OpenGeoSys 6: Implementation of the Unsaturated Component Transport Process

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1 Unsaturated Component Transport Process

Used literature: [1] [3] [4] [2] [5] [7] [8] [6]

1.1 General Balance Equations

Let Ω be a domain, Γ the boundary of the domain and let u be an intrinsic quantity (for instance mass or heat) and the volume density is described by a function $S(u)$. The amount of the quantity in the domain can vary within time by two reasons. Firstly, new quantity 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

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

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

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

Applying the theorem of Gauss yields to

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

Finally,

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

Since the domain is arbitrary it holds:

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

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

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

which describes diffusive flow and

$$J^{(2)} = cu \quad \text{(where } c \text{ is a velocity vector)} \tag{1.7}$$

which describes advective flow or a combination of (1.6) and (1.7). For instance, substituting (1.6) in (1.5) leads to the following parabolic partial differential equation:

$$\frac{\partial S(u(x,t))}{\partial t} - \nabla \cdot [\boldsymbol{K}(x,t)\nabla u(x,t)] - Q(x,t) = 0, \tag{1.8}$$

while the description of the flow by a combination of (1.6) and (1.7) yields to

$$\frac{\partial S(u(x,t))}{\partial t} - \nabla \cdot [\boldsymbol{K}(x,t)\nabla u(x,t) - cu(x,t)] - Q(x,t) = 0. \tag{1.9}$$

1.2 Unsaturated Flow - The Richards Equation

todo

- explain
  - porous medium,
  - saturated / unsaturated
  - wet and gas phase,
- mention all assumptions

Literature: [6, chapter 6], [2, chapter 6]

$$
\begin{aligned}
0 &= \frac{\partial \phi \rho_w S}{\partial t} - \nabla \cdot \left(\rho_w \frac{k_{\text{rel}} \boldsymbol{\kappa}}{\mu_w} \left(\nabla p_w + \rho_w g e_z \right) \right) - Q_w && (1.10) \\
&= \frac{\partial \phi}{\partial t} \rho_w S + \phi \frac{\partial \rho_w}{\partial t} S + \phi \rho_w \frac{\partial S}{\partial t} - \nabla \cdot \left(\rho_w \frac{k_{\text{rel}} \boldsymbol{\kappa}}{\mu_w} \left(\nabla p + \rho_w g e_z \right) \right) - Q_w && (1.11)
\end{aligned}
$$

Under the assumptions

- that the porosity is constant (i.e., the first term vanishes),
- and that the pressure of the gas phase is zero, that allows for $p_c = -p$

the above equation takes the following form

$$
0 = \phi \frac{\partial \rho_w}{\partial p} \frac{\partial p}{\partial t} S - \phi \rho_w \frac{\partial S}{\partial p_c} \frac{\partial p_c}{\partial t} - \nabla \cdot \left(\rho_w \frac{k_{\text{rel}} \boldsymbol{\kappa}}{\mu_w} \left(\nabla p_w + \rho_w g e_z \right) \right) - Q_w \tag{1.12}
$$

where

$$
p_c = \frac{\rho_w g}{\alpha} \left[S_{\text{eff}}^{-\frac{1}{m}} - 1 \right]^{\frac{1}{n}} \tag{1.13}
$$

is the capillary pressure and

$$
S_{\text{eff}} = \frac{S - S_r}{S_{\max} - S_r} \tag{1.14}
$$

is the effective saturation.

1.2.1 Boundary Conditions

$$
\begin{aligned}
p_w - g_D^{p_w} &= 0 \quad \text{on} \quad \Gamma_D \quad \text{(Dirichlet type boundary conditions)} && (1.15) \\
\rho_w \frac{k_{\text{rel}} \boldsymbol{\kappa}}{\mu_w} \nabla^T p_w \cdot n + g_N^{p_w} &= 0 \quad \text{on} \quad \Gamma_N \quad \text{(Neumann type boundary conditions)} && (1.16)
\end{aligned}
$$

1.2.2 Evaluating Dominance of Effects

Substitution of variables from the first term of (1.12) results in

see 7.7 in [2]

$$
\begin{aligned}
\phi \frac{\partial \rho_w}{\partial p} \frac{\partial p}{\partial t} S &= \phi_c \left(\frac{\partial p}{\partial t} \right)_c \left(\frac{\partial \rho_w}{\partial p} \right)_c S_c \phi^* \left(\frac{\partial \rho_w}{\partial p} \right)^* \left(\frac{\partial p}{\partial t} \right)^* S^* = \phi_c \frac{\Delta (\rho_w)_c}{(\Delta t)_c} S_c \phi^* \left(\frac{\partial \rho_w}{\partial p} \right)^* \left(\frac{\partial p}{\partial t} \right)^* S^* \\
&= \phi_c \frac{\Delta (\rho_w)_c}{t_c} S_c \phi^* \left(\frac{\partial \rho_w}{\partial p} \right)^* \left(\frac{\partial p}{\partial t} \right)^* S^*
\end{aligned} \tag{1.17}
$$

The second term of (1.12) yields

$$\begin{aligned}\phi\rho_w\frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t} &= \phi^*\phi_c\rho_w^*\left(\rho_w\right)_c\left(\frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\right)^*\left(\frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\right)_c = \phi_c\left(\rho_w\right)_c\left(\frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\right)_c\phi^*\rho_w^*\left(\frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\right)^*\\ &= \phi_c\left(\rho_w\right)_c\frac{(\Delta S)_c}{(\Delta t)_c}\phi^*\rho_w^*\left(\frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\right)^* = \phi_c\left(\rho_w\right)_c\frac{(\Delta S)_c}{t_c}\phi^*\rho_w^*\left(\frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\right)^*\end{aligned}\tag{1.18}$$

$$\begin{aligned}\nabla\cdot\left(\rho_w\frac{k_{\text{rel}}\boldsymbol{\kappa}}{\mu_w}\left(\nabla p_w+\rho_w g e_z\right)\right) &= \frac{\partial}{\partial x_i}\cdot\left(\rho_w\frac{k_{\text{rel}}\boldsymbol{\kappa}}{\mu_w}\left(\frac{\partial}{\partial x_i}p_w+\rho_w g e_z\right)\right)\\ &= \frac{(\rho_w)_c}{L_c}\frac{(k_{\text{rel}})_c\boldsymbol{\kappa}_c}{(\mu_w)_c}\left(\frac{(\Delta p_w)_c}{L_c}+(\rho_w)_c g e_z\right)\frac{\partial}{\partial x_i^*}\left(\rho_w^*\frac{k_{\text{rel}}^*\boldsymbol{\kappa}^*}{\mu_w^*}\left(\frac{\partial p_w^*}{\partial x_i^*}+\rho_w^* g e_z\right)\right)\end{aligned}\tag{1.19}$$

$$\begin{aligned}0 &= \phi_c\frac{\Delta(\rho_w)_c}{t_c}S_c\phi^*\left(\frac{\partial\rho_w}{\partial p}\right)^*\left(\frac{\partial p}{\partial t}\right)^*S^* - \phi_c\left(\rho_w\right)_c\frac{(\Delta S)_c}{t_c}\phi^*\rho_w^*\left(\frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\right)^*\\ &\quad - \frac{(\rho_w)_c}{L_c}\frac{(k_{\text{rel}})_c\boldsymbol{\kappa}_c}{(\mu_w)_c}\left(\frac{(\Delta p_w)_c}{L_c}+(\rho_w)_c g e_z\right)\frac{\partial}{\partial x_i^*}\left(\rho_w^*\frac{k_{\text{rel}}^*\boldsymbol{\kappa}^*}{\mu_w^*}\left(\frac{\partial p_w^*}{\partial x_i^*}+\rho_w^* g e_z\right)\right)\\ &= \phi_c\frac{\Delta(\rho_w)_c}{t_c}S_c\phi^*\left(\frac{\partial\rho_w}{\partial p}\right)^*\left(\frac{\partial p}{\partial t}\right)^*S^* - \phi_c\left(\rho_w\right)_c\frac{(\Delta S)_c}{t_c}\phi^*\rho_w^*\left(\frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\right)^*\\ &\quad - \frac{(\rho_w)_c}{L_c^2}\frac{(k_{\text{rel}})_c\boldsymbol{\kappa}_c}{(\mu_w)_c}\left((\Delta p_w)_c+L_c(\rho_w)_c g e_z\right)\frac{\partial}{\partial x_i^*}\left(\rho_w^*\frac{k_{\text{rel}}^*\boldsymbol{\kappa}^*}{\mu_w^*}\left(\frac{\partial p_w^*}{\partial x_i^*}+\rho_w^* g e_z\right)\right)\end{aligned}\tag{1.20}$$

1.2.3 Weak Formulation

Multiplying (1.12) and (1.16) with test functions $v_p, \bar{v}_p \in H_0^1(\Omega)$, integration over Ω, Γ_N and adding the results leads to

$$\begin{aligned}0 &= \int_\Omega v_p\cdot\phi\frac{\partial\rho_w}{\partial p}\frac{\partial p}{\partial t}S\mathrm{d}x - \int_\Omega v_p\cdot\phi\rho_w\frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\mathrm{d}x\\ &\quad - \int_\Omega v_p\cdot\nabla\cdot\rho_w\frac{k_{\text{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla p_w\mathrm{d}x\\ &\quad - \int_\Omega v_p\cdot\nabla\cdot\rho_w\frac{k_{\text{rel}}\boldsymbol{\kappa}}{\mu_w}\rho_w g e_z\mathrm{d}x - \int_\Omega v_p\cdot Q_w\mathrm{d}x + \int_{\Gamma_N}\bar{v}_p\cdot\left[\rho_w\frac{k_{\text{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla^T p_w\cdot n + g_N^{p_w}\right]\mathrm{d}\sigma.\end{aligned}\tag{1.21}$$

Partial integration of the third integral of (1.21) leads to

$$\int_\Omega v_p\cdot\nabla\cdot\rho_w\frac{k_{\text{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla p_w\mathrm{d}x = \int_\Omega\nabla\cdot\left[v_p\cdot\rho_w\frac{k_{\text{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla p_w\right]\mathrm{d}x - \int_\Omega\nabla^T v_p\cdot\rho_w\frac{k_{\text{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla p_w\mathrm{d}x\tag{1.22}$$

The application of the theorem of Gauss to the first integral of the right hand side of (1.22) leads to

$$\begin{aligned}\int_\Omega\nabla\cdot\left[v_p\cdot\rho_w\frac{k_{\text{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla p_w\right]\mathrm{d}x &= \int_\Gamma v_p\cdot\rho_w\frac{k_{\text{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla p_w\cdot n\,\mathrm{d}\sigma\\ &= \underbrace{\int_{\Gamma_D} v_p\cdot\rho_w\frac{k_{\text{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla^T p_w\cdot n\,\mathrm{d}\sigma}_{=0,\text{ since } v_p\in H_0^1(\Omega)} + \int_{\Gamma_N} v_p\cdot\rho_w\frac{k_{\text{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla^T p_w\cdot n\,\mathrm{d}\sigma\end{aligned}\tag{1.23}$$

Substituting (1.23) in (1.22) and substituting the result in (1.21) yields

$$
\begin{aligned}
0 = &\int_\Omega v_p \cdot \phi \frac{\partial \rho_w}{\partial p}\frac{\partial p}{\partial t} S \mathrm{d}x - \int_\Omega v_p \cdot \phi \rho_w \frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\mathrm{d}x \\
&- \int_{\Gamma_N} v_p \cdot \rho_w \frac{k_{\mathrm{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla^T p_w \cdot n \,\mathrm{d}\sigma + \int_\Omega \nabla^T v_p \cdot \rho_w \frac{k_{\mathrm{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla p_w \mathrm{d}x \\
&- \int_\Omega v_p \cdot \nabla \cdot \rho_w \frac{k_{\mathrm{rel}}\boldsymbol{\kappa}}{\mu_w}\rho_w g e_z \mathrm{d}x - \int_\Omega v_p \cdot Q_w \mathrm{d}x + \int_{\Gamma_N} \bar{v}_p \cdot \left[\rho_w \frac{k_{\mathrm{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla^T p_w \cdot n + g_N^{p_w}\right] \mathrm{d}\sigma.
\end{aligned}
\tag{1.24}
$$

Since the $\bar{v}_p$ and v_p are arbitrary test functions it is possible to set $\bar{v}_p = v_p$. This results in

$$
\begin{aligned}
0 = &\int_\Omega v_p \cdot \phi \frac{\partial \rho_w}{\partial p}\frac{\partial p}{\partial t} S \mathrm{d}x - \int_\Omega v_p \cdot \phi \rho_w \frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\mathrm{d}x \\
&+ \int_\Omega \nabla^T v_p \cdot \rho_w \frac{k_{\mathrm{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla p_w \mathrm{d}x \\
&- \int_\Omega v_p \cdot \nabla \cdot \rho_w \frac{k_{\mathrm{rel}}\boldsymbol{\kappa}}{\mu_w}\rho_w g e_z \mathrm{d}x - \int_\Omega v_p \cdot Q_w \mathrm{d}x + \int_{\Gamma_N} v_p \cdot g_N^{p_w} \mathrm{d}\sigma.
\end{aligned}
\tag{1.25}
$$

1.2.4 Finite Element Discretization

The pressure of the wet phase p_w is approximated by

$$
p_w \approx \widetilde{p_w} = \sum N_j \widehat{p_j} = N\widehat{p},
\tag{1.26}
$$

using the shape functions N_j and time dependent coefficients $\widehat{p_j}$. Using the shape functions again as test functions (Galerkin principle) the discretization of (1.25)) takes the following form

$$
\begin{aligned}
0 = &\int_\Omega N \cdot \phi \frac{\partial \rho_w}{\partial p}\frac{\partial p}{\partial t} S \mathrm{d}x - \int_\Omega N \cdot \phi \rho_w \frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\mathrm{d}x \\
&+ \int_\Omega \nabla^T N \cdot \rho_w \frac{k_{\mathrm{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla N\widehat{p} \mathrm{d}x \\
&- \int_\Omega N \cdot \nabla \cdot \rho_w \frac{k_{\mathrm{rel}}\boldsymbol{\kappa}}{\mu_w}\rho_w g e_z \mathrm{d}x - \int_\Omega N \cdot Q_w \mathrm{d}x + \int_{\Gamma_N} N \cdot g_N^{p_w} \mathrm{d}\sigma.
\end{aligned}
\tag{1.27}
$$

This is a set of equations of the form

$$
\boldsymbol{M}_{pp}\widehat{\dot{p}} + \boldsymbol{K}_{pp}\widehat{p} + \boldsymbol{\Psi}_p = 0
\tag{1.28}
$$

with

$$
\boldsymbol{M}_{pp} = \int_\Omega N \cdot \phi \frac{\partial \rho_w}{\partial p}\frac{\partial p}{\partial t} S \mathrm{d}x - \int_\Omega N \cdot \phi \rho_w \frac{\partial S}{\partial p_c}\frac{\partial p_c}{\partial t}\mathrm{d}x
\tag{1.29}
$$

$$
\boldsymbol{K}_{pp} = \int_\Omega \nabla^T N \cdot \rho_w \frac{k_{\mathrm{rel}}\boldsymbol{\kappa}}{\mu_w}\nabla N \mathrm{d}x
\tag{1.30}
$$

$$
\boldsymbol{\Psi}_p = -\int_\Omega N \cdot \nabla \cdot \rho_w \frac{k_{\mathrm{rel}}\boldsymbol{\kappa}}{\mu_w}\rho_w g e_z \mathrm{d}x - \int_\Omega N \cdot Q_w \mathrm{d}x + \int_{\Gamma_N} N \cdot g_N^{p_w} \mathrm{d}\sigma.
\tag{1.31}
$$

1.3 Mass Diffusion Equation

The primary variable in the mass diffusion process is the concentration C. In the general balance equation (1.5) the function $S(u(x,t))$ is substituted by $\phi R C$, where ϕ is the porosity and R denotes the retardation factor. The term J, describing the mass flow, is substituted by

$$
qC - \boldsymbol{D}\,\boldsymbol{grad}\,C,
\tag{1.32}
$$

i.e., there is advective and diffusive flow. The advective part qC is driven by the Darcy velocity q of the coupled groundwater flow. Finally, the term

$$\phi R \vartheta C \tag{1.33}$$

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 balance equation reads:

$$\frac{\partial}{\partial t}(\phi R C) + \operatorname{div}(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C) + \phi R \vartheta C - Q_C = 0 \tag{1.34}$$

where

- $\boldsymbol{D}$ hydrodynamic dispersion tensor,

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

  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

- ϑ is the decay rate

Incompressible solid, i.e. $\dfrac{\partial \phi}{\partial t} = 0$, and the retardation factor is not time dependent:

$$\phi R \frac{\partial C}{\partial t} + \operatorname{div}(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C) + \phi R \vartheta C - Q_C = 0 \tag{1.35}$$

1.3.1 Boundary Conditions

$$C = g_D^C \quad \text{on} \quad \Gamma_D \quad \text{(Dirichlet type boundary conditions)} \tag{1.36}$$

$$-\langle \boldsymbol{D}\,\boldsymbol{grad}\,C | n \rangle = g_N^C \quad \text{on} \quad \Gamma_N \quad \text{(Neumann type boundary conditions)} \tag{1.37}$$

1.3.2 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 (1.35), multiplying with arbitrary test functions $v, \bar{v} \in H_0^1(\Omega)$ and integration over Ω results in

$$\begin{aligned} 0 = & \int_\Omega v \cdot \phi \cdot R \cdot \frac{\partial C}{\partial t} \mathrm{d}\Omega + \int_\Omega v \cdot \operatorname{div}(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C)\,\mathrm{d}\Omega \\ & + \int_\Omega v \cdot [\vartheta \cdot \phi \cdot R \cdot C]\,\mathrm{d}\Omega - \int_\Omega v \cdot Q_C \mathrm{d}\Omega + \int_{\Gamma_N} \bar{v} \cdot \left[\langle \boldsymbol{D}\,\boldsymbol{grad}\,C|n\rangle + g_N^C\right] \mathrm{d}\sigma \end{aligned} \tag{1.38}$$

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

$$\int_\Omega v \cdot \operatorname{div}(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C)\,\mathrm{d}\Omega = -\int_\Omega \langle \boldsymbol{grad}\,v | qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\rangle\,\mathrm{d}\Omega + \int_\Omega \operatorname{div}[v(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C)]\,\mathrm{d}\Omega \tag{1.39}$$

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

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

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

$$\int_\Omega v{\cdot}\operatorname{div}\left(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right)\mathrm{d}\Omega = -\int_\Omega \left\langle \boldsymbol{grad}\,v|qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right\rangle \mathrm{d}\Omega + \int_{\Gamma_N} \left\langle v\left(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right)|n\right\rangle \mathrm{d}\sigma \tag{1.40}$$

Thus (1.38) reads:

$$\begin{aligned} 0 = &\int_\Omega v\cdot\phi\cdot R\cdot\frac{\partial C}{\partial t}\mathrm{d}\Omega - \int_\Omega \left\langle \boldsymbol{grad}\,v|qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right\rangle \mathrm{d}\Omega + \int_{\Gamma_N} \left\langle v\left(qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right)|n\right\rangle \mathrm{d}\sigma \\ &+ \int_\Omega v\cdot\left[\vartheta\cdot\phi\cdot R\cdot C\right]\mathrm{d}\Omega - \int_\Omega v\cdot Q_C \mathrm{d}\Omega + \int_{\Gamma_N} \bar{v}\cdot\left[\left\langle \boldsymbol{D}\,\boldsymbol{grad}\,C|n\right\rangle + g_N^C\right]\mathrm{d}\sigma \end{aligned} \tag{1.41}$$

Setting $v = \bar{v}$:

$$\begin{aligned} 0 = &\int_\Omega v\cdot\phi\cdot R\cdot\frac{\partial C}{\partial t}\mathrm{d}\Omega - \int_\Omega \left\langle \boldsymbol{grad}\,v|qC - \boldsymbol{D}\,\boldsymbol{grad}\,C\right\rangle \mathrm{d}\Omega + \int_{\Gamma_N} \left\langle vqC|n\right\rangle \mathrm{d}\sigma \\ &+ \int_\Omega v\cdot\left[\vartheta\cdot\phi\cdot R\cdot C\right]\mathrm{d}\Omega - \int_\Omega v\cdot Q_C \mathrm{d}\Omega + \int_{\Gamma_N} v\cdot g_N^C \mathrm{d}\sigma \end{aligned} \tag{1.42}$$

1.3.3 Finite Element Discretization

The concentration is approximated by:

$$C \approx \sum N_j^C c_j = N^C c \tag{1.43}$$

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 (1.42)) takes the following form

$$\begin{aligned} 0 = &\int_\Omega N_i^C\cdot\phi\cdot R\cdot N_j\frac{\partial c_j}{\partial t}\mathrm{d}\Omega - \int_\Omega \nabla^T N_i^C\cdot q\cdot N_j^C c_j \mathrm{d}\Omega + \int_\Omega \nabla^T N_i^C \boldsymbol{D}\nabla N_j^C c_j \mathrm{d}\Omega + \int_{\Gamma_N} \left(N_i^C q^T N_j^C c_j\right) n\,\mathrm{d}\sigma \\ &+ \int_\Omega N_i^C\cdot\left[\vartheta\cdot\phi\cdot R\cdot N_j^C c_j\right]\mathrm{d}\Omega - \int_\Omega N_i^C\cdot Q_C \mathrm{d}\Omega + \int_{\Gamma_N} N_i^C\cdot g_N^C \mathrm{d}\sigma \end{aligned} \tag{1.44}$$

This is a set of equations of the form

$$\boldsymbol{C}^{CC}\dot{c} + \boldsymbol{K}^{CC}c + f^C = 0 \tag{1.45}$$

with

$$\begin{aligned} \boldsymbol{K}_{ij}^{CC} = &-\int_\Omega \nabla^T N_i^C\cdot q\cdot N_j^C \mathrm{d}\Omega + \int_\Omega \nabla^T N_i^C \boldsymbol{D}\nabla N_j^C \mathrm{d}\Omega + \int_{\Gamma_N} \left(N_i^C\cdot q^T N_j^C\right)^T n\mathrm{d}\sigma \\ &+ \int_\Omega N_i^C\cdot\left[\vartheta\cdot\phi\cdot R\cdot N_j^C\right]\mathrm{d}\Omega, \end{aligned} \tag{1.46}$$

$$f_i^C = -\int_\Omega N_i^C Q_C \mathrm{d}\Omega + \int_{\Gamma_N} N_i^C g_N^C \mathrm{d}\sigma, \tag{1.47}$$

$$\boldsymbol{C}_{ij}^{CC} = \int_\Omega N_i^C\cdot\phi\cdot R\cdot N_j^C \mathrm{d}\Omega. \tag{1.48}$$

In (1.46) 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

$$q = \frac{\kappa}{\mu} \boldsymbol{grad}\,(p + \varrho \cdot g \cdot z) \approx \frac{\kappa}{\mu} \left(\nabla N_i^p + \varrho \cdot g \cdot e_z\right). \tag{1.49}$$

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

$$\boldsymbol{K}_{ij}^{Cp} = -\int_\Omega \nabla^T N_i^C \cdot \frac{\kappa}{\mu} \left(\nabla N_i^p + \varrho \cdot g \cdot e_z\right) \cdot N_j^C \mathrm{d}\Omega \tag{1.50}$$

1.4 Evaluating Dominance of Effects

Substitute variables and coefficients that appear in (1.35): see 7.7 in [2]

$$\phi R \frac{\partial C}{\partial t} = \phi^* \phi_c R^* R_c \left(\frac{\partial C}{\partial t}\right)^* \left(\frac{\partial C}{\partial t}\right)_c = \phi^* \phi_c R^* R_c \left(\frac{\partial C}{\partial t}\right)^* \frac{(\Delta C)_c}{(\Delta t)_c} = \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* \phi_c R_c \frac{(\Delta C)_c}{t_c} \tag{1.51}$$

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

$$\begin{aligned}\operatorname{div}(qC) &= \frac{\partial qC}{\partial x_i} = \frac{\partial q}{\partial x_i} C + \frac{\partial C}{\partial x_i} q = \left(\frac{\partial q}{\partial x_i}\right)^* \frac{(\Delta q)_c}{L_c^{(q)}} C^* C_c + \left(\frac{\partial C}{\partial x_i}\right)^* \frac{(\Delta C)_c}{L_c^{(C)}} q^* q_c \\ &= \frac{\partial q^*}{\partial x_i^*} C^* \frac{(\Delta q)_c}{L_c^{(q)}} C_c + q^* \frac{\partial C^*}{\partial x_i^*} \frac{q_c (\Delta C)_c}{L_c^{(C)}}\end{aligned} \tag{1.52}$$

$$\begin{aligned}\operatorname{div}(\boldsymbol{D}\,\boldsymbol{grad}\,C) &= \frac{\partial}{\partial x_i}\left(\boldsymbol{D}\frac{\partial C}{\partial x_i}\right) = \left(\frac{\partial}{\partial x_i}\right)^* \frac{1}{L_c^{(C)}} \left(\boldsymbol{D}^* D_c \left(\frac{\partial C}{\partial x_i}\right)^* \frac{(\Delta C)_c}{L_c^{(C)}}\right) \\ &= \frac{\partial}{\partial x_i^*}\left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right) \frac{D_c (\Delta C)_c}{{L_c^{(C)}}^2}\end{aligned} \tag{1.53}$$

$$\phi R \vartheta C = \phi^* \phi_c R^* R_c \vartheta^* \vartheta_c C^* C_c = \phi^* R^* \vartheta^* C^* \phi_c R_c \vartheta_c C_c \tag{1.54}$$

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

$$\begin{aligned}0 = {}& \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* \phi_c R_c \frac{(\Delta C)_c}{t_c} + \frac{(\Delta q)_c}{L_c} C_c \frac{\partial q^*}{\partial x_i^*} C^* + \frac{q_c (\Delta C)_c}{L_c} q^* \frac{\partial C^*}{\partial x_i^*} - \frac{D_c (\Delta C)_c}{L_c^2} \frac{\partial}{\partial x_i^*}\left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right) \\ &+ \phi_c R_c \vartheta_c C_c \phi^* R^* \vartheta^* C^*\end{aligned} \tag{1.55}$$

$$\begin{aligned}0 = {}& \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* + \frac{1}{\phi_c R_c} \left(\frac{(\Delta q)_c}{(\Delta C)_c} C_c \frac{t_c}{L_c} \frac{\partial q^*}{\partial x_i^*} C^* + q_c \frac{t_c}{L_c} q^* \frac{\partial C^*}{\partial x_i^*} - D_c \frac{t_c}{L_c^2} \frac{\partial}{\partial x_i^*}\left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right)\right) \\ &+ \frac{\vartheta_c C_c t_c}{(\Delta C)_c} \phi^* R^* \vartheta^* C^*\end{aligned} \tag{1.56}$$

$$\begin{aligned}0 = {}& \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* + \frac{D_c t_c}{\phi_c R_c L_c^2} \left(\frac{(\Delta q)_c}{(\Delta C)_c} C_c \frac{L_c}{D_c} \frac{\partial q^*}{\partial x_i^*} C^* + q_c \frac{L_c}{D_c} q^* \frac{\partial C^*}{\partial x_i^*} - \frac{\partial}{\partial x_i^*}\left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right)\right) \\ &+ \frac{\vartheta_c C_c t_c}{(\Delta C)_c} \phi^* R^* \vartheta^* C^*\end{aligned} \tag{1.57}$$

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

$$\begin{aligned} 0 = \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* + \frac{D_c t_c}{\phi_c R_c L_c^2}\left(q_c \frac{L_c}{D_c}\frac{\partial q^*}{\partial x_i^*} C^* + q_c \frac{L_c}{D_c} q^* \frac{\partial C^*}{\partial x_i^*} - \frac{\partial}{\partial x_i^*}\left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right)\right) \\ + \vartheta_c t_c \phi^* R^* \vartheta^* C^* \end{aligned} \tag{1.58}$$

$$0 = \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* + \frac{D_c t_c}{\phi_c R_c L_c^2}\left(q_c \frac{L_c}{D_c}\frac{\partial q^* C^*}{\partial x_i^*} - \frac{\partial}{\partial x_i^*}\left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right)\right) + \vartheta_c t_c \phi^* R^* \vartheta^* C^* \tag{1.59}$$

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

$$0 = \phi^* R^* \left(\frac{\partial C}{\partial t}\right)^* + \frac{\mathrm{Fo}}{\phi_c R_c}\frac{\partial}{\partial x_i^*}\left(\mathrm{Pe} \cdot q^* C^* - \left(\boldsymbol{D}^* \frac{\partial C^*}{\partial x_i^*}\right)\right) + \vartheta_c t_c \phi^* R^* \vartheta^* C^* \tag{1.60}$$

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