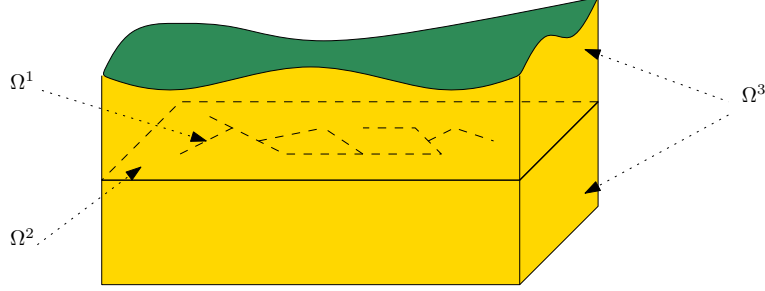


# 1 Transport of substances

Flow123d can simulate transport of substances dissolved in water. The transport mechanism is governed by the *advection*, and the *hydrodynamic dispersion*. Moreover the substances can move between ground and fractures.



## 1.1 Physical model

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

$$\delta^d \partial_t (\vartheta c^i) + \operatorname{div}(\mathbf{q}^d c^i) - \operatorname{div}(\vartheta \delta^d \mathbb{D}^i \nabla c^i) = F_S + F_C(c^i) + F_R(c^1, \dots, c^s). \quad (1)$$

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:

- $\delta^d$  represents the cross-cut, i.e.  $\delta^1$  [ $m^2$ ] stands for the cross-section,  $\delta^2$  [ $m$ ] for the thickness, and  $\delta^3 = 1$  [ $-$ ].
- $\vartheta$  [ $-$ ] is the porosity, i.e. fraction of space occupied by water and the total volume.
- $\mathbf{q}^d$  [ $m^{4-d}\ s^{-1}$ ] is the Darcy flux, defined as the product of the *macroscopic* water velocity and the cross-cut. It is related to the *microscopic* water velocity  $\mathbf{v}$  [ $m\ s^{-1}$ ] by the relation  $\mathbf{q}^d = \vartheta \delta^d \mathbf{v}$ .
- The hydrodynamic dispersivity tensor  $\mathbb{D}^i$  [ $m^2\ s^{-1}$ ] has the form

$$\mathbb{D}^i = D_m^i \tau \mathbb{I} + |\mathbf{v}| (\alpha_L^i \mathbb{I} + (\alpha_L^i - \alpha_T^i) \frac{\mathbf{v} \otimes \mathbf{v}}{|\mathbf{v}|^2}),$$

representing (isotropic) molecular diffusion, and dispersion in longitudinal and transversal direction to the flow. Here  $D_m^i$  [ $m^2\ s^{-1}$ ] 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]),  $\alpha_L^i$  and  $\alpha_T^i$  is the longitudinal and the transversal dispersivity [ $m$ ], respectively. The value of  $D_m^i$  for specific substances can be found in literature (see e.g. Císlerová and Vogel [1998]). For instructions on how to determine  $\alpha_L^i$ ,  $\alpha_T^i$  we refer to De Marsily [1986], Domenico and Schwartz [1990].

- $F_S$  [ $kg\ m^{-d}\ s^{-1}$ ] is the density of concentration sources.

- $F_C(c^i)$  [ $kg\ m^{-d}\ s^{-1}$ ] is the density of concentration sources due to exchange between regions with different dimensions, see (3) below.
- The reaction term  $F_R(\dots)$  [ $kg\ m^{-d}\ s^{-1}$ ] is currently neglected.

**Initial and boundary conditions.** At time  $t = 0$  the concentration is determined by the initial condition

$$c^i(0, \mathbf{x}) = c_0^i(\mathbf{x}).$$

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

$$\begin{aligned}\Gamma_D(t) &= \{\mathbf{x} \in \partial\Omega^d \mid \mathbf{q}(t, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) < 0\}, \\ \Gamma_N(t) &= \{\mathbf{x} \in \partial\Omega^d \mid \mathbf{q}(t, \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) \geq 0\},\end{aligned}$$

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

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

while on  $\Gamma_N$  we impose homogeneous Neumann boundary condition:

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

**Communication between dimensions.** Transport of substances is considered also on interfaces of physical domains with adjacent dimensions (i.e. 3D-2D and 2D-1D, but not 3D-1D). Denoting  $c_{d+1}$ ,  $c_d$  the concentration of a given substance in  $\Omega^{d+1}$  and  $\Omega^d$ , respectively, the communication on the interface between  $\Omega^{d+1}$  and  $\Omega^d$  is described by:

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

where

- $q^c$  [ $kg\ m^{-d}\ s^{-1}$ ] is the density of concentration flux from  $\Omega^{d+1}$  to  $\Omega^d$ ,
- $\sigma^c$  [ $m\ s^{-1}$ ] is a transition parameter, (hint:  $\sigma^c \approx \frac{\delta^{d+1}}{\delta^d}|\mathbb{D}|$ ?)
- $q^w$  [ $m^{3-d}\ s^{-1}$ ] is the water flux from  $\Omega^{d+1}$  to  $\Omega^d$ .

Equation (2) is incorporated as a boundary condition for the problem on  $\Omega^{d+1}$ :

$$-\vartheta\delta^{d+1}\mathbb{D}\nabla c_{d+1} \cdot \mathbf{n} + q^w c_{d+1} = q^c,$$

and a source term in  $\Omega^d$ :

$$F_d^c = (\sigma^c + |q^w|)(c_{d+1} - c_d). \quad (3)$$

## 2 Numerical solution

For the numerical approximation of the advection-dispersion equation (1) we distinguish whether the dispersion  $\mathbb{D}$  is present or not. Since the true solution has qualitatively different properties, we also choose different numerical methods for each case.

## 2.1 Pure advection

## 2.2 Advection with dispersion

For the general case we use the discontinuous Galerkin space approximation and implicit Euler time discretization. Let  $\tau, h$  be the time step and the space discretization parameter, respectively. We assume that  $\mathcal{T}_h^d$  is a regular partition of the domain  $\Omega^d$  into simplices,  $d = 1, 2, 3$ . We define the set  $\mathcal{E}_h^d$  of all edges of elements in  $\mathcal{T}_h$  (triangles for  $d = 3$ , line segments for  $d = 2$  and points for  $d = 1$ ). Further,  $\mathcal{E}_{h,I}^d$  will denote interior edges,  $\mathcal{E}_{h,D}^d(t)$  edges that coincide with  $\Gamma_D^d(t)$  and  $\mathcal{E}_{h,C}^d$  stands for edges on interface with  $\Omega^{d-1}$ .

Let us fix one substance and the space dimension  $d$ . At each time instant  $t_k = k\tau$  we search for the concentration field  $c_d^{h,k} \in V_d^h$ , where

$$V_d^h = \{v : \overline{\Omega^d} \rightarrow \mathbb{R} \mid v|_T \in P_1(T) \ \forall T \in \mathcal{T}_h^d\}$$

is the space of functions piecewise affine on the elements of  $\mathcal{T}_h^d$ , possibly discontinuous across the element interfaces. The initial concentration  $c_d^{h,0}$  is set to the projection of the initial data  $c_0$ . For  $k = 1, 2, \dots$ , the discrete problem reads:

$$\left( \vartheta \frac{c_d^{h,k} - c_d^{h,k-1}}{\tau}, v \right)_{\Omega^d} + a_d^{h,k}(c_d^{h,k}, v) = b_d^{h,k}(v) \quad \forall v \in V_d^h.$$

Here  $(f, g)_{\Omega^d} = \int_{\Omega^d} fg$ ,  $c_d^{h,k-1}$  is the solution from the previous time step and the forms  $a_d^{h,k}$ ,  $b_d^{h,k}$  are defined as follows:

$$\begin{aligned} a_d^{h,k}(u, v) &= (\vartheta \mathbb{D} \nabla u, \nabla v)_{\Omega^d} + ((\operatorname{div} \mathbf{q})u, v)_{\Omega^d} + (\mathbf{q} \cdot \nabla u, v)_{\Omega^d} \\ &\quad - \sum_{E \in \mathcal{E}_{h,I}^d} ((\{\vartheta \mathbb{D} \nabla u\}_\omega \cdot \mathbf{n}, [v])_E + (\{\vartheta \mathbb{D} \nabla v\}_\omega \cdot \mathbf{n}, [u])_E) \\ &\quad - \sum_{E \in \mathcal{E}_{h,I}^d} (\mathbf{q} \cdot \mathbf{n} \{v\}_\omega, [u])_E + \sum_{E \in \mathcal{E}_{h,I}^d} \gamma_E ([u], [v])_E + \sum_{E \in \mathcal{E}_{h,D}^d(t_k)} \gamma_E (u, v)_E, \\ b_d^{h,k}(v) &= \sum_{E \in \mathcal{E}_{h,D}^d(t_k)} \gamma_E (c_D, v)_E. \end{aligned}$$

For an interior edge  $E$  we denote by  $T^-(E)$  and  $T^+(E)$  the elements sharing  $E$ . By  $\mathbf{n}$  we mean the unit normal vector to  $E$  pointing from  $T^-(E)$  towards  $T^+(E)$ , the inter-element jump is defined as  $[f] = f|_{T^-(E)} - f|_{T^+(E)}$ , and  $\{f\}_\omega = \omega f|_{T^-(E)} + (1 - \omega) f|_{T^+(E)}$  denotes a weighted average of the quantity  $f$ . The weight  $\omega$  is chosen in a specific way (see Ern et al. [2009] for details) taking into account possible inhomogeneity of  $\mathbb{D}$ . The stabilization parameter  $\gamma_E > 0$  is user dependent; its value affects the inter-element jumps of the solution.

In case that lower dimensional domains ( $\Omega^1, \Omega^2$ ) have complex topology, e.g. if there are more triangles sharing one line segment, then we consider ideal mixing, i.e. the concentration entering the edge through every inlet element ( $\mathbf{q}$  points out of this element) is divided among all outlet elements proportionally to their fluxes.

If there are interfaces between adjacent dimensions, then the following terms are added to the bilinear form and the right hand side, respectively:

$$a_{d,C}^{h,k}(u, v) = \sum_{E \in \mathcal{E}_{h,C}^d} (\sigma^c + (q^w)^-) (u, v)_E - \sum_{T \in \mathcal{T}_h^d \cap \mathcal{E}_{h,C}^{d+1}} \frac{\delta_{d+1}}{\delta_d} (\sigma^c + |q^w|) (u, v)_T,$$

$$b_{d,C}^{h,k}(v) = \sum_{E \in \mathcal{E}_{h,C}^d} (\sigma^c + (q^w)^-) (c_{d-1}^h, v)_E - \sum_{T \in \mathcal{T}_h^d \cap \mathcal{E}_{h,C}^{d+1}} \frac{\delta_{d+1}}{\delta_d} (\sigma^c + |q^w|) (c_{d+1}^h, v)_T.$$

Here we obviously set  $\mathcal{E}_{h,C}^4 = \mathcal{E}_{h,C}^1 = \emptyset$ .

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