Mass Transport Processes in Porous Media
Part II – Numerical Simulation

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01 July 2011, TU Dresden, Lecture for Hydro-system Analysis
Hoersaalzentrum 403H, 11:30 – 12:40 and 13:15 – 14:30.

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Topics for today

- Basic procedure of numerical simulation
- A 2D mass transport example in MatLab
  - Mesh data-structure
  - Assembly
  - Boundary conditions
  - Source term
- Implicit and explicit scheme
- Peclet and Courant numbers
- Stability and accuracy control

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Basic procedure of FEM simulation

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Basic procedure of FEM simulation

Pre-processing
Mesh
Time loop
ST IC BC
Assembly
Solve Ax=b
Output result
Post-Processing (Visualization)

In simple words, we convert the PDE from

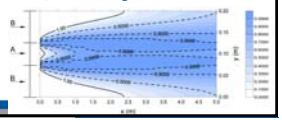
$$\frac{\partial c}{\partial t} + \nabla \cdot \left(-D\,\nabla \vec{c} + \vec{v}\,c\right) = s.$$

, using the topology:

, so that it is converted to linear equation Ax = b:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \cdot \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \cdot \\ b_m \end{bmatrix}$$

, and solve it, so that we get:



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Let's show it in a MatLab script.

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Software preparation

OpenGeoSys to run the model
Recommended version >= 5.0.13

Paraview to view the results
Freely downloadable from:
http://www.paraview.org/paraview/resources/software.html

A good Notepad program to edit ASCII files
Eg. Notepad++, freely downloadable from:
http://notepad-plus-plus.org/release/5.8.7

The OGS executable file for windows users are located at **\all_data\OGS**

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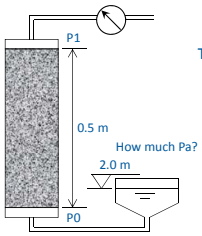
Exercise 1: Darcy flow experiment Using liquid flow

Already provided

Keep the 1 m3/d flow rate.
How much Pressure it will be?



- The 1D mesh file. 1d_darcy_liq.msh
- The time step setting. 1d_darcy_liq.tim
- The solid density. 1d_darcy_liq.msp

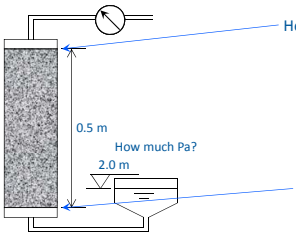
TODO List

- We use LIQUID_FLOW.
  - change *.pcs file
- Fixed pressure boundaries, using PRESSURE1.
  - change 1d_darcy_liq.bc file
- Fixed pressure initial condition.
  - change 1d_darcy_liq.ic file
- The permeability and viscosity has been given, give your flow rate.
  - Check 1d_darcy_liq.mmp, .mfp and .st file
- We want to print out the pressure values
  - set 1d_darcy_liq.out file
- Run OGS and compare your result to your Ex 1.1 result.

Exercise 1: Darcy flow experiment Using liquid flow

My simulation shows:

Keep the same flow rate.
How much Pa it will be?

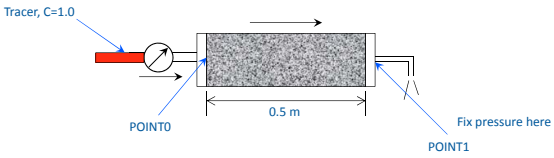


Here is 99947.5Pa

Here is 10240 Pa

Do you get the same thing?

Exercise 2: Conservative mass transport



Already provided

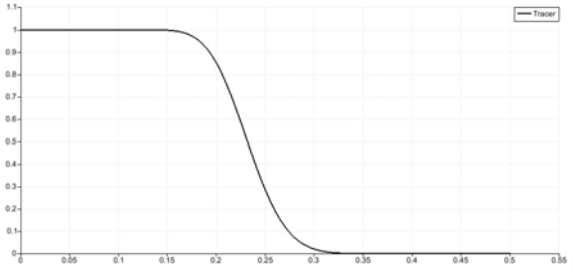
- 1d_cons_trans.gli
- 1d_cons_trans.msh
- 1d_cons_trans.mmp
- 1d_cons_trans.msp
- 1d_cons_trans.mfp
- 1d_cons_trans.tim
- 1d_cons_trans.num

TODO List

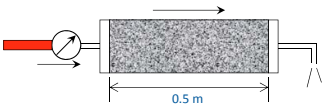
- Add a MASS_TRANSPORT process
  - change 1d_cons_trans.pcs file
- Define the transported components.
  - change 1d_cons_trans.mcp file
- Set a fixed concentration boundaries.
  - change 1d_cons_trans.bc file
- Set initial concentration to zero.
  - change 1d_cons_trans.ic file
- We also print out the concentration values.
  - set 1d_cons_trans.out file

Exercise 2: Conservative mass transport

My simulation shows the following at 5th output, that time is 5*20*60/86400 = 0.069 days. Check with the flow rate.



Peclet and Courant number



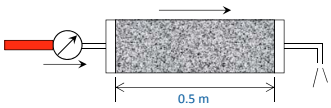
Peclet number: $Pe = \frac{Lv}{D}$ What's the unit of Pe?

Physical meaning: The ratio of advection part versus dispersion part!

Courant number: $Cr = \frac{v\Delta t}{\Delta x} \leq 1$

Physical meaning: A particle can not travel more than one grid!

Exercise 3: Peclet and Courant number



Analytical solution for Ex 3:

$$C = \frac{C_0}{2}[erfc(\frac{L - v_x t}{2\sqrt{D_L t}}) + exp(\frac{v_x L}{D_L})erfc(\frac{L + v_x t}{2\sqrt{D_L t}})]$$

Solution is provided under: \all_data\exercises\ex_3\analytical

Both maple script and result data file.

Make some oscillation in our model:

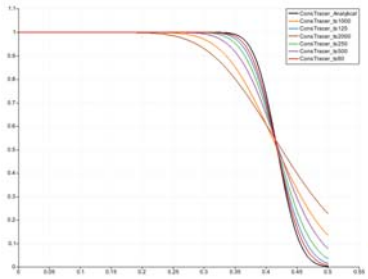
Let's use the current velocity and grid settings

How big the time step size will be enough? (Change your TIM file.)

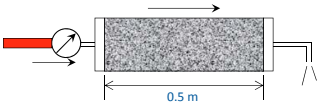
If we want to keep Courant number around one.

Exercise 3: Peclet and Courant number

Be careful, you can induce numerical dispersion by setting a large time step.



Exercise 4: Sorption isotherm Henry



Already provided

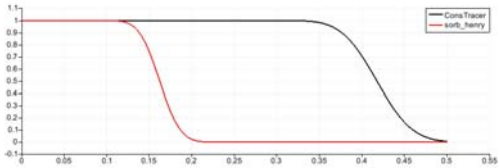
- 1d_henry.gli
- 1d_henry.msh
- 1d_henry.mmp
- 1d_henry.msp
- 1d_henry.mfp
- 1d_henry.tim
- 1d_henry.num

TODO List

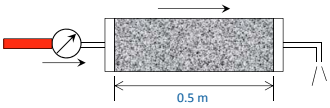
- Give two MASS_TRANSPORT process
  - change 1d_henry.pcs file
- Define the 2nd sorption components.
  - change 1d_henry.mcp file
- Set a fixed concentration boundaries also for 2nd component.
  - change 1d_henry.bc file
- Set initial concentration to zero.
  - change 1d_henry.ic file
- Print out the 2nd component concentration.
  - set 1d_henry.out file

Exercise 4: Sorption isotherm Henry

Are the curves same as you have estimated?



Exercise 5: Sorption isotherm Freundlich



Already provided

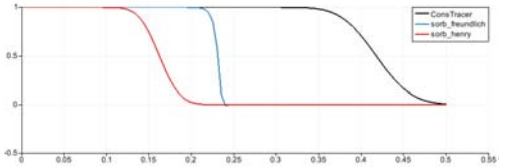
- 1d_freundlich.gli
- 1d_freundlich.msh
- 1d_freundlich.mmp
- 1d_freundlich.msp
- 1d_freundlich.mfp
- 1d_freundlich.tim
- 1d_freundlich.num

TODO List

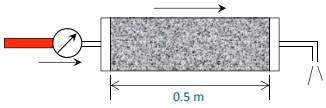
- Give three MASS_TRANSPORT process
  - change 1d_freundlich.pcs file
- Define the 3rd sorption components.
  - change 1d_freundlich.mcp file
- Set a fixed concentration boundaries also for 3rd component.
  - change 1d_freundlich.bc file
- Set initial concentration to zero.
  - change 1d_freundlich.ic file
- Print out the 3rd component concentration.
  - set 1d_freundlich.out file

Exercise 5: Sorption isotherm Freundlich

Are the curves same as you have estimated?



Exercise 6: Sorption isotherm Langmuir



Already provided

- 1d_langmuir.gli
- 1d_langmuir.msh
- 1d_langmuir.mmp
- 1d_langmuir.msp
- 1d_langmuir.mfp
- 1d_langmuir.tim
- 1d_langmuir.num

TODO List

- Add the 4th MASS_TRANSPORT process
  - change 1d_langmuir.pcs file
- Define the 4nd sorption components.
  - change 1d_langmuir.mcp file
- Set a fixed concentration boundaries also for 4th component.
  - change 1d_langmuir.bc file
- Set initial concentration to zero.
  - change 1d_langmuir.ic file
- Print out the 4th component concentration.
  - set 1d_langmuir.out file

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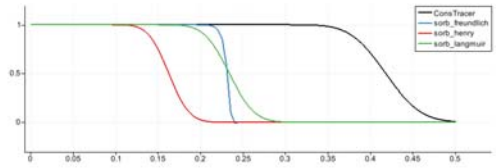
Exercise 6: Sorption isotherm Langmuir

Are the curves same as you have estimated?



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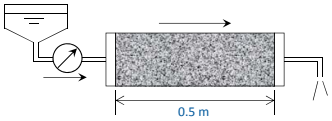
Exercise 7: Sorption isotherm 1st order decay



TODO List

- Add the 5th MASS_TRANSPORT process
  - change 1d_decay.pcs file
- Define the 5th decay components.
  - change 1d_decay.mcp file
- Set a fixed concentration boundaries also for 5th component.
  - change 1d_decay.bc file
- Set initial concentration to zero.
  - change 1d_decay.ic file
- Print out the 5th component concentration.
  - set 1d_decay.out file

Let's assume it undergoes both decay and Henry sorption

With K_D = 6.8e-4 m3/kg
And λ = 2.0e-5 1/sec
Half-life ≈ 0.5 days

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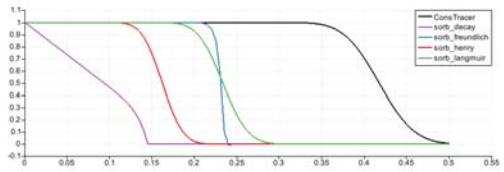
Exercise 7: Sorption isotherm with 1st oder decay

Are the curves same as you have estimated?



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That's a lot for today. Hope you enjoyed.
Thanks for your attention.