1 Advection-diffusion-reaction equation in Flow123d

1.1 Physical model

On the domain Ω^d of dimension $d \in \{1,2,3\}$, we consider a system of mass balance equations in the following form:

$$\partial_t(\vartheta c^i) + \mathrm{div}(\boldsymbol{q} c^i) - \mathrm{div}(\vartheta \mathbb{D}^i \nabla c^i) = F(c^1, \dots, c^s) \quad \text{on } \Omega^d. \tag{1}$$

The principal unknown is the concentration c^i $[kg/m^3]$ of a substance $i \in \{1, \dots, s\}$, which means weight of the substance in unit volume of the water. Other quantities are:

- ϑ $[-]$ is the porosity, i.e. fraction of space occupied by water and the total volume.
- $\boldsymbol{q}$ $[ms^{-1}]$ is the Darcy flux or the *macroscopic* water velocity. It is related to the *microscopic* water velocity $\boldsymbol{v}$ by the relation $\boldsymbol{q} = \vartheta \boldsymbol{v}$.
- The hydrodynamic dispersivity tensor $\mathbb{D}^i$ $[m^2 s^{-1}]$ has the form

  $$\mathbb{D}^i = D^i_m \tau \mathbb{I} + |\boldsymbol{v}| \big(\alpha^i_T \mathbb{I} + (\alpha^i_L - \alpha^i_T)\big) \frac{\boldsymbol{v} \times \boldsymbol{v}}{|\boldsymbol{v}|^2},$$

  which models (isotropic) molecular diffusion, and dispersion in longitudal and transversal direction to the flow. Here D^i_m $[m^2 s^{-1}]$ is the molecular diffusion coefficient of the i-th substance (usual magnitude in clear water is 10^{-9}), $\tau = \vartheta^{1/3}$ is the tortuosity (by Millington and Quirk [1961]), α^i_L and α^i_T is the longitudal and the transversal dispersivity $[m]$, respectively.
- The reaction term $F(\dots)$ is currently neglected.

In lower dimensions $d = 1, 2$, equation (1) represents transport processes in planar or channel fractures whose cross-cut δ^d ($[m]$ for 2D and $[m^2]$ for 1D) is negligible with respect to the dimensions of the physical domain.

Boundary conditions. The physical boundary $\partial\Omega^d$ is decomposed into two parts:

$$\Gamma_D(t) = \{\boldsymbol{x} \in \partial\Omega^d \,|\, \boldsymbol{q}(t,\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x}) < 0\},$$
$$\Gamma_N(t) = \{\boldsymbol{x} \in \partial\Omega^d \,|\, \boldsymbol{q}(t,\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x}) \geq 0\},$$

where $\boldsymbol{n}$ stands for the unit outward normal vector to $\partial\Omega^d$. On the inflow part Γ_D, concentrations have to be prescribed (Dirichlet boundary condition):

$$c^i(t,\boldsymbol{x}) = c^i_D(t,\boldsymbol{x}) \text{ on } \Gamma_D(t),$$

while on Γ_N we impose homogeneous Neumann boundary condition:

$$-\mathbb{D}^i(t,\boldsymbol{x}) \nabla c^i(t,\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x}) = 0 \text{ on } \Gamma_N(t).$$

Communication between dimensions. Transport of substances is considered also on interfaces of physical domains with adjacent dimensions. Denoting c_{d+1}, c_d the concentration of a given substance in Ω^{d+1} and Ω^d, respectively, the comunication on the interface between Ω^{d+1} and Ω^d is described by:

$$q^c = \sigma^c(c_{d+1} - c_d) + \begin{cases} q^w c_{d+1} & \text{if } q^w \geq 0, \\ q^w c_d & \text{if } q^w < 0, \end{cases} \tag{2}$$

where q^c is the concentration flux from $d+1$ to d dimensions, σ^c is a transition parameter, q^w is water flux from $d+1$ to d dimensions. Equation (2) is incorporated as a boundary condition for the problem on Ω^{d+1}:

$$-\mathbb{D}\nabla c_{d+1} \cdot \boldsymbol{n} + q^w c_{d+1} = q^c$$

and a source term in Ω^d:

$$f_d^c = \frac{\delta_{d+1}}{\delta_d}(\sigma^c + |q^w|)(c_{d+1} - c_d).$$