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 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".

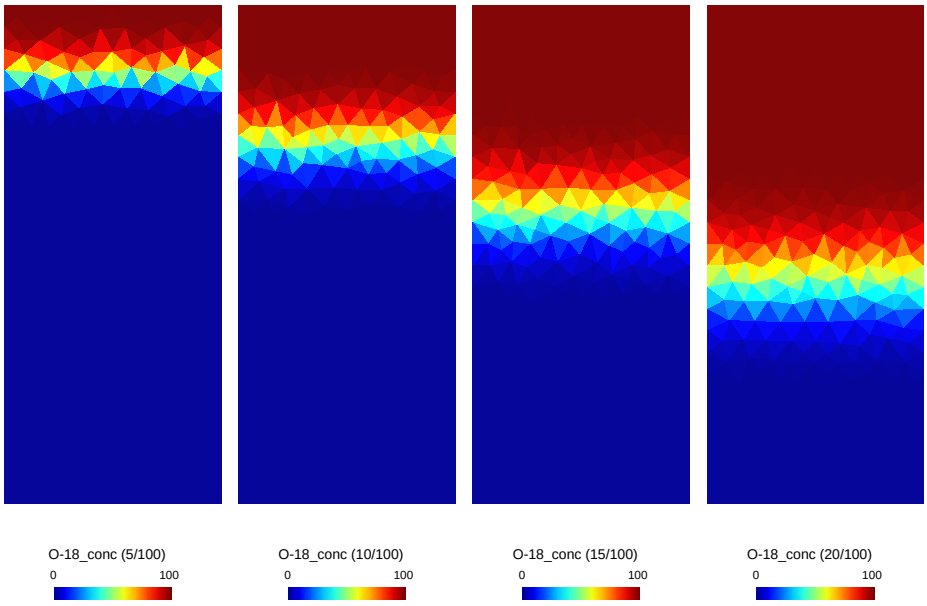

Figure 1: Tracer concentration after 5, 10, 15 and 20 time steps.

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

time	region	quantity [kg]	flux	flux_in	flux_out	mass	error
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 `water_balanced.txt` – selected columns in two time steps.

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
    transport: !Solute_Advection_FV
      input_fields:
        - region: .surface
          bc_conc: 100
    substances:
```

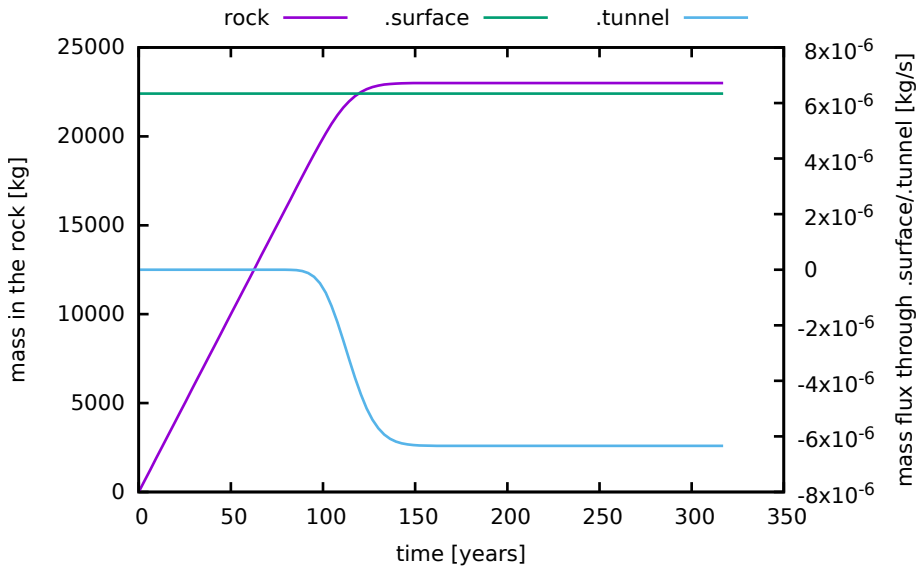

Figure 2: Results of evolution of mass in the volume and flux through boundaries.

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