Modeling the dispersion of a pollutant in a two-layer porous medium

General problem

Following pollution in a saturated environment subject to the hydrodynamic conditions reported in Figure 1, we want to understand and investigate the transport of this pollutant within the environment.

To do this, we are going to apply upscaling techniques allowing us to better understand the situation, and above all to be able to provide engineering support for the exploitation of water resources in situ.

In order to determine dangerous regions we will have to investigate the medium in which the concentration is more or equal to 0.000001 kg/m$^3$

1. Presentation of the experience

A pollutant dispersion experiment carried out in the laboratory is presented in Figure 1. The domain consists of different types of porous medium (homogeneous or heterogeneous) 200m m wide, 200 m long and 100 m thick. We introduce at time $t_0$ a polluting volume in its concentrated form in a block of 2mx2mx2m located at x=49m, y=49m and z=49m with c=1kg/m$^3$. We impose a flow (V = Vinj and the p=0 at the outlet) and we measure the concentrations in the whole domain according to time.

According to some previous work, and studying short courses, we are going to study this case.

The objective is to reproduce this experiment numerically under COMSOL. For this, two samples of porous media were taken and on which numerical scaling techniques will be applied to obtain equivalent properties (permeability and dispersion coefficient). With the help of these properties and a pre-built numerical experiment model, we will feed the model with the different properties and we will simulate the experiment.

So, we will have to determine both the permeability and the dispersivity of some samples in order to carry out the large scale simulation. Anyway it requires some previous knowledges we will try to get before starting.

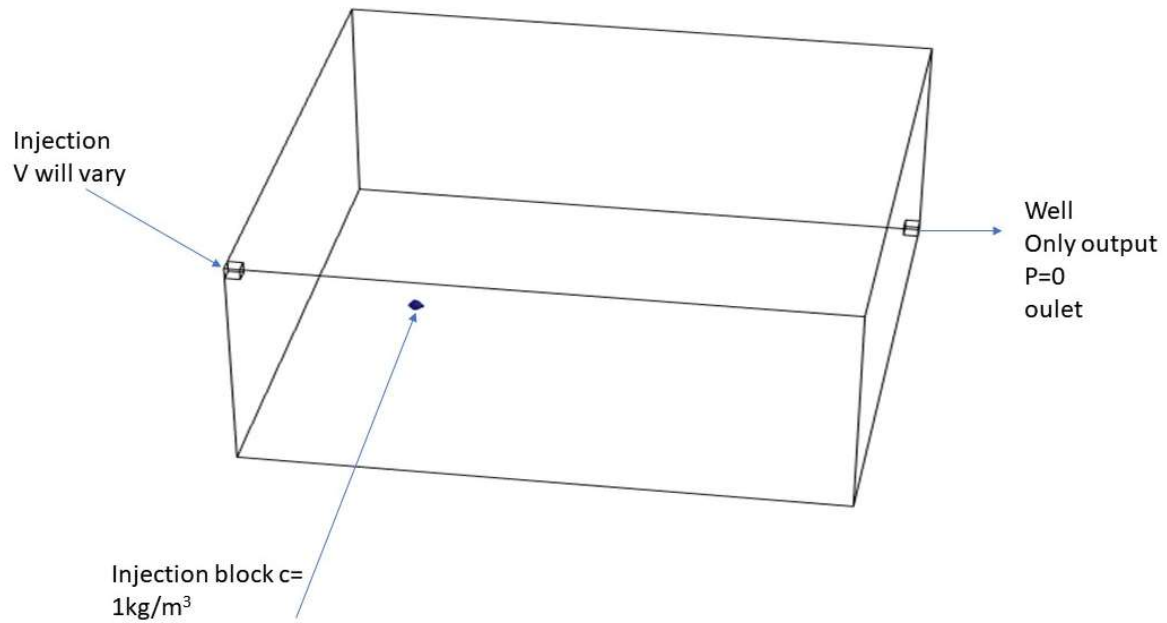Two samples will be taken from the ground, a homogeneous medium and an heterogeneous medium.

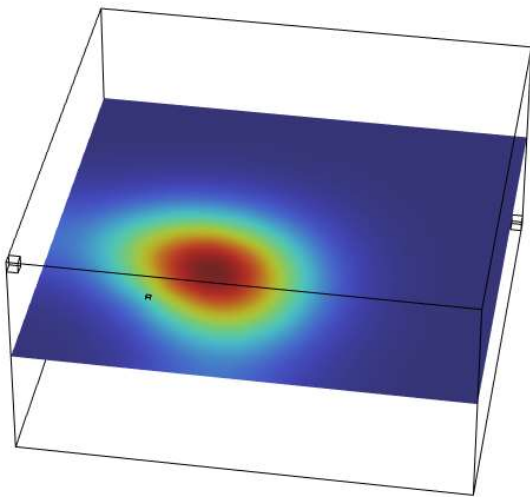Figure 1 : polluted soil and boundary conditions applied.



Figure 2: example of the concentration field obtained with a set of experimental parameters

## 2 Upscaling parameters determination

### 2.1 Determination of the properties of the homogeneous medium

A sample of the porous medium of a few centimeters of the whole reservoir was taken to estimate the properties of the soil using numerical modeling (permeability and dispersion). Using the sample provided (see Figure 3 and the sample file eta.mph), we seek to perform the upscaling process to calculate the permeability of the medium and the dispersion coefficient.



Figure 3 Homogeneous medium whose dimensions are L=0.05625m, l=0.005m the cylinders have a diameter of 0.0025m.

#### 2.1.1 Determination of permeability K

By solving the flow at the microscale on the digital sample, we will first determine the permeability of the provided sample using Darcy's law (will do that together)

#### 2.1.2 Determination of dispersion D (U)

We will see in class that we can estimate the permeability of a porous medium, but also the dispersion of a constituent at a Peclet number Pe given with:

Pe= Ud/D

With U the average speed (speed imposed in the medium at the entrance), d the diameter of the cylinders and D the molecular diffusion coefficient of the species transported in the water.

Plot of the reference curves. Using the real geometry of the medium, we impose a concentration at the entrance (a step) for a certain time (the duration depending on the flow velocity, see Table 1).

| Pe | 0.125 | 1.25 | 12.5 | 125 | 1250 |
|---|---|---|---|---|---|
| Concentration window duration (s) | 1e4 | 1e3 | 100 | 10 | 1 |
| Total simulation time (s) | 1e6 | 1e5 | 1e4 | 1000 | 100 |

Table 1 Injection and simulation times at various Peclet numbers

A concentration signal C(t) or outflow of solute QC (t) = C(t) U (see Figure 4) is obtained for each flow velocity.
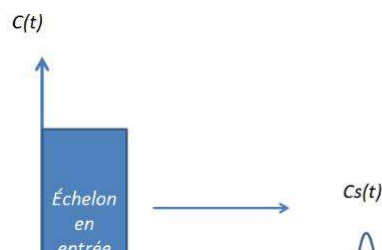
Figure 4 Example of output concentration profile as a function of time C(t)

The velocity field is not homogeneous at the output of the simulation domain, the concentration at the output is not directly integrated on the output edge. The concentration value has the x coordinate and at time t and l the width of the exit edge). It is necessary to integrate according to the flow, i.e.:

$$C(t) = \frac{1}{\overline{U}} \int_l U_x C_x(t) dl$$

with U the average output speed.

**Darcy scale 1D model**
To evaluate the dispersion coefficient, it is sought to reproduce the reference curves using a 1D model (for each flow velocity) by adjusting the dispersion coefficient D*. The 1D transport of a concentration C can be solved on the Darcy scale using the equation:

$$\varepsilon \frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = \varepsilon D^* \frac{\partial^2 C}{\partial x^2}$$

This equation is almost identical to transport at the microscopic scale with however the porosity " and the coefficient of dispersion D . The 1D model of transport allowing to solve this equation will be developed under COMSOL (by building a 1D model of length equivalent to the A correlation can be found by using the values D as a function of U to estimate the value of the coefficient for any value of U.

A few tips....For a first estimate of the dispersion coefficient, please refer to Figure 5 where the changes in the longitudinal dispersion coefficients (flow direction) are given as a function of the Peclet number. It is recalled that effective dispersion at low Peclet number is lower than molecular diffusion. This is due to the tortuosity of the medium which penalizes transport and slows down diffusion. When the Peclet number increases, then the dispersion is a function of $Pe^\gamma$ with $1 < \gamma < 2$.

To impose an input slot, define the following relationship:
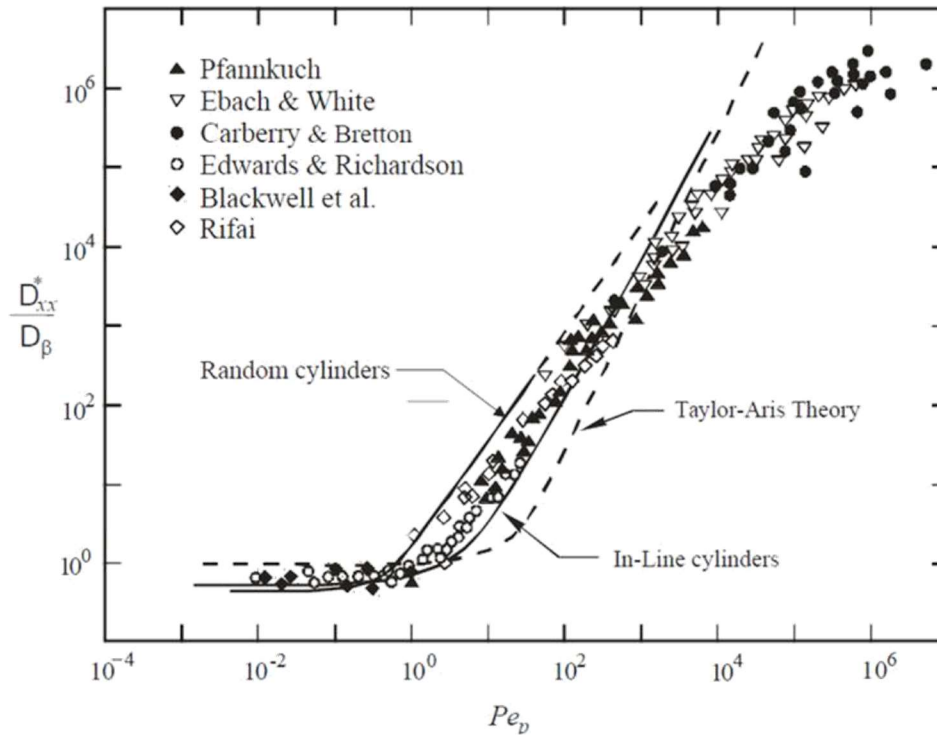
$$if\,(t{<}tps\,,1\,,0)$$

Figure 5 Longitudinal dispersion coefficient as a function of the Peclet number

## 2.2 Heterogeneous medium

### 2.2.1 Determination of the properties of the heterogeneous medium

We consider in this part the second sample of porous medium called heterogeneous presenting a fast zone (a sinusoidal channel) and a slow zone (tangle of close cylinders), see Figure 6. In the same way as for scenario 1, we seek to scale using the gamma.mph sample le.
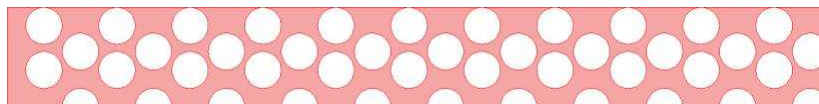


Figure 6: Heterogeneous medium: The dimensions are L=0.05625m, l=0.00675m, the cylinders have a diameter of 0.0025m

### 2.2.2 Calculation of permeability K

Same as section 1.1.1.

### 2.2.3 Calculation of the dispersion curve D (U)

Plot of reference curves          Same as section 1.1.2.

**Darcy scale 1D model**
For this second sample, a double-medium effect can be observed with a slow flow rate zone (upper part of the sample) and a fast flow zone (lower part). The simplified 1D model proposed in the previous part (known as the local equilibrium model) is not adapted to this new environment and it is necessary to resort to a two-equation model, the so-called local non-equilibrium model.

It is considered in this model that there are two distinct zones and it is therefore necessary to follow 2 concentrations, a concentration in the mobile phase $C_M$ occupying the mobile porosity $\varepsilon_M$ and a concentration $C_{im}$ in the immobile phase $C_{im}$ occupying the immobile porosity $\varepsilon_{im}$, with of course the equality $\varepsilon = \varepsilon_M + \varepsilon_{im}$. The system has two equations and can be written:

$$\frac{\varepsilon_M \partial C_M}{\partial t} + V\frac{\partial C_M}{\partial x} = \varepsilon_M D^* \frac{\partial^2 C_M}{\partial x^2} - \alpha(C_M - C_{im})$$

$$\frac{\varepsilon_{im} \partial C_{im}}{\partial t} = \alpha(C_M - C_{im})$$

The exchange between the two zones is characterized by an exchange speed that should be determined (depending on the speed or not, it's up to you to explore the space of parameters). We can start from the 1D model built previously by adding the second equation.

**A few tips....**
If you want to program the term $\alpha(CM - Cim)$ , it should be written in the R term of a convection/diffusion equation: if($C_M > 0$, $\alpha(CM - Cim)$,0). This avoids numerical oscillations when Cm becomes slightly lower than 0 during simulation.
To facilitate the calibration of the model, we can proceed step by step. It is for example possible to adjust the temporal position of the concentration peak by adjusting $\varepsilon_M$ and $\varepsilon_{im}$, then the coefficient D for the spreading and finally the coefficient for the residual concentration at the end of the event.

## 4 COMSOL guide

To simulate transport on a sample

For each con guration (number of Peclet):

1. Impose in input the speed allowing to obtain the number of Peclet reported in the table.

2. Solve the flow (stationary) then the transport in the medium by convection-diffusion:

   (a) slot time in Component 1 -> Laminar Flow -> Inlet 1 and in Component 1 -> Transport Of Diluted Species -> Inflow 1.

   (b) the simulation time in Study 1 -> Step 2: Time Dependent

   (c) Create Output Average Concentration Temporal Table Results -> Derived Values -> Line Average 1 (right click) -> Evaluate

   (d) Visualize the output curve of the domain Results -> 1D Plot Group 1 -> Table Graph 1

3. Use the local equilibrium formulation of the macroscopic 1D model and determine the coefficient of dispersion allowing to observe the output signal QC (t).