OpenGeoSys 6: Implementation of the HC Process

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1 Component Transport Process

[5] [6] [3] [4]

1.1 Mass Diffusion Equation

1.1.1 Balance Equation

This subsection is similar to [1]. Let Ω be a domain, Γ the boundary of Ω. Let C be the concentration and the volume density is described by a function $\phi\rho$, where ϕ is the porosity and ρ is the fluid density. The amount of concentration in the domain can vary within time by two reasons. Firstly, new concentration can accumulate by flow over Γ or secondly it can be generated due to the presence of sources or sinks within Ω. Consequently, the balance reads

$$\frac{\partial}{\partial t}\int_{\Omega}\phi\rho \mathrm{d}x = -\int_{\Gamma}\langle J(x,t)|n(x)\rangle \,\mathrm{d}\sigma + \int_{\Omega} Q(x,t)\mathrm{d}x, \tag{1.1}$$

where $J(x,t)$ is the flow over the boundary, n is normal vector pointing outside of Ω, $\mathrm{d}\sigma$ is an infinitesimal small surface element and $Q(x,t)$ describes sources and sinks within Ω. Further mathematical manipulations leads to

$$\int_{\Omega}\frac{\partial\phi\rho}{\partial t}\mathrm{d}x + \int_{\Gamma}\langle J(x,t)|n(x)\rangle \,\mathrm{d}\sigma - \int_{\Omega} Q(x,t)\mathrm{d}x = 0. \tag{1.2}$$

Applying the theorem of Gauss yields to

$$\int_{\Omega}\frac{\partial\phi\rho}{\partial t}\mathrm{d}x + \int_{\Omega}\operatorname{div} J(x,t)\mathrm{d}x - \int_{\Omega} Q(x,t)\mathrm{d}x = 0. \tag{1.3}$$

Finally,

$$\int_{\Omega}\left[\frac{\partial\phi\rho}{\partial t} + \operatorname{div} J(x,t) - Q(x,t)\right]\mathrm{d}x = 0. \tag{1.4}$$

Since the domain is arbitrary it holds:

$$\frac{\partial\phi\rho}{\partial t} + \operatorname{div} J(x,t) - Q(x,t) = 0. \tag{1.5}$$

1.1.2 Constitutive Law

Depending on the constitutive law that describes the flow J, we obtain the balance equation of the considered process. Important practical laws are

$$J^{(1)} = -\boldsymbol{D}\,\boldsymbol{grad}\,C = -\boldsymbol{D}\nabla C, \tag{1.6}$$

where $\boldsymbol{D}$ is the hydrodynamic dispersion tensor. (1.6) describes diffusive flow and

$$J^{(2)} = qC \quad \text{(where } q \text{ is a Darcy velocity vector)} \tag{1.7}$$

describes advective flow. It is also possible to combine (1.6) and (1.7). The description of the flow by a combination of (1.6) and (1.7) yields to

$$\frac{\partial \phi \rho}{\partial t} - \nabla \cdot [\boldsymbol{D}(x,t)\nabla C(x,t) - qC(x,t)] - Q(x,t) = 0. \tag{1.8}$$

The advective part qC is driven by the Darcy velocity q of the coupled groundwater flow process.

For the process at hand the density is substituted by RC, where R denotes the retardation factor. Finally, the term

$$\phi R \vartheta C \tag{1.9}$$

describing the decay of the chemical species is integrated into the equation which acts similarly to a sink term. Here ϑ is the decay rate. The final mass diffusion equation reads:

$$\frac{\partial}{\partial t}(\phi R C) + \operatorname{div}(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C) + \phi R \vartheta C - Q_C = 0. \tag{1.10}$$

The hydrodynamic dispersion tensor is

$$\boldsymbol{D} = (\phi D_d + \beta_T \|q\|)\,\boldsymbol{I} + (\beta_L - \beta_T)\frac{qq^T}{\|q\|},$$

where

- β_L is the longitudinal dispersivity of chemical species,
- β_T is the transverse dispersivity of chemical species,
- D_d is the molecular diffusion coefficient.

Porosity variations and solid motions are neglected, i.e., $\frac{\partial \phi}{\partial t} = 0$. Furthermore, it is assumed that the retardation factor is not time dependent:

$$\phi R \frac{\partial C}{\partial t} + \operatorname{div}(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C) + \phi R \vartheta C - Q_C = 0 \tag{1.11}$$

1.1.3 Boundary Conditions

$$C = g_D^C \quad \text{on} \quad \Gamma_D \quad \text{(Dirichlet type boundary conditions)} \tag{1.12}$$

$$-\langle \boldsymbol{D}\,\boldsymbol{grad}\,C | n \rangle = g_N^C \quad \text{on} \quad \Gamma_N \quad \text{(Neumann type boundary conditions)} \tag{1.13}$$

1.1.4 Weak Formulation

The integration of the reformulated Neumann type boundary condition, i.e., $\langle \boldsymbol{D}\,\boldsymbol{grad}\,C | n \rangle + g_N^C = 0$, into (1.11), multiplying with arbitrary test functions $v, \bar{v} \in H_0^1(\Omega)$ and integration over Ω results in

$$\begin{aligned} 0 = &\int_\Omega v \cdot \phi \cdot R \cdot \frac{\partial C}{\partial t} \mathrm{d}\Omega + \int_\Omega v \cdot \operatorname{div}(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C)\,\mathrm{d}\Omega \\ &+ \int_\Omega v \cdot [\vartheta \cdot \phi \cdot R \cdot C]\,\mathrm{d}\Omega - \int_\Omega v \cdot Q_C \mathrm{d}\Omega + \int_{\Gamma_N} \bar{v} \cdot \left[\langle \boldsymbol{D}\,\boldsymbol{grad}\,C | n \rangle + g_N^C\right] \mathrm{d}\sigma \end{aligned} \tag{1.14}$$

Integration by parts of the second term in the above equation yields:

$$\int_\Omega v \cdot \operatorname{div}(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C)\,\mathrm{d}\Omega = -\int_\Omega \langle \boldsymbol{grad}\,v | qC - \boldsymbol{D}\,\boldsymbol{grad}\,C \rangle\,\mathrm{d}\Omega + \int_\Omega \operatorname{div}[v\,(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C)]\,\mathrm{d}\Omega \tag{1.15}$$

Using Green's formula for the last term of the above expression

$$\int_\Omega \operatorname{div}\left[v\left(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right)\right]\mathrm{d}\Omega = \oint_\Gamma \langle v\left(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right)|n\rangle\,\mathrm{d}\sigma$$
$$= \int_{\Gamma_D} \langle v\left(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right)|n\rangle\,\mathrm{d}\sigma + \int_{\Gamma_N} \langle v\left(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right)|n\rangle\,\mathrm{d}\sigma$$

and since v vanishes on Γ_D the integral over Γ_D also vanishes, this leads to

(1.16)
$$\int_\Omega v \cdot \operatorname{div}\left(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right)\mathrm{d}\Omega = -\int_\Omega \langle \boldsymbol{grad}\,v | qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\rangle\,\mathrm{d}\Omega + \int_{\Gamma_N} \langle v\left(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right)|n\rangle\,\mathrm{d}\sigma$$

Thus (1.14) reads:

(1.17)
$$0 = \int_\Omega v\cdot\phi\cdot R\cdot\frac{\partial C}{\partial t}\mathrm{d}\Omega - \int_\Omega \langle \boldsymbol{grad}\,v | qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\rangle\,\mathrm{d}\Omega + \int_{\Gamma_N} \langle v\left(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right)|n\rangle\,\mathrm{d}\sigma$$
$$+ \int_\Omega v\cdot\left[\vartheta\cdot\phi\cdot R\cdot C\right]\mathrm{d}\Omega - \int_\Omega v\cdot Q_C\mathrm{d}\Omega + \int_{\Gamma_N} \bar{v}\cdot\left[\langle \boldsymbol{D}\,\boldsymbol{grad}\,C|n\rangle + g_N^C\right]\mathrm{d}\sigma$$

Setting $v = \bar{v}$:

$$0 = \int_\Omega v\cdot\phi\cdot R\cdot\frac{\partial C}{\partial t}\mathrm{d}\Omega - \int_\Omega \langle \boldsymbol{grad}\,v | qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\rangle\,\mathrm{d}\Omega + \int_{\Gamma_N} \langle vqC|n\rangle\,\mathrm{d}\sigma$$
$$+ \int_\Omega v\cdot\left[\vartheta\cdot\phi\cdot R\cdot C\right]\mathrm{d}\Omega - \int_\Omega v\cdot Q_C\mathrm{d}\Omega + \int_{\Gamma_N} v\cdot g_N^C\mathrm{d}\sigma \tag{1.18}$$

1.1.5 Finite Element Discretization

The concentration is approximated by:

$$C \approx \sum N_j^C c_j = N^C c \tag{1.19}$$

using the shape functions N_j^C and time dependent coefficients c_j. Using the shape functions again as test functions (Galerkin principle) the discretization of (1.18)) takes the following form

(1.20)
$$0 = \int_\Omega N_i^C\cdot\phi\cdot R\cdot N_j\frac{\partial c_j}{\partial t}\mathrm{d}\Omega - \int_\Omega \nabla^T N_i^C\cdot q\cdot N_j^C c_j\mathrm{d}\Omega + \int_\Omega \nabla^T N_i^C\boldsymbol{D}\nabla N_j^C c_j\mathrm{d}\Omega + \int_{\Gamma_N}\left(N_i^C q^T N_j^C c_j\right)n\,\mathrm{d}\sigma$$
$$+ \int_\Omega N_i^C\cdot\left[\vartheta\cdot\phi\cdot R\cdot N_j^C c_j\right]\mathrm{d}\Omega - \int_\Omega N_i^C\cdot Q_C\mathrm{d}\Omega + \int_{\Gamma_N} N_i^C\cdot g_N^C\mathrm{d}\sigma$$

This is a set of equations of the form

$$\boldsymbol{C}^{CC}\dot{c} + \boldsymbol{K}^{CC}c + f^C = 0 \tag{1.21}$$

with

$$\boldsymbol{K}_{ij}^{CC} = -\int_\Omega \nabla^T N_i^C\cdot q\cdot N_j^C\mathrm{d}\Omega + \int_\Omega \nabla^T N_i^C\boldsymbol{D}\nabla N_j^C\mathrm{d}\Omega + \int_{\Gamma_N}\left(N_i^C\cdot q^T N_j^C\right)^T n\mathrm{d}\sigma$$
$$+ \int_\Omega N_i^C\cdot\left[\vartheta\cdot\phi\cdot R\cdot N_j^C\right]\mathrm{d}\Omega, \tag{1.22}$$

$$f_i^C = -\int_\Omega N_i^C Q_C\mathrm{d}\Omega + \int_{\Gamma_N} N_i^C g_N^C\mathrm{d}\sigma, \tag{1.23}$$

$$\boldsymbol{C}_{ij}^{CC} = \int_\Omega N_i^C\cdot\phi\cdot R\cdot N_j^C\mathrm{d}\Omega. \tag{1.24}$$

In (1.22) the Darcy velocity q is assumed to be known from the hydrological process. In contrast to this approach pressure p in the Darcy velocity can be expressed as an approximation by shape functions N_i^p

$$q = \frac{\kappa}{\mu} \boldsymbol{grad}\, (p + \varrho \cdot g \cdot z) \approx \frac{\kappa}{\mu} \left(\nabla N_i^p + \varrho \cdot g \cdot e_z\right). \tag{1.25}$$

Thus, some terms of $\boldsymbol{K}_{ij}^{CC}$ are moved to the coupling matrix:

$$\boldsymbol{K}_{ij}^{Cp} = - \int_{\Omega} \nabla^T N_i^C \cdot \frac{\kappa}{\mu} \left(\nabla N_i^p + \varrho \cdot g \cdot e_z\right) \cdot N_j^C \mathrm{d}\Omega \tag{1.26}$$

1.2 Evaluating Dominance of Effects

Substitute variables and coefficients that appear in (1.11): see 7.7 in [2]

$$\phi R \frac{\partial C}{\partial t} = \phi^* \phi_c R^* R_c \left(\frac{\partial C}{\partial t}\right)^* \left(\frac{\partial C}{\partial t}\right)_c = \phi^* \phi_c R^* R_c \left(\frac{\partial C}{\partial t}\right)^* \frac{(\Delta C)_c}{(\Delta t)_c} = \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* \phi_c R_c \frac{(\Delta C)_c}{t_c} \tag{1.27}$$

where $t_c = (\Delta t)_c$.

$$\begin{aligned} \operatorname{div}(qC) &= \frac{\partial qC}{\partial x_i} = \frac{\partial q}{\partial x_i} C + \frac{\partial C}{\partial x_i} q = \left(\frac{\partial q}{\partial x_i}\right)^* \frac{(\Delta q)_c}{L_c^{(q)}} C^* C_c + \left(\frac{\partial C}{\partial x_i}\right)^* \frac{(\Delta C)_c}{L_c^{(C)}} q^* q_c \\ &= \frac{\partial q^*}{\partial x_i^*} C^* \frac{(\Delta q)_c}{L_c^{(q)}} C_c + q^* \frac{\partial C^*}{\partial x_i^*} \frac{q_c (\Delta C)_c}{L_c^{(C)}} \end{aligned} \tag{1.28}$$

$$\begin{aligned} \operatorname{div}(\boldsymbol{D}\, \boldsymbol{grad}\, C) &= \frac{\partial}{\partial x_i} \left(\boldsymbol{D} \frac{\partial C}{\partial x_i}\right) = \left(\frac{\partial}{\partial x_i}\right)^* \frac{1}{L_c^{(C)}} \left(\boldsymbol{D}^* D_c \left(\frac{\partial C}{\partial x_i}\right)^* \frac{(\Delta C)_c}{L_c^{(C)}}\right) \\ &= \frac{\partial}{\partial x_i^*} \left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right) \frac{D_c (\Delta C)_c}{{L_c^{(C)}}^2} \end{aligned} \tag{1.29}$$

$$\phi R \vartheta C = \phi^* \phi_c R^* R_c \vartheta^* \vartheta_c C^* C_c = \phi^* R^* \vartheta^* C^* \phi_c R_c \vartheta_c C_c \tag{1.30}$$

With $L_c^{(C)} = L_c^{(q)} = L_c$

$$\begin{aligned} 0 = {} & \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* \phi_c R_c \frac{(\Delta C)_c}{t_c} + \frac{(\Delta q)_c}{L_c} C_c \frac{\partial q^*}{\partial x_i^*} C^* + \frac{q_c (\Delta C)_c}{L_c} q^* \frac{\partial C^*}{\partial x_i^*} - \frac{D_c (\Delta C)_c}{L_c^2} \frac{\partial}{\partial x_i^*} \left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right) \\ & + \phi_c R_c \vartheta_c C_c \phi^* R^* \vartheta^* C^* \end{aligned} \tag{1.31}$$

$$\begin{aligned} 0 = {} & \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* + \frac{1}{\phi_c R_c} \left(\frac{(\Delta q)_c}{(\Delta C)_c} C_c \frac{t_c}{L_c} \frac{\partial q^*}{\partial x_i^*} C^* + q_c \frac{t_c}{L_c} q^* \frac{\partial C^*}{\partial x_i^*} - D_c \frac{t_c}{L_c^2} \frac{\partial}{\partial x_i^*} \left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right)\right) \\ & + \frac{\vartheta_c C_c t_c}{(\Delta C)_c} \phi^* R^* \vartheta^* C^* \end{aligned} \tag{1.32}$$

$$\begin{aligned} 0 = {} & \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* + \frac{D_c t_c}{\phi_c R_c L_c^2} \left(\frac{(\Delta q)_c}{(\Delta C)_c} C_c \frac{L_c}{D_c} \frac{\partial q^*}{\partial x_i^*} C^* + q_c \frac{L_c}{D_c} q^* \frac{\partial C^*}{\partial x_i^*} - \frac{\partial}{\partial x_i^*} \left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right)\right) \\ & + \frac{\vartheta_c C_c t_c}{(\Delta C)_c} \phi^* R^* \vartheta^* C^* \end{aligned} \tag{1.33}$$

With $C_c = (\Delta C)_c$ and $q_c = (\Delta q)_c$

$$0 = \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* + \frac{D_c t_c}{\phi_c R_c L_c^2}\left(q_c \frac{L_c}{D_c}\frac{\partial q^*}{\partial x_i^*} C^* + q_c \frac{L_c}{D_c} q^* \frac{\partial C^*}{\partial x_i^*} - \frac{\partial}{\partial x_i^*}\left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right)\right) + \vartheta_c t_c \phi^* R^* \vartheta^* C^* \tag{1.34}$$

$$0 = \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* + \frac{D_c t_c}{\phi_c R_c L_c^2}\left(q_c \frac{L_c}{D_c}\frac{\partial q^* C^*}{\partial x_i^*} - \frac{\partial}{\partial x_i^*}\left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right)\right) + \vartheta_c t_c \phi^* R^* \vartheta^* C^* \tag{1.35}$$

Setting $\mathrm{Pe} = q_c \dfrac{L_c}{D_c}$, the Peclet number and $\mathrm{Fo} = q_c \dfrac{t_c D_c}{L_c^2}$ the Fourier number

$$0 = \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* + \frac{\mathrm{Fo}}{\phi_c R_c}\frac{\partial}{\partial x_i^*}\left(\mathrm{Pe} \cdot q^* C^* - \left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right)\right) + \vartheta_c t_c \phi^* R^* \vartheta^* C^* \tag{1.36}$$

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