Flow123d tutorial 2 – "1D column transport"

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1 Description and input

This is a variant of O1_column.yaml. The user will learn how to:

- Use flux boundary conditions;
- Set up the advective transport model.

For the fluid flow model we change the atmospheric pressure on the surface to the more realistic infiltration 200 mm/yr (= 6.34e-9 m/s):

```
- region: .surface
 bc_type: total_flux
 bc_flux: 6.34E-09
```

In the resulting file water_balance.txt we can see that the value of the input and output flux changes to 6.34e-8. The visual results are similar to the case O1_column.yaml.

Next we demonstrate a simulation of the transport of a tracer. The equation of advective transport (no diffusion/dispersion) is specified by:

```
solute_equation: !Coupling_OperatorSplitting
transport: !Solute_Advection_FV
```

The boundary condition of concentration is prescribed on the surface region:

```
input_fields:
    region: .surface
    bc_conc: 100
```

The default type of boundary condition is inflow, i.e. prescribed concentration is applied where water flows into the domain.

We provide the name of the transported substance (in general there can be multiple transported substances):

substances: 0-18

The end time of the simulation is set in the section time to value 1e10 second (381 years):

time:

end_time: 1e10

The output files can be generated for specific time values. We set the time step for output to 1e8 second (=3 years and 2 months):

output_stream:
 time_step: 1e8

Finally, we turn on computation of mass balance with cumulative sums over the simulation time interval.

balance:

cumulative: true

2 Results

The results of the mass balance computation are in the output folder in the file mass_balance.txt. The evolution of concentration is depicted in Figure 1. A selected part of numerical results of mass balance is in the Table 1. On the region "surface", the mass flux of the tracer is still identical $(6 \times 10\text{-}6 \text{ kg/s})$. On "tunnel", the mass flux is zero at the beginning and then it changes within around 100 years to the opposite value of inflow $-6 \times 10\text{-}6 \text{ kg/s}$. Figure 2 depicts results from the file mass_balance.txt for mass transported through the boundaries "surface" and "tunnel" and in the volume of "rock".

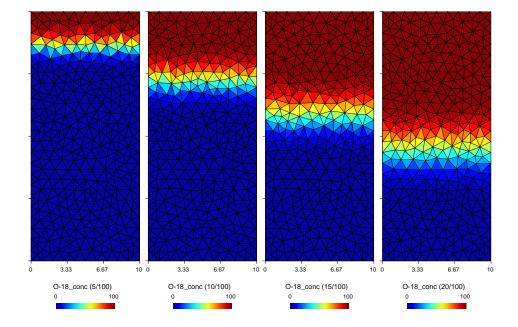


Figure 1: Tracer concentration after 5, 10, 15 and 20 time steps.

time	region	quantity [kg]	flux	flux_in	flux_out	mass	error
3.9e + 09	rock	O-18	0	0	0	22654.4	0
3.9e+09	.surface	O-18	6.34 e-06	6.34 e-06	0	0	0
3.9e+09	.tunnel	O-18	-4.99e-06	0	-4.99e-06	0	0
3.9e + 09	IMPLICIT BOUNDARY	O-18	-1.02e-19	0	-1.02e-19	0	
3.9e + 09	ALL	O-18	1.34 e-06	6.34 e-06	-4.99e-06	22654.4	-5.78e-10
4e + 09	rock	O-18	0	0	0	22774.9	0
4e + 09	.surface	O-18	6.34 e-06	6.34 e-06	0	0	0
4e + 09	.tunnel	O-18	-5.39e-06	0	-5.39e-06	0	0
4e + 09	IMPLICIT BOUNDARY	O-18	-1.02e-19	0	-1.02e-19	0	0
4e + 09	ALL	O-18	9.40 e - 07	6.34 e-06	-5.39e-06	22774.9	-6.03e-10

Table 1: Illustration of the results in mass_balance.txt - selected columns in two time steps.

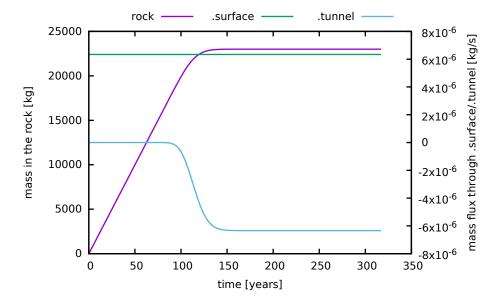


Figure 2: Results of evolution of mass in the volume and flux through boundaries.

3 The control file

Below is the complete YAML source.

```
flow123d_version: 1.8.9
problem: !Coupling_Sequential
  description: Example 1 of real locality - column 1D model with transport
  mesh:
    mesh_file: ./01_mesh.msh
```

```
flow_equation: !Flow_Darcy_MH
 nonlinear_solver:
   linear_solver: !Petsc
     a_tol: 1e-15
     r_tol: 1e-15
  input_fields:
   - region: rock
     conductivity: 1e-8
    - region: .tunnel
     bc_type: dirichlet
     bc_pressure: 0
    - region: .surface
     bc_type: total_flux
     bc_flux: 6.34E-09
 balance: true
 output:
    output_stream:
     file: flow.msh
     format: !gmsh
        variant: ascii
    output_fields:
     - piezo_head_p0
      - pressure_p0
      - pressure_p1
      - velocity_p0
solute_equation: !Coupling_OperatorSplitting
 transport: !Solute_Advection_FV
    input_fields:
      - region: .surface
        bc_conc: 100
  substances: 0-18
 time:
    end_time: 1e10
 output_stream:
   time_step: 1e8
   file: transport.msh
   format: !gmsh
     variant: ascii
 balance:
    cumulative: true
```