Head contours in the REV under vertical flow.

3.2 Pollutant transfer and transport

For this problem, the governing equation is the mass balance of the species taking into account advection, diffusion, dispersion and possibly sorption:

$$r\frac{\partial c}{\partial t} - \underline{\nabla} \cdot (-\underline{\underline{D}} \cdot \underline{\nabla} c) + \underline{v} \cdot \underline{\nabla} c = 0 \qquad (8)$$

where c is the concentration of the pollutant, $\underline{v}$ is the advection transport velocity ($\underline{v} = \underline{V_r}/\theta$, $\underline{\underline{D}}$ takes into account diffusion and dispersion and is given by:

$$\underline{\underline{D}} = \underline{\underline{D}}_0 + \alpha_L \underline{e}_L \otimes \underline{e}_L + \alpha_T \underline{e}_T \otimes \underline{e}_T \qquad (9)$$

where $\underline{\underline{D}}_0$ denotes the bulk diffusion of the medium, α_L and α_T are the longitudinal and transversal dispersivity coefficients and $\underline{e}_A$ represents the unit vector along the A direction. In absence of adsorption the retardation factor r should be taken equal to one.

Response R1:
The model (Figure 8) will be limited to the substratum in the vertical direction. The boundary conditions are given below.

Neumann condition with no diffusive flux:

$$\underline{n} \cdot (D_n \underline{\nabla}_n c) = 0 \quad \underline{x} \in \Gamma_{c_1}, \Gamma_{c_3}, \Gamma_{c_5} \qquad (10)$$

advective flux boundary:

$$\underline{n} \cdot (D_n \frac{\partial c}{\partial n}) + v_n \cdot c = v_n \cdot c \quad \underline{x} \in \Gamma_{c_2}, \Gamma_{c_6} \quad (11)$$

Dirichlet condition:

$$c(\underline{x}, t) = 1 \quad \underline{x} \in \Gamma_{c_4} \qquad (12)$$

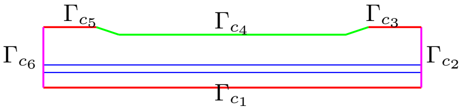


Figure 8: The domain and its boundaries for the solute transport problem.

The contours of concentration after 10 years are given in Figure 9. It should be noticed that due to the dominance of advection, numerical oscillations may occur. These oscillations can be eliminated using regularization methods such as numerical damping or up-wind schemes.

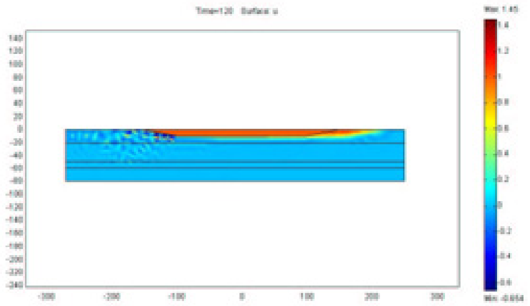


Figure 9: Contours of concentration after 10 years.

Response 2:
Once the confinement and the trench executed, the water flow will be modified on the site. The corresponding boundary conditions for the hydraulic head are given below:

Neumann boundary condition:

$$\underline{n} \cdot (k_n \underline{\nabla}_n h) = 0 \tag{13}$$

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

Dirichlet conditions:

$$h = H_1 \quad \underline{x} \in \Gamma_{h_{2a}}, \Gamma_{h_{6a}} \tag{14}$$

$$h = H_1 - 10m \quad \underline{x} \in \Gamma_{h_7} \tag{15}$$

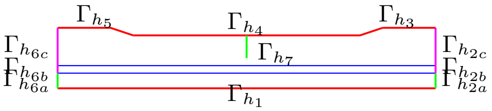


Figure 10: The domain and its boundaries for the water flow.

The resolution of the two equation systems is easily conducted in COMSOL. The flux of water to be pumped in the trench is 10 $m^3/month/m$ when no sandy lenses are considered in the clay layer. However, this value is multiplied almost by 10 with the presence of sandy lenses. The contours of concentration as well as the water streamlines are given in Figure 11.

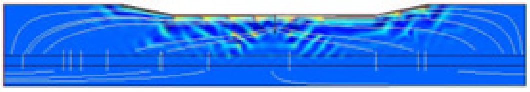


Figure 11: Contours of concentration and the streamlines after 10 months.

4 Conclusion

To get familiar with the different aspects of ground water pollution and its modelling a step by step approach using COMSOL is presented. A waste disposal site is used as the case study. First, the water flow problem, usefull in many engineering situations, is adressed. Many remediation techniques are available and may be modelled. In this paper, we limit our presentation to the confinement technique as it one of the most commonly used methods. Other techniques, generally more sofisticated are available and can be modelled by COMSOL. The numerical modelling is an efficient tool for cost effective design. However, for practical applications as in many other hydrogeotechnical problems, the availability of data is essential.

References

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Appendix

	k $[m/s]$	θ	D_0 $[m^2/s]$
Sand	10^{-4}	0.4	10^{-9}
Clay	10^{-8}	0.7	10^{-9}

Table 2: Characteristic values for properties of different layers.