Flow123d tutorial 3 – "1D column transport"

Contents

1 Description and input

This is a variant of `01_column.yaml` and `02_column_infiltration.yaml`. See therein for details.

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 any number of 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 1e7 second (=3.8 months):

```
output_stream:
  time_step: 1e7
```

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".

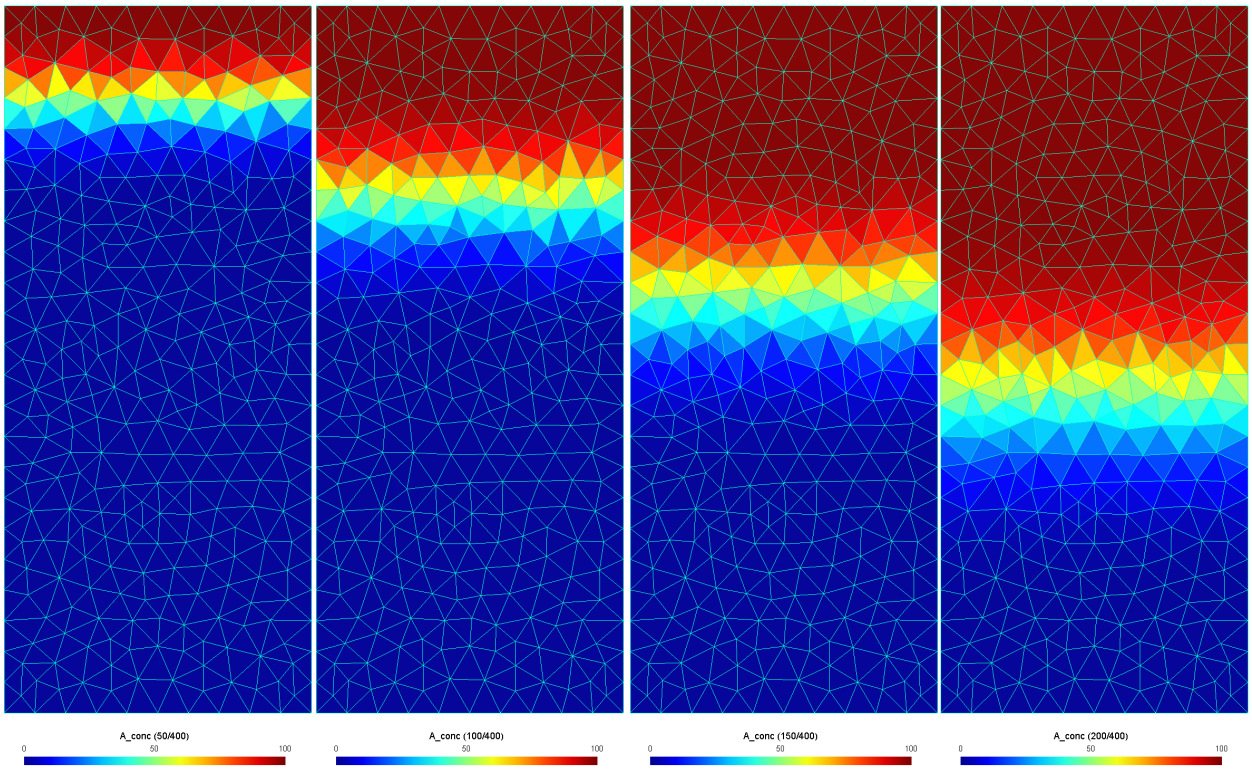

Figure 1: Results of transport.

time	region	quantity [kg]	flux	flux_in	flux_out	mass	error
3.96E+09	rock	A	0	0	0	22544.1	0
3.96E+09	.surface	A	6.34E-06	6.34E-06	0	0	0
3.96E+09	.tunnel	A	-4.88E-06	0	-4.88E-06	0	0
3.96E+09	IMPLICIT BOUNDARY	A	-1.02E-19	0	-1.02E-19	0	0

time	region	quantity [kg]	flux	flux_in	flux_out	mass	error
3.96E+09	ALL	A	1.46E-06	6.34E-06	-4.88E-06	22544.1	-7.39E-10
3.97E+09	rock	A	0	0	0	22558.7	0
3.97E+09	.surface	A	6.34E-06	6.34E-06	0	0	0
3.97E+09	.tunnel	A	-4.92E-06	0	-4.92E-06	0	0
3.97E+09	IMPLICIT BOUNDARY	A	-1.02E-19	0	-1.02E-19	0	0
3.97E+09	ALL	A	1.42E-06	6.34E-06	-4.92E-06	22558.7	-7.53E-10

Table 1: Illustration of the results in "water_balanced.txt" – selected columns in two time steps (edited table, extract from the file).

3 The control file

Below is the complete YAML file `03_column_transport.yaml`.

```
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
```

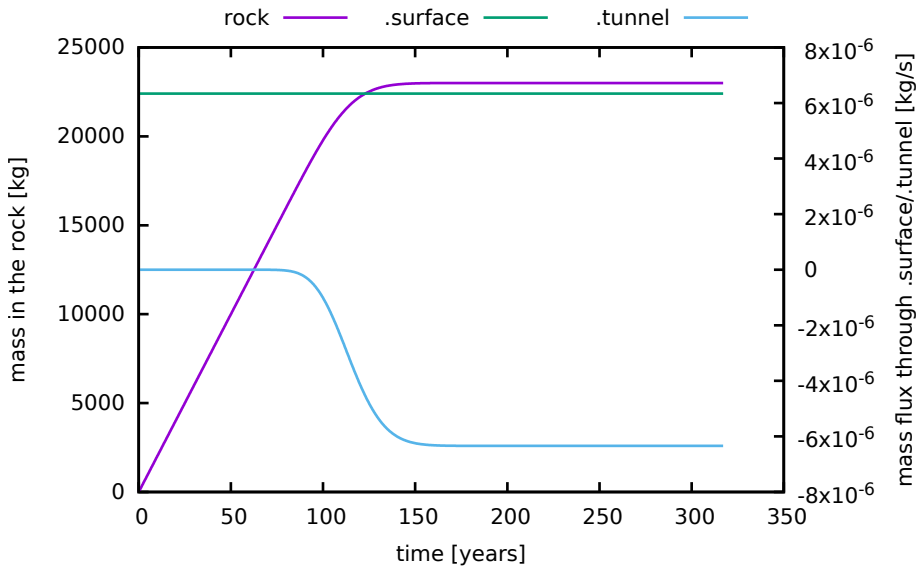

Figure 2: Results of evolution of mass in the volume and flux through boundaries.

```
transport: !Solute_Advection_FV
  input_fields:
    - region: .surface
      bc_conc: 100
      time: 0
    - region: .surface
      bc_conc: 100
      time: 1e7
substances:
  - tracer
time:
  end_time: 1e10
output_stream:
  time_step: 1e7
  file: transport.msh
  format: !gmsh
    variant: ascii
balance:
  cumulative: true
```