Flow123d tutorial 2 – "1D column transport"

Contents

1 Description and input

This is a variant of `01_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 `01_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: O-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 × 10-6 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 × 10-6 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".

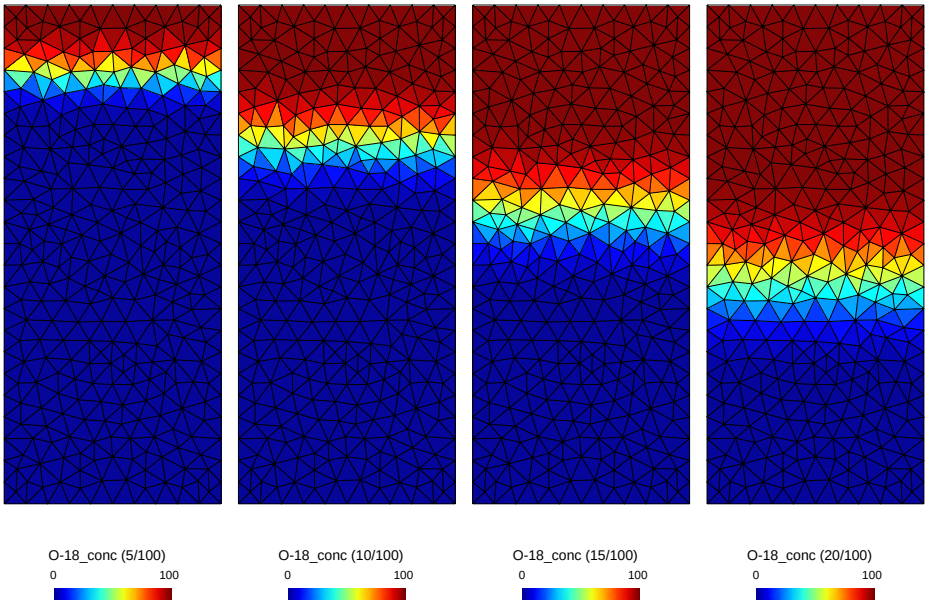

Figure 1: Tracer concentration after 5, 10, 15 and 20 time steps.

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	6.34e-06	6.34e-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	1.34e-06	6.34e-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	6.34e-06	6.34e-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	9.40e-07	6.34e-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.

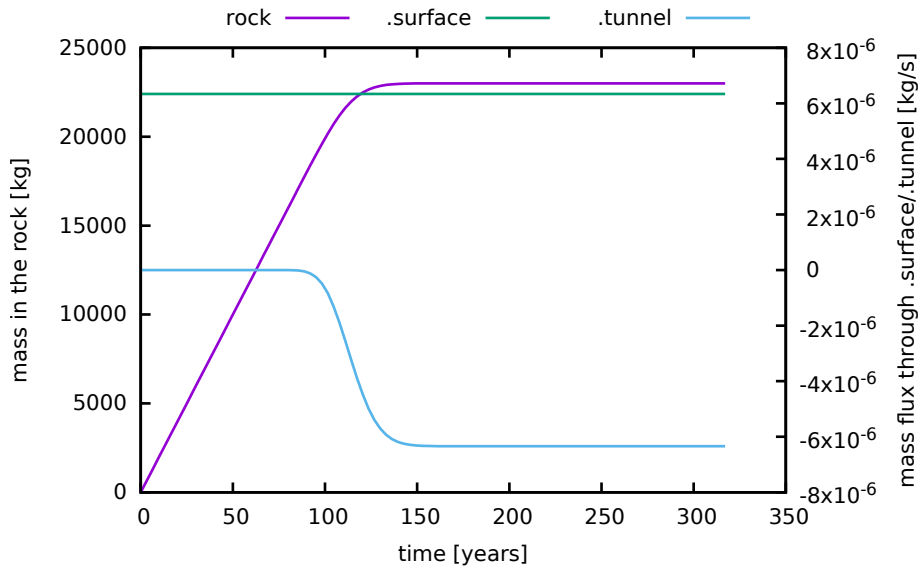

Figure 2: Results of evolution of mass in the volume and flux through boundaries.

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: O-18
  time:
    end_time: 1e10
  output_stream:
    time_step: 1e8
    file: transport.msh
    format: !gmsh
      variant: ascii
  balance:
    cumulative: true
```