Non-isothermal single phase flow in partially saturated deformable porous media

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1. Balance equations of THM coupled systems

The governing equations, which are essential for the analysis, are detailed hereafter.

1.1. Energy balance equation

For heat transport problem, we consider the convective transport, i.e. the transport of heat by flow. There are two basic kinds of convection recognized such as *forced convection* and *free convection*. In the former, the velocity of convective motion does not has any impact on the temperature on the fluids and the heat energy transport is forced by the flow movement. In the latter, flow velocities are driven solely by buoyancy effects in the fluid, and these are related to temperature change through the coefficient of thermal expansion. In real ground water systems, there is a mixture of both types of convection. The simple expression of heat flux in forced convection is given by

$$\mathbf{q}^{\mathrm{T}} = -\boldsymbol{\lambda}_{T}{}^{\mathrm{eff}}\nabla T + \phi\varrho_w c_p T \mathbf{v}_{\mathrm{w}} \tag{1}$$

where $\boldsymbol{\lambda}_{T}{}^{\mathrm{eff}}$ is the effective heat conductivity tensor, $\phi(\varrho c_p)T\mathbf{v}_{\mathrm{w}}$ is the flux of heat transported by water velocity $\mathbf{v}_{\mathrm{w}}$ per unit area, and across the entire rock face this flux is reduced by the effective porosity, ϕ. With the definition of heat flux (1), the governing equation of the convective heat transport can be derived for any point $\mathbf{x} \in \Omega \in \mathbb{R}^{\mathrm{n}}$ as

$$(\varrho c_p)\frac{\partial T}{\partial t} - \nabla\mathbf{q}^{\mathrm{T}} + Q_T = 0 \tag{2}$$

with boundary condition

$$-\mathbf{q}^{\mathrm{T}} \cdot \mathbf{n} = q_{\mathrm{r}}|_{\Gamma}, \text{ or } \quad T = T_{\Gamma}, \forall \mathbf{x} \in \partial\Omega \tag{3}$$

and initial condition

$$T(\mathbf{x}) = T_0(\mathbf{x}), \forall \mathbf{x} \in \Omega \tag{4}$$

1.2. Mass balance equation

Consider a general case of a flow problem in deformable porous media under the Richard's approximation. With the classical Darcy's law, the large scale water flow $\mathbf{q}^{\mathrm{w}}$ is defined as

$$\mathbf{q}^{\mathrm{w}} = -\phi S \varrho_w \frac{\mathbf{k}\mathbf{k}_{\mathrm{rel}}}{\mu}(\nabla p - \varrho_w \mathbf{g}) \tag{5}$$

where S is the water saturation, p is the water pressure, ϱ_w is the water density, ϕ is the effective porosity of the media, μ is the viscosity of flow, $\mathbf{k}$ denotes intrinsic permeability, $\mathbf{k}_{\mathrm{rel}}$ is the relative permeability, and $\mathbf{g}$ is the gravity force by density. Meanwhile, we consider vapor flow filled pores due to

molecular diffusion, which is coupled with temperature. Similar to what is defined in [4], the vapor flow is given by

$$\mathbf{q}^{\mathrm{v}} = -D_{pv}\nabla p - f_{Tv}D_{Tv}\nabla T \tag{6}$$

where f_Tv is a thermal diffusion enhancement factor takes value of 1.0 in the present simulation, D_{pv} and D_{Tv} are diffusion coefficients takes form as

$$\begin{aligned} D_{pv} &= \frac{D_v\varrho_v}{\varrho_w R T_{abs}} \\ D_{Tv} &= D_v\left(h\frac{\partial\varrho_{vS}}{\partial T} - \frac{\varrho_v p}{\varrho_w R T_{abs}^2}\right) \end{aligned} \tag{7}$$

with h, the relative humidity according to

$$h = e^{p/\varrho_w R T_{abs}} \tag{8}$$

$R = 461.6 J/kgK$, the specific gas constant for water vapor, ϱ_{vS}, the saturated vapor density given by

$$\varrho_{vS} = 10^{-3} e^{19.891 - 4975/T_{abs}} \tag{9}$$

and vapor density $\varrho_v = h \, \varrho_{vS}$.

The factor D_v is the water vapor diffusion coefficient, which is determined experimentally [2, 3, 1], and its empirical expression takes the form of

$$D_v = 2.16 \cdot 10^{-5} \left(\frac{T_{abs}}{273.15} \right)^{1.8} D_{vr} \tag{10}$$

for bentonite material with D_{vr} the relative diffusion coefficient. So far, D_{vr} has two assumptions as

- $D_{vr} = \tau \phi (1 - S)$, with tortuosity $\tau = 0.8$ for the FEBEX bentonite [4].

- $D_{vr} = 0.66 \phi (1 - S)^2$, the Penman-Millington-Quirk (PMQ) model[1] with tortuosity $\tau = 0.66$.

The expressions of flow defined in (5) and (6) lead the governing equation of flow field in the terms of mass balance equation given by

$$\phi \left[\frac{\varrho_w - \varrho_v}{\varrho_w} \frac{\partial S}{\partial p} + S \beta_p + (1 - S) \frac{\varrho_v}{\varrho_w^2 R T_{abs}} \right] \frac{d_S p}{dt}$$
$$- \left[H(1 - S) \phi \alpha_T^{\text{L}} + 3(1 - \phi) \alpha_T^{\text{S}} \right] \frac{d_S T}{dt}$$
$$\phi \frac{1 - S}{\varrho_w} \left(h \frac{\partial \varrho_{vS}}{\partial T} + \frac{\varrho_v P}{R T_{abs}^2} \right) \frac{d_S T}{dt}$$
$$+ \nabla \cdot (\mathbf{q}^{\text{w}} + \mathbf{q}^{\text{v}}) / \varrho_w + S \frac{\partial}{\partial t} (\nabla \cdot \mathbf{u}) = Q_H \tag{11}$$

for any point $\mathbf{x} \in \Omega \in \mathbb{R}^{\text{n}}$ with n the dimension of the real space, where $H(1 - S)$ is the Heaviside step functionα_T^{L} is the volumetric thermal expansion of fluid, α_T^{S} is the linear thermal expansion of the solid, and Q_H is the sink or source term of the fluid field. In eqn. (11), β_p is the storitivity. The unknown of eqn. (11) to be solved are saturation of the phase S, fluid pressure p and the coupling term, i.e. temperature and displacement $\mathbf{u}$, deduced by solid deformation. The boundary conditions for this problem can be simplified for this Richard's flow model

$$-(\mathbf{q}^{\text{w}} + \mathbf{q}^{\text{v}}) \cdot \mathbf{n} = q_\Gamma, \forall \mathbf{x} \in \partial \Omega \tag{12}$$

or Dirichlet type as

$$p = p_\Gamma, \forall \mathbf{x} \in \partial \Omega \tag{13}$$

This initial-boundary-value-problem can be solved with the corresponding initial condition of unknowns.

1.3. Momentum balance equation

Deformations in porous media can be described by the momentum balance equation in the terms of stress as

$$\nabla \cdot \boldsymbol{\sigma} + \varrho \mathbf{g} = 0 \tag{14}$$

with $\boldsymbol{\sigma}$ the total stress, which can be defined for different mechanical sceneries. For example, under the assumption of linear elasticity and non-swelling in the porous media, the total stress is given by

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\text{eff}} - \alpha_{\text{B}} S p \, \mathbf{I} \tag{15}$$

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with $\boldsymbol{\sigma}^{\text{eff}}$, the effective stress, and α_{B} the Biot's constant. The Bishop models can be considered in expression (15) for the pore pressure contribution to the total stress.

Considering the solid thermal expansion, the effective stress given by

$$\boldsymbol{\sigma}^{\text{eff}} = \mathcal{C}(\boldsymbol{\epsilon} - \alpha_T \Delta T)$$

with $\mathcal{C}$ the fourth order elastic tensor, $\boldsymbol{\epsilon}$ the train tensor, and α_T the thermal expansion coefficient.

References

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