Diffusion and Seepage of Mixture Fluid in Porous Media

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1. Introduction

In the field of geomechanics the diffusion problem in porous media saturated with multi-component solution has been treated independently of the seepage problem [1], [2]. This is a strange context since both problems must be established on the basis of mass conservation. We here discuss a relation of diffusion and seepage on the basis of mixture theory [3]. In the seepage problem we shed light on a physical implication of seepage velocity. In the diffusion problem we show sorption can be introduced on concepts of a source term, a distribution factor or an equation of adsorption isotherm. Note that we can apply a multi-scale homogenization analysis [4] for this diffusion problem, and the molecular dynamics (MD) simulation is essentially important to specify the local properties of the porous media [5]. Notation: "!α" implies "do not sum over the subscript repeated α".

2. Diffusion and Seepage Theory in Porous Media Saturated with Multi-component Solution

Diffusion equation in fluid phase

If n_α is the amount of substance of the αth species of the mixture fluid, the volume-molar concentration or fraction Ω_α and mass density ρ_α are defined as follows:

$$n_\alpha = \int_\Omega n\,\omega_\alpha dv = \int_\Omega n\frac{\rho_\alpha}{m_\alpha}dv \qquad (!\alpha) \tag{1}$$

where n is the porosity and m_α is the molecular weight of the αth species.

Let γ_α be the mass supply of the αth species caused by, for example, a chemical reaction, and ζ_α be an adsorption at each local grain surface Γ^i_{fs}. Then the mass conservation law of the αth species can be written by

$$\frac{d_{(\alpha)}(n\rho_\alpha)}{dt} + n\rho_\alpha \operatorname{div} v_\alpha = \frac{\partial(n\rho_\alpha)}{\partial t} + \operatorname{div}(n\rho_\alpha v_\alpha) = n\gamma_\alpha - \varsigma^*_\alpha \qquad (!\alpha) \tag{2}$$

where v_α is the velocity of the αth species in mixture fluid and ζ^*_α is the volumetrically estimated adsorption derived from ζ_α. We sum up (2) for all the αth species and get

$$\frac{d(n\rho)}{dt} + n\rho \operatorname{div} v = \frac{\partial(n\rho)}{\partial t} + \operatorname{div}(n\rho v) = 0; \qquad v = \frac{1}{\rho}\sum_\alpha \rho_\alpha v_\alpha,\quad \rho = \sum_\alpha \rho_\alpha \quad \varsigma^* = \sum_\alpha \varsigma^*_\alpha \tag{3}$$

We define the diffusion velocity $\bar{v}_\alpha = v_\alpha - v$ and the mass concentration $c_\alpha = \rho_\alpha / \rho$, then by substituting these into (2) we get the following diffusion equation:

$$n\rho\frac{dc_\alpha}{dt} = n\rho\left(\frac{\partial c_\alpha}{\partial t} + v\cdot\operatorname{grad} c_\alpha\right) = -\operatorname{div}(n\rho_\alpha \bar{v}_\alpha) + n\gamma_\alpha - \varsigma^*_\alpha \qquad (!\alpha) \tag{4}$$

Note that we have the constrain condition $\sum_\alpha c_\alpha = 1$, and we can introduce Fick's law as $n\rho_\alpha \bar{v}_\alpha = -\sum_\beta D_{\alpha\beta} \operatorname{grad} c_\beta$.

Diffusion equation in solid phase

Similar to the above discussion we the diffusion equations of solid phase corresponding to (1), (2), (3) and (4):

$$n^*_\alpha = \int_\Omega (1-n)\,\omega^*_\alpha dv = \int_\Omega (1-n)\frac{\rho^*_\alpha}{m_\alpha} dv \qquad (!\alpha) \tag{5}$$

$$\frac{d_{(*\alpha)}\left((1-n)\rho^*_\alpha\right)}{dt} + (1-n)\rho^*_\alpha \operatorname{div} v^*_\alpha = \frac{\partial\left((1-n)\rho^*_\alpha\right)}{\partial t} + \operatorname{div}\left((1-n)\rho^*_\alpha v^*_\alpha\right) = (1-n)\gamma^*_\alpha - \varsigma^*_\alpha \qquad (!\alpha) \tag{6}$$

$$\frac{d_*\left((1-n)\rho^*\right)}{dt} + (1-n)\rho^* \operatorname{div} v^* = \frac{\partial\left((1-n)\rho^*\right)}{\partial t} + \operatorname{div}\left((1-n)\rho^* v^*\right) = 0;\quad v^* = \frac{1}{\rho^*}\sum_\alpha \rho^*_\alpha v^*_\alpha,\ \rho^* = \sum_\alpha \rho^*_\alpha \tag{7}$$

$$(1-n)\rho^* \frac{d_* c^*_\alpha}{dt} = (1-n)\rho^*\left(\frac{\partial c^*_\alpha}{\partial t} + v^* \cdot \operatorname{grad} c^*_\alpha\right) = -\operatorname{div}\left((1-n)\rho^*_\alpha \bar{v}^*_\alpha\right) + (1-n)\gamma^*_\alpha - \varsigma^*_\alpha \qquad (!\alpha) \tag{8}$$

where we have the constraint $\sum_\alpha c^*_\alpha = 1$ and define the velocity gradient $\boldsymbol{L}^*$, stretching tensor $\boldsymbol{D}^*$ and spin tensor $\boldsymbol{W}^*$ of the solid phase as

$$\boldsymbol{L}^* = \operatorname{grad} v^* = \boldsymbol{D}^* + \boldsymbol{W}^*;\qquad \boldsymbol{D}^* = \left(\boldsymbol{L}^* + \boldsymbol{L}^{*T}\right)/2,\quad \boldsymbol{W}^* = \left(\boldsymbol{L}^* - \boldsymbol{L}^{*T}\right)/2 \tag{9}$$

Seepage equation

When we solve the diffusion equation (4), it is a question how to specify the mean velocity $\boldsymbol{v}$. For this purpose in geomechanics it is common to derive the seepage equation from (3) and (7) under the incompressible condition of fluid and intrinsic solid part, i.e., ρ=constant, ρ^*=constant. Under these conditions (3) and (7) become

$$\frac{dn}{dt} + \operatorname{div}(n\boldsymbol{v}) - \boldsymbol{v} \cdot \operatorname{grad} n = 0 \tag{10}$$

$$-\frac{d_* n}{dt} + (1-n)\operatorname{tr} \boldsymbol{D}^* = 0 \tag{11}$$

We have the following relation

$$\frac{d_* n}{dt} = \frac{dn}{dt} - (\boldsymbol{v} - \boldsymbol{v}^*) \cdot \operatorname{grad} n = 0 \tag{12}$$

and by substituting (12) into (11) we get

$$\frac{dn}{dt} = (1-n)\operatorname{tr} \boldsymbol{D}^* + \boldsymbol{v}^* \cdot \operatorname{grad} n \tag{13}$$

We substitute (13) into (10) and get the following seepage equation:

$$(1-n)\operatorname{tr} \boldsymbol{D}^* + \operatorname{div}(n\boldsymbol{v}) - \boldsymbol{v}^* \cdot \operatorname{grad} n = 0 \tag{14}$$

We can use Darcy's law for (14).

3. Conclusion

We derived the diffusion equations in fluid phase and solid phase based on the mass conservation law, and then we showed the seepage equation from these diffusion equations. Thus both diffusion and seepage phenomena can be drawn in the same framework.

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