

# OpenGeoSys 6: Implementation of the *HC* Process

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# 1 Model Formulation

## 1.1 Balance Equations

This is a general motivation to parabolic partial differential equations which is very similar to [?] and is here repeated for a complete representation.

Let  $\Omega$  be a stationary domain,  $\Gamma$  the boundary of  $\Omega$ . Let  $\mathbf{u}$  be an extensive quantity (for instance mass or heat). The corresponding intensive quantity (e.g. density) of  $\mathbf{u}$  may be described by a function  $S(\mathbf{u})$ . The amount of the quantity in the domain can vary within time by two reasons. Firstly, new quantity can accumulate by flow over  $\Gamma$  or secondly it can be generated due to the presence of sources or sinks within  $\Omega$ . Consequently, the balance reads

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

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

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

Applying the theorem of Gauss yields to

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

Finally, since the integral operator is linear, it holds

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

Since the domain is arbitrary it holds:

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

### 1.1.1 Mass Balance Equations

Hydrodynamics and mechanics within porous media are described on a semimacroscopic level, in order to include the highly heterogenous microscopic material properties as volume averages.

Let  $V[m^3]$  be a representative elementary volume (REV). The quotient of mass  $m[kg]$  and  $V$  defines the apparent density  $\rho = \frac{m}{V}$ .  $V_{\text{void}} = \phi V$  represents the pore or void volume of the porous medium. The real density  $\rho_R = \frac{m}{V_{\text{void}}}$  is related to the apparent density by the porosity.

For the problem at hand we consider a two component fluid consisting of a solvent of total mass  $m_s$  and a solved component of mass  $m_C$ . Here the subscripts  $s$  and  $C$  denote solvent and solved component, respectively. In general all quantities do depend on space and time. For convenience, this dependency is not indicated explicitly in the following. The intensive functions  $S(m_s)$  and  $S(m_C)$  as well as the total mass density  $\left[\frac{kg}{m^3}\right] S(m_t)$ , with corresponding mass fractions  $\omega_i = \rho_i/\rho_R$  and the identity  $\sum_i \omega_i = 1$ , read

$$(1.6) \quad S(m_s) = \phi \rho_R \omega_s$$

$$(1.7) \quad S(m_C) = \phi \rho_R \omega_C$$

$$(1.8) \quad S(m_t) = \phi \rho_R.$$

Here  $\rho_i$  denotes the density of component  $i$  and  $\rho_R$  denotes the total mass density. Using Equation (1.5) the conservation law for the component  $i$  can be written as

$$(1.9) \quad \frac{\partial (\phi \rho_R \omega_i)}{\partial t} + \text{div} (J (\phi \rho_R \omega_i)) + Q_i = 0.$$

Making use of the average bulk velocity  $v$  within an REV we can decompose the flux of component  $i$  in advective flux and dispersive flux, which captures all deviations induced by dispersion or diffusion

$$(1.10) \quad J (\phi \rho_R \omega_i) = \phi \rho_R \omega_i v + J_i^{\text{dis}}.$$

By definition the following identity holds

$$(1.11) \quad \sum_i J_i^{\text{dis}} = 0.$$

The sum of all component mass balances leads to the balance equation of total mass density

$$(1.12) \quad \frac{\partial (\phi \rho_R)}{\partial t} + \text{div} (\phi \rho_R v) + Q_p = 0.$$

Inserting Equation (1.12) the component wise mass balance equation (1.9) can be rewritten in its advective form into

$$(1.13) \quad \phi \rho_R \frac{\partial (\omega_i)}{\partial t} + \phi \rho_R \left\langle v \left| \nabla \omega_i \right. \right\rangle + \nabla J_i^{\text{dis}} + Q_i - \omega_i Q_p = 0.$$

### 1.1.2 Momentum Balance Equation

The momentum density  $S(M) = \phi \rho_R v$  needs to be conserved according to Equation (1.5). We define the momentum density flux as

$$(1.14) \quad J(S(M)) = \phi \rho_R v v - \sigma,$$

where  $\sigma$  is a viscous stress density tensor in units of  $\frac{kg}{m \cdot s^2}$ . Using  $F$  as an interfacial drag term of momentum exchange and  $g$  as gravitational acceleration the macroscopic momentum balance equation reads

$$(1.15) \quad \frac{\partial \phi \rho_R v}{\partial t} + \text{div}(\phi \rho_R v^2) - \text{div}(\sigma) = \phi(\rho_R g + F).$$

## 1.2 Simplifications

### 1.2.1 Phenomenological Laws

For the nonadvective (dispersive) fluxes of mass  $J_i^{\text{dis}}$  and momentum  $\sigma$  phenomenological laws are available. Dispersive mass flux is expressed as an Fickian type law

$$(1.16) \quad J_i^{\text{dis}} = -\rho_R \mathbf{D}_h \nabla \omega_i$$

with  $\mathbf{D}_h$   $\left[\frac{m^2}{s}\right]$  denoting the hydrodynamic dispersion tensor, which is assumed to be independent of the concentration and its gradient. According to the *Bear-Scheidegger* dispersion relationship for isotropic porous media it reads

$$(1.17) \quad \mathbf{D}_h = \phi \left( \mathbf{D}_D + \beta_T \|v\| \mathbf{I} + (\beta_L - \beta_T) \frac{vv^T}{\|v\|} \right)$$

with molecular diffusion coefficient  $\mathbf{D}_D$ , longitudinal  $\beta_L$  and transversal  $\beta_T$  dispersivity coefficients and the identity tensor  $\mathbf{I}$ .

The stress tensor for the fluid phase can be expressed assuming the validity of *Newton's viscosity law*, with hydrostatic pressure  $p$  and  $\sigma^l$  denoting the deviatoric stress tensor depending on the dynamic viscosity  $\mu$   $\left[\frac{kg}{ms}\right]$  and the velocity gradient  $\nabla v$ ,

$$(1.18) \quad \sigma = -\phi \left( p \mathbf{I} + \sigma^l(\mu, \nabla v) \right).$$

### 1.2.2 Density Differential

The density function  $\rho_R(p, \omega_C)$  is regarded as a function of pressure and component concentration. Hence, its total differential reads

$$(1.19) \quad d\rho_R = \frac{\partial \rho_R}{\partial p} dp + \frac{\partial \rho_R}{\partial \omega_C} d\omega_C.$$

From the relation above the density function can be obtained immediately by integration.

### 1.2.3 Constitutive Equations

The interfacial drag term  $F$  of momentum exchange can be developed up to the 2nd order in  $q$  with  $q$  being the filtration or Darcy velocity  $q = \phi v$ , with  $\kappa$   $[m^2]$  being a permeability tensor and the Forchheimer coefficient  $\mathcal{I}_F$ ,

$$(1.20) \quad F = -\frac{\mu}{\kappa} q - \frac{\mu}{\kappa} \mathcal{I}_F \|q\| q.$$

Additionally the dynamic viscosity can be regarded as a function of concentration  $\mu = \mu(\omega_C)$ .

### 1.2.4 Incompressible Porous Medium

The porous medium is considered not to vary in space and time. Thus, all derivatives of  $\phi$  vanish.

### 1.2.5 Component Mass Balance Assumptions

A scenario might be considered, where a certain fraction of component mass is stored within the solid matrix, incapable of moving with the fluid. If there is an equilibrium reaction between the amount of bound component mass with the amount of solved mass within an REV, their proportion is constant

$$(1.21) \quad \frac{\omega_C^{\text{solid}} \rho_S}{\omega_C^{\text{fluid}} \rho_R} = K_d \phi = \text{const},$$

with proportionality factor  $K_d$ . Hence, by definition the amount of component bound to the solid matrix can only change by components getting solved within the fluid or vice versa. Thus, the total component mass change is reads

$$(1.22) \quad \frac{\partial (\omega_C^{\text{solid}} \rho_S + \phi \rho_R \omega_C^{\text{fluid}})}{\partial t} = \frac{\partial ((K_d \phi \rho_R + \phi \rho_R) \omega_C^{\text{fluid}})}{\partial t}.$$

Since both, the solid matrix and the void space are assumed to be constant the expression can be further simplified as

$$(1.23) \quad \frac{\partial (K_d \phi \rho_R + \phi \rho_R) \omega_C^{\text{fluid}}}{\partial t} = (K_d + 1) \frac{\partial \phi \rho_R \omega_C}{\partial t}.$$

For convenience  $\omega_C^{\text{fluid}} = \omega_C$  is set and a retardation factor  $R = 1 + K_d$  is introduced. In the following, there is no energetic cost for the transition of components from bound state to solved state taken into account.

Often, a process might be of interest, where the component concentration decays in time. This could be a consequence for radioactive decay. Hence, we add this decay term permanently to the equations. The widely used description of decay processes include such as sink terms  $R_C$  and read

$$(1.24) \quad R_C = R\theta\phi\rho_R\omega_C$$

with  $\theta$  [ $\frac{1}{s}$ ] denoting a decay rate. Note, both the bound and solved parts of the component mass are exposed to the decay process here.

### 1.2.6 Momentum Balance Assumptions

Within ground water flow models, inertia is generally neglected. Additionally, forces are only regarded in linear order of  $q$  and no derivatives of  $q$  are considered. Taking those simplifications into account, the momentum balance Equation (1.15) simplifies to

$$(1.25) \quad \text{div}(p\mathbf{I}) = \left( \rho_R g - \frac{\mu}{\kappa} q \right)$$

which can be used to calculate the filtration velocity

$$(1.26) \quad q = -\frac{\kappa}{\mu} (\nabla p - \rho_R g).$$

## 1.3 Complete Equations

Here, all assumptions made in the previous chapter are taken into account. Using Equation (1.26) to rewrite (1.12) the total mass balance reads

$$(1.27) \quad \phi \frac{\partial \rho_R}{\partial t} - \text{div} \left( \frac{\kappa}{\mu} \rho_R (\nabla p - \rho_R g) \right) + Q_p = 0$$

and can be rewritten using (1.19)

$$(1.28) \quad \underbrace{\phi \frac{\partial \rho_R}{\partial p}}_{\alpha_p} \frac{\partial p}{\partial t} + \underbrace{\phi \frac{\partial \rho_R}{\partial \omega_C}}_{\beta_p} \frac{\partial \omega_C}{\partial t} - \operatorname{div} \left( \underbrace{\frac{\kappa}{\mu} \rho_R (\nabla p - \rho_R g)}_{\gamma_p} \right) + \underbrace{Q_p}_{\delta_p} = 0.$$

Inserting (1.26) and (1.16) into the advective form for component mass balance Equation (1.13) for the solved component mass and adding the decay term (1.24) as well as the retardation factor introduced above leads to

$$(1.29) \quad \underbrace{\phi \rho_R R}_{\beta_{\omega_C}} \frac{\partial \omega_C}{\partial t} - \operatorname{div} \left( \underbrace{\rho_R \mathbf{D}_h \nabla \omega_C}_{\gamma_{\omega_C}} \right) + \underbrace{Q_{\omega_C} - \rho_R \left\langle \frac{\kappa}{\mu} (\nabla p - \rho_R g) \middle| \nabla \omega_C \right\rangle - R \omega_C Q_p + R \theta \phi \rho_R \omega_C}_{\delta_{\omega_C}} = 0.$$

The abbreviations  $\alpha_i, \beta_i, \gamma_i, \delta_i$  are introduced to simplify calculations. The system can be solved by the parallel solution of Equation (1.28) and Equation (1.29).

### 1.3.1 Boundary Conditions

Dirichlet and Neumann conditions are defined at the boundary  $\Gamma$  of  $\Omega$ . The corresponding areas, where the boundary conditions are defined are denoted with  $\Gamma_D$  and  $\Gamma_N$ , respectively, with  $\Gamma = \Gamma_D \cup \Gamma_N$  and  $\Gamma_D \cap \Gamma_N = \emptyset$ .

#### Pressure Boundary Conditions

For the pressure Boundary conditions we can note, that flow boundary conditions are equivalent in it's form to Neumann type boundary conditions, hence the boundary conditions can be defined as

$$(1.30) \quad p - g_D^p = 0 \quad \text{on } \Gamma_D \quad (\text{Dirichlet type boundary condition}),$$

$$(1.31) \quad \left\langle \underbrace{\frac{\kappa}{\mu} \rho_R (\nabla p - \rho_R g)}_{\gamma_p^N} \middle| n \right\rangle + g_N^p = 0 \quad \text{on } \Gamma_N \quad (\text{Neumann type boundary condition}).$$

### 1.3.2 Concentration Boundary Conditions

For component concentration boundary conditions are implemented as

$$(1.32) \quad \omega_C - g_D^{\omega_C} = 0 \quad \text{on } \Gamma_D \quad (\text{Dirichlet type boundary condition}),$$

$$(1.33) \quad \left\langle \underbrace{\rho_R \mathbf{D}_h \nabla \omega_C}_{\gamma_{\omega_C}^N} \middle| n \right\rangle + g_N^{\omega_C} = 0 \quad \text{on } \Gamma_N \quad (\text{Neumann type boundary condition}).$$

## 2 Weak Formulation and FEM Discretization

### 2.1 General Derivation of Weak Formulation

Adding the Neumann type boundary conditions to the whole domain boundaries and adding the expression to Equation (1.29) or Equation (1.28) leads to a partial differential equation of the form

$$(2.1) \quad \alpha \frac{\partial p}{\partial t} + \beta \frac{\partial \omega_C}{\partial t} - \operatorname{div} \gamma + \delta = 0.$$

Since Equation (2.1) holds for arbitrary points of the domain, the equations stays valid if it is multiplied by a test function  $\Psi \in H_0^1(\Omega)$  which is chosen, such that it vanishes on the Dirichlet boundary of  $\Omega$

$$(2.2) \quad 0 = \int_{\Omega} \Psi \left( \alpha \frac{\partial p}{\partial t} + \beta \frac{\partial \omega_C}{\partial t} - \operatorname{div} \gamma + \delta \right) dx$$

or equivalently

$$(2.3) \quad 0 = \int_{\Omega} \Psi \alpha \frac{\partial p}{\partial t} dx + \int_{\Omega} \Psi \beta \frac{\partial \omega_C}{\partial t} dx - \int_{\Omega} \Psi \operatorname{div} \gamma dx + \int_{\Omega} \Psi \delta dx.$$

Applying partial integration and using Gauss theorem on the third part of Equation (2.3) leads to

$$(2.4) \quad - \int_{\Omega} \Psi \operatorname{div} \gamma dx = \int_{\Omega} \langle \mathbf{grad} \Psi | \gamma \rangle dx - \int_{\Gamma_N} \langle \Psi \gamma | n \rangle d\sigma - \int_{\Gamma_D} \langle \Psi \gamma | n \rangle d\sigma.$$

The integral over the Dirichlet boundaries  $\Gamma_D$  vanishes, since we choose  $\Psi$  accordingly. Inserting the remaining parts of Equation (2.4) into Equation (2.3) yields

$$(2.5) \quad 0 = \int_{\Omega} \Psi \alpha \frac{\partial p}{\partial t} dx + \int_{\Omega} \Psi \beta \frac{\partial \omega_C}{\partial t} dx + \int_{\Omega} \langle \mathbf{grad} \Psi | \gamma \rangle dx - \int_{\Gamma_N} \langle \Psi \gamma | n \rangle d\sigma + \int_{\Omega} \Psi \delta dx.$$

To this, we can add a Neumann boundary condition integrated at the domain boundary and use the linearity of scalar products. Using the notation from the previous section, the weak form of an Equation in the form of Equation (2.1) reads

$$(2.6) \quad \begin{aligned} 0 = & \int_{\Omega} \Psi \alpha \frac{\partial p}{\partial t} dx + \int_{\Omega} \Psi \beta \frac{\partial \omega_C}{\partial t} dx + \int_{\Omega} \langle \mathbf{grad} \Psi | \gamma \rangle dx + \int_{\Omega} \Psi \delta dx \\ & + \int_{\Gamma_N} \langle \Psi (\gamma^N - \gamma) | n \rangle d\sigma + \int_{\Gamma_N} \Psi g_N d\sigma. \end{aligned}$$

## 2.2 Total Mass Flow

### 2.2.1 Weak Formulation

For the bulk flow, we can replace the coefficients in Equation (2.6) with

$$\underbrace{\phi \frac{\partial \rho_R}{\partial p}}_{\alpha=\alpha_p} \frac{\partial p}{\partial t} + \underbrace{\phi \frac{\partial \rho_R}{\partial \omega_C}}_{\beta=\beta_p} \frac{\partial \omega_C}{\partial t} - \operatorname{div} \left( \underbrace{\frac{\kappa}{\mu} \rho_R (\nabla p - \rho_R g)}_{\gamma=\gamma_p} \right) + \underbrace{Q_p}_{\delta=\delta_p} = 0,$$

and  $\gamma_p^N - \gamma_p = 0$ .

Hence the weak form of Equation (1.28) reads

$$(2.7) \quad 0 = \int_{\Omega} \Psi^p \phi \frac{\partial \rho_R}{\partial p} \frac{\partial p}{\partial t} dx + \int_{\Omega} \Psi^p \phi \frac{\partial \rho_R}{\partial \omega_C} \frac{\partial \omega_C}{\partial t} dx + \int_{\Omega} \left\langle \mathbf{grad} \Psi^p \left| \frac{\kappa}{\mu} \rho_R (\nabla p - \rho_R g) \right. \right\rangle dx \\ + \int_{\Omega} \Psi^p Q_p dx + \int_{\Gamma_N} \Psi^p g_N^p d\sigma.$$

### 2.2.2 Finite Element Discretization

The solutions for  $p$  and  $\omega_C$  will be approximated by shape functions

$$(2.8) \quad p \approx \sum N_j^p \hat{p}_j = N^p \hat{p}, \quad \omega_C \approx \sum N_j^{\omega} \hat{\omega}_j = N^{\omega} \hat{\omega}$$

where  $N_j^p(x, y, z)$  and  $N_j^{\omega}(x, y, z)$  are the *shape functions* and  $\hat{p}(t), \hat{\omega}(t)$  are coefficients. The case where the test functions are approximated by the same shape function, i.e.

$$(2.9) \quad \Psi^p = \sum_i N_i^p, \quad \Psi^{\omega} = \sum_i N_i^{\omega},$$

is denoted as Galerkin principle. With this, the whole system is a set of equations of the form

$$(2.10) \quad \mathbf{M} \dot{\mathbf{a}} + \mathbf{K} \mathbf{a} + \mathbf{b} = 0$$

with

$$(2.11) \quad \mathbf{M} = \begin{bmatrix} \mathbf{M}^{\omega_C \omega_C} & \mathbf{M}^{\omega_C p} \\ \mathbf{M}^{p \omega_C} & \mathbf{M}^{pp} \end{bmatrix}, \quad \mathbf{a} = \begin{bmatrix} \hat{\omega} \\ \hat{p} \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} \mathbf{K}^{\omega_C \omega_C} & \mathbf{K}^{\omega_C p} \\ \mathbf{K}^{p \omega_C} & \mathbf{K}^{pp} \end{bmatrix}, \quad \text{and} \quad \mathbf{f} = \begin{bmatrix} \mathbf{b}^{\omega_C} \\ \mathbf{b}^p \end{bmatrix}.$$

Substituting (2.8) and (2.9) in (2.7) leads to

$$(2.12) \quad 0 = \left[ \int_{\Omega} N_i^p \phi \frac{\partial \rho_R}{\partial p} N_j^p dx \right] \frac{\partial \hat{p}_j}{\partial t} + \left[ \int_{\Omega} N_i^p \phi \frac{\partial \rho_R}{\partial \omega_C} N_j^{\omega_C} dx \right] \frac{\partial \hat{\omega}_j}{\partial t} + \left[ \int_{\Omega} \nabla^T N_i^p \rho_R \frac{\kappa}{\mu} \nabla N_j^p dx \right] \hat{p}_j \\ - \int_{\Omega} \nabla^T N_i^p \rho_R \frac{\kappa}{\mu} \rho_R g e_z dx + \int_{\Omega} N_i^p Q_p dx + \int_{\Gamma_N} N_i^p g_N^p d\sigma, \\ = \mathbf{M}_{ij}^{pp} \frac{\partial \hat{p}_j}{\partial t} + \mathbf{M}_{ij}^{p \omega_C} \frac{\partial \hat{\omega}_j}{\partial t} + \mathbf{K}_{ij}^{pp} \hat{p}_j + b_i^p$$

with components  $i, j = 1, \dots, n$ , and coefficients

$$(2.13) \quad M_{ij}^{pp} = \int_{\Omega} N_i^p \phi \frac{\partial \rho_R}{\partial p} N_j^p dx \\ M_{ij}^{p \omega_C} = \int_{\Omega} N_i^p \phi \frac{\partial \rho_R}{\partial \omega_C} N_j^{\omega_C} dx \\ K_{ij}^{pp} = \int_{\Omega} \nabla^T N_i^p \rho_R \frac{\kappa}{\mu} \nabla N_j^p dx \\ b_i^p = \int_{\Omega} N_i^p Q_p dx + \int_{\Gamma_N} N_i^p g_N^p d\sigma - \int_{\Omega} \nabla^T N_i^p \rho_R \frac{\kappa}{\mu} \rho_R g e_z dx.$$

## 2.3 Component Flow - Advective Form

### 2.3.1 Weak Formulation

For the component flow, we can replace the coefficients in Equation (2.6) with

$$\underbrace{\phi \rho_R R}_{\beta = \beta_{\omega_C}} \frac{\partial \omega_C}{\partial t} - \operatorname{div} \left( \underbrace{\rho_R \mathbf{D}_h \nabla \omega_C}_{\gamma = \gamma_{\omega_C}} \right) + \underbrace{Q_{\omega_C} - \rho_R \left\langle \frac{\kappa}{\mu} (\nabla p - \rho_R g) \middle| \nabla \omega_C \right\rangle - R \omega_C Q_p + R \theta \phi \rho_R \omega_C}_{\delta = \delta_{\omega_C}} = 0.$$

and  $\gamma_{\omega_C}^N - \gamma_{\omega_C} = 0$ . Hence the weak solution of Equation (1.28) reads

$$\begin{aligned} 0 &= \int_{\Omega} \Psi^{\omega_C} R \phi \rho_R \frac{\partial \omega_C}{\partial t} \, dx \\ &\quad + \int_{\Omega} \left\langle \mathbf{grad} \Psi^{\omega_C} \middle| (\rho_R \mathbf{D}_h \nabla \omega_C) \right\rangle \, dx \\ &\quad + \int_{\Omega} \Psi^{\omega_C} (Q_{\omega_C} + R \theta \phi \rho_R \omega_C - R \omega_C Q_p) \, dx \\ &\quad - \int_{\Omega} \Psi^{\omega_C} \rho_R \left\langle \frac{\kappa}{\mu} (\nabla p - \rho_R g) \middle| \nabla \omega_C \right\rangle \, dx \\ &\quad + \int_{\Gamma_N} \Psi^{\omega_C} g_N^{\omega_C} \, d\sigma \end{aligned} \tag{2.14}$$

### 2.3.2 Finite Element Discretization

Using the shape functions defined in Section 2.2.2 the finite element discretization of equation (2.21) reads

$$\begin{aligned} 0 &= \left[ \int_{\Omega} N_i^{\omega} R \phi \rho_R N_j^{\omega} \, dx \right] \frac{\partial \hat{\omega}_j}{\partial t} \\ &\quad + \left[ \int_{\Omega} \left\langle \nabla^T N_i^{\omega} \middle| \rho_R \mathbf{D}_h \nabla N_j^{\omega} \right\rangle \, dx \right] \hat{\omega}_j \\ &\quad + \int_{\Omega} N_i^{\omega} Q_{\omega_C} \, dx + \left[ \int_{\Omega} N_i^{\omega} R \theta \phi \rho_R N_j^{\omega} \, dx \right] \hat{\omega}_j - \left[ \int_{\Omega} N_i^{\omega} R Q_p N_j^{\omega} \, dx \right] \hat{\omega}_j \\ &\quad + \int_{\Omega} N_i^{\omega} \rho_R \left\langle q \middle| \nabla \omega_C \right\rangle \, dx + \int_{\Gamma_N} N_i^{\omega} g_N^{\omega_C} \, d\sigma \\ &= \mathbf{M}_{ij}^{\omega_C p} \frac{\partial \hat{p}_j}{\partial t} + \mathbf{M}_{ij}^{\omega_C \omega_C} \frac{\partial \hat{\omega}_j}{\partial t} + \mathbf{K}_{ij}^{\omega_C \omega_C} \hat{\omega}_j + b_i^{\omega} \end{aligned} \tag{2.15}$$

where we used the abbreviation

$$q(t) = -\frac{\kappa}{\mu} (\nabla p - \rho_R g). \tag{2.16}$$

The coefficients for the shape matrices read

$$(2.17) \quad \mathbf{M}_{ij}^{\omega_C \omega_C} = \int_{\Omega} N_i^{\omega} R \phi \rho_R N_j^{\omega} \, dx$$

$$(2.18) \quad \mathbf{K}_{ij}^{\omega_C \omega_C} = \int_{\Omega} \left\langle \nabla^T N_i^{\omega} \left| \rho_R \mathbf{D}_h \nabla N_j^{\omega} \right. \right\rangle dx + \int_{\Omega} N_i^{\omega} R \theta \phi \rho_R N_j^{\omega} \, dx$$

$$(2.19) \quad - \int_{\Omega} N_i^{\omega} R Q_p N_j^{\omega} \, dx$$

$$(2.20) \quad b_i^{\omega_C} = \int_{\Omega} N_i^{\omega} Q_{\omega_C} \, dx + \int_{\Gamma_N} N_i^{\omega} g_N^{\omega_C} \, d\sigma + \int_{\Omega} N_i^{\omega} \rho_R \left\langle q \left| \nabla \omega_c \right. \right\rangle \, dx.$$

## 2.4 Component Flow - Non Advective Form

### 2.4.1 Weak Formulation

For the component flow, we can replace the coefficients in Equation (2.6) with

$$\underbrace{\omega_C R \phi \frac{\partial \rho_R}{\partial p} \frac{\partial p}{\partial t}}_{\alpha = \alpha_{\omega_C}} + \underbrace{\omega_C R \phi \left( \frac{\rho_R}{\omega_C} + \frac{\partial \rho_R}{\partial \omega_C} \right) \frac{\partial \omega_C}{\partial t}}_{\beta = \beta_{\omega_C}} - \operatorname{div} \underbrace{\left( \frac{\kappa}{\mu} \rho_R \omega_C (\nabla p - \rho_R g) + \rho_R \mathbf{D}_h \nabla \omega_C \right)}_{\gamma = \gamma_{\omega_C}} + \underbrace{Q_{\omega_C} + R \theta \phi \rho_R \omega_C}_{\delta = \delta_{\omega_C}} = 0,$$

and  $\gamma_{\omega_C}^N - \gamma_{\omega_C} = 0$ . Hence the weak solution of Equation (1.28) reads

$$(2.21) \quad \begin{aligned} 0 &= \int_{\Omega} \Psi^{\omega_C} \left( \omega_C R \phi \frac{\partial \rho_R}{\partial p} \right) \frac{\partial p}{\partial t} \, dx \\ &+ \int_{\Omega} \Psi^{\omega_C} \left( \omega_C R \phi \left( \frac{\rho_R}{\omega_C} + \frac{\partial \rho_R}{\partial \omega_C} \right) \right) \frac{\partial \omega_C}{\partial t} \, dx \\ &+ \int_{\Omega} \left\langle \mathbf{grad} \Psi^{\omega_C} \left| \left( \frac{\kappa}{\mu} \rho_R \omega_C (\nabla p - \rho_R g) + \rho_R \mathbf{D}_h \nabla \omega_C \right) \right. \right\rangle dx \\ &+ \int_{\Omega} \Psi^{\omega_C} (Q_{\omega_C} + R \theta \phi \rho_R \omega_C) \, dx \\ &+ \int_{\Gamma_N} \Psi^{\omega_C} g_N^{\omega_C} \, d\sigma. \end{aligned}$$

## 2.4.2 Finite Element Discretization

Using the shape functions defined in Section 2.2.2 the finite element discretization of equation (2.21) reads

$$\begin{aligned}
(2.22) \quad 0 &= \left[ \int_{\Omega} N_i^{\omega} \left( \omega_C R \phi \frac{\partial \rho_R}{\partial p} \right) N_j^p \, dx \right] \frac{\partial \hat{p}_j}{\partial t} \\
&+ \left[ \int_{\Omega} N_i^{\omega} \left( R \phi \left( \rho_R + \omega_C \frac{\partial \rho_R}{\partial \omega_C} \right) \right) N_j^{\omega} \, dx \right] \frac{\partial \hat{\omega}_j}{\partial t} \\
&+ \left[ \int_{\Omega} \left\langle \nabla^T N_i^{\omega} \left| (-q \rho_R N_j^{\omega} + \rho_R \mathbf{D}_h \nabla N_j^{\omega}) \right. \right\rangle dx \right] \hat{\omega}_j \\
&+ \int_{\Omega} N_i^{\omega} Q_{\omega_C} \, dx + \left[ \int_{\Omega} N_i^{\omega} R \theta \phi \rho_R N_j^{\omega} \, dx \right] \hat{\omega}_j \\
&+ \int_{\Gamma_N} N_i^{\omega} g_N^{\omega_C} \, d\sigma \\
&= \mathbf{M}_{ij}^{\omega_C p} \frac{\partial \hat{p}_j}{\partial t} + \mathbf{M}_{ij}^{\omega_C \omega_C} \frac{\partial \hat{\omega}_j}{\partial t} + \mathbf{K}_{ij}^{pp} \hat{p}_j + b_i^{\omega}
\end{aligned}$$

where we used the abbreviation

$$(2.23) \quad q(t) = -\frac{\kappa}{\mu} (\nabla p - \rho_R g).$$

The coefficients for the shape matrices read

$$(2.24) \quad \mathbf{M}_{ij}^{\omega_C p} = \int_{\Omega} N_i^{\omega} \left( \omega_C R \phi \frac{\partial \rho_R}{\partial p} \right) N_j^p \, dx$$

$$(2.25) \quad \mathbf{M}_{ij}^{\omega_C \omega_C} = \int_{\Omega} N_i^{\omega} \left( R \phi \left( \rho_R + \omega_C \frac{\partial \rho_R}{\partial \omega_C} \right) \right) N_j^{\omega} \, dx$$

$$(2.26) \quad \mathbf{K}_{ij}^{\omega_C \omega_C} = \int_{\Omega} \left\langle \nabla^T N_i^{\omega} \left| (-q \rho_R N_j^{\omega} + \rho_R \mathbf{D}_h \nabla N_j^{\omega}) \right. \right\rangle dx$$

$$(2.27) \quad + \int_{\Omega} N_i^{\omega} R \theta \phi \rho_R N_j^{\omega} \, dx$$

$$(2.28) \quad b_i^{\omega_C} = \int_{\Omega} N_i^{\omega} Q_{\omega_C} \, dx + \int_{\Gamma_N} N_i^{\omega} g_N^{\omega_C} \, d\sigma.$$