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On one model of solute transport in poroelastic shale*

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Abstract. A chemically inert deformable rock is considered, taking into account only changes in stress and pore pressure: the chemistry of a porous fluid has no direct effect on deformation. Accounting the chemical effects leads to changes in the pore pressure and in the strain of rocks. This theory is applied to mathematical modeling of the transfer of solvent and solute through a semi-permeable shale.

Keywords: porous medium, saturated fluid, elastic parameters, stress tensor, partial density, Darcy law, chemical potential.

1. Introduction

Cations may exchange in a shale between the clay surfaces and the pore fluid involved. Other solutes can also be adsorbed or desorbed at the pore walls. These effects can be neglected [1]. The resulting transfer analysis is valid only for the molecules that are not inclined to adsorb, or for the molecules whose amount is already sufficient in the pores, so that the balance between the rock and the pore fluid is not disturbed. An example is the transfer of sodium through clay, which contains only sodium counterions. Neglecting adsorption/desorption and direct chemical effects in the theory of poroelasticity, the stress-strain, simplifies the basic equations.

For simplicity, let us consider a porous liquid following [1], that consists of one uncharged solute with a molar fraction x^s in a solvent (water) with a molar fraction $x^w = 1 - x^s$. In this case, the solution is considered to be ideal. The chemical potentials of the solute μ^s and the solvent μ^w are the following:

$$\mu^s = pV_s + RT \ln x^s, \qquad \mu^w = pV_w + RT \ln x^w,$$

where p is the pressure, R is the gas constant, T is the temperature and V_s, V_w are the partial molar volumes of solute and solvent, respectively. The molar volume of the solution (at the atmosphere pressure) is

$$V_{\text{soln}} = (1 - x^s)V_w + x^s V_s.$$

Assume, just like [1], that the bulk modulus K of the solution does not depend on x^s, and we confine ourselves to the isothermal case with the constant T.

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2. Transport across a membrane

Consider two solutions separated by a membrane. We denote the pressure on sides 1 and 2 of the membrane as p_1 and p_2; the mole fractions are x_1^s, x_2^s [1]. The equations of transport for the fluxes f_w and f_s of water and solute, respectively, from side 1 to side 2 per unit area of the membrane can be written down as [2]:

$$f_w = L_{ww}\Delta\mu^w + L_{ws}\Delta\mu^s, \qquad f_s = L_{sw}\Delta\mu^w + L_{ss}\Delta\mu^s,$$

where $\Delta\mu = \mu_1 - \mu_2$ means the jumps of the chemical potential and $L_{sw} = L_{ws}$ by Onsager's principle. Consequently, these fluxes can be written down as follows:

$$\begin{aligned} f_w &= (V_w L_{ww} + V_s L_{ws})\Delta p + RT(L_{ww}\Delta \ln x^w + L_{ws}\Delta \ln x^s), \\ f_s &= (V_w L_{sw} + V_s L_{ss})\Delta p + RT(L_{sw}\Delta \ln x^w + L_{ss}\Delta \ln x^s). \end{aligned}$$

Assume that the jump in the mole fraction x^s across the membrane is small, then we can set

$$\Delta \ln x^s = \frac{\Delta x^s}{x_0^s}, \qquad \Delta \ln x^w = \frac{\Delta x^s}{1 - x_0^s},$$

where x_0^s is some mean mole fraction.

There are three independent transport coefficients, L_{ww}, L_{ss}, and $L_{sw} = L_{ws}$. Instead, we will use the three transfer coefficients k, D, and γ. The fluxes f_w and f_s have the following form:

$$\begin{gathered} f_w = (1 - x_0^s)k\Delta p - V_w^{-1}[(1-\gamma)RTk + \gamma V_s D]\Delta x^s, \\ f_s = \gamma x_0^s k \Delta p + \gamma D \Delta x^s. \end{gathered}$$

Here γ is the transmission coefficient. The flux of salt due to changes in concentration is controlled by the diffusion coefficient D and is also modified by γ.

If $\gamma = 1$, then the flux of water and solute due to the pressure difference in Δp is controlled by the coefficient of the hydraulic resistance k, and the flux of each type is proportional to the mole fraction of this type. In the limit $\gamma = 0$, the following relations are valid:

$$f_w = V_w^{-1}(1 - x_0^s)k\Delta\mu^w, \qquad f_s = 0,$$

and the flux of water depends solely on the jump $\Delta\mu^w$ in the chemical potential of water.

Let us now consider a system in which the volume of the reservoir V_2 on side 2 of the membrane is kept fixed, so that any transfer to this reservoir will result in an increase in the pressure p_2. Suppose that the pressure p_1 is kept constant and the volume V_1 is sufficiently large, so that any change in the concentration of the solute x_1^s is negligible.

As is shown in [1], the rate of a change in pressure and molar fraction satisfy the one-dimensional system of diffusion equations

$$\frac{\partial p}{\partial t} = A\frac{\partial^2 p}{\partial x^2} + H\frac{\partial^2 x^s}{\partial x^2}, \qquad \frac{\partial x^s}{\partial t} = C\frac{\partial^2 p}{\partial x^2} + E\frac{\partial^2 x^s}{\partial x^2}, \tag{1}$$

where

$$A = \frac{K_e k[(1-x_0^s)V_w + \gamma x_0^s V_s]S}{\phi_0}, \qquad C = -\frac{x_0^s(1-x_0^s)(1-\gamma)V_{\text{soln}}k}{\phi_0},$$
$$H = -\frac{K_e k(1-\gamma)RT}{\phi_0}, \qquad E = \frac{[x_0^s RTk(1-\gamma) + D\gamma V_{\text{soln}}]V_{\text{soln}}}{\phi_0 V_w},$$

ϕ_0 is a certain mean porosity, S is the membrane area.

The solution of the system of diffusion equations (1) is the following:

$$\begin{aligned} p = p_2 &+ \frac{\lambda_2}{\lambda_2-\lambda_1}\left[p_1 - p_2 + \lambda_1(x_1^s - x_2^s)\right]\operatorname{erf}\Big(\frac{1}{2}x(k_1 t)^{-1/2}\Big) - \\ &\frac{\lambda_1}{\lambda_2-\lambda_1}\left[p_1 - p_2 + \lambda_2(x_1^s - x_2^s)\right]\operatorname{erf}\Big(\frac{1}{2}x(k_2 t)^{-1/2}\Big), \\ x^s = x_2^s &+ \frac{1}{\lambda_1-\lambda_2}\left[p_1 - p_2 + \lambda_1(x_1^s - x_2^s)\right]\operatorname{erf}\Big(\frac{1}{2}x(k_1 t)^{-1/2}\Big) - \\ &\frac{1}{\lambda_1-\lambda_2}\left[p_1 - p_2 + \lambda_2(x_1^s - x_2^s)\right]\operatorname{erf}\Big(\frac{1}{2}x(k_2 t)^{-1/2}\Big), \end{aligned}$$

where $\operatorname{erf}(x)$ is the error function, with $\operatorname{erf}(0) = 0$ and $\operatorname{erf}(x) \to 1$ as $x \to \infty$,

$$\lambda_1 = \frac{E - A + ((E-A)^2 + 4HC)^{1/2}}{2C}, \tag{2}$$
$$\lambda_2 = \frac{E - A - ((E-A)^2 + 4HC)^{1/2}}{2C}; \tag{3}$$

two relaxation rates are determined as follows

$$k_1 = A + \lambda_1 C = \frac{E + A + ((E-A)^2 + 4HC)^{1/2}}{2}, \tag{4}$$
$$k_2 = A + \lambda_2 C = \frac{E + A - ((E-A)^2 + 4HC)^{1/2}}{2}. \tag{5}$$

3. Poroelasticity theory

In order to connect changes in the rock deformation e_{ij} with changes in the applied stress σ_{ij} and changes in the chemical potentials of the components of the porous fluid, we use the modified poroelasticity theory. If the pore fluid contains chemicals with the chemical potentials μ^i, $i = 1, \dots, n$, and with the mass m^i (per unit volume of a porous material), then [3]

$$de_{ij} = S_{ijkl} d\sigma_{kl} + \sum_p Q^p_{ij} d\mu^p, \tag{6}$$

$$dm^p = Q^p_{ij} d\sigma_{ij} + \sum_q B^{pq} d\mu^q, \tag{7}$$

where the cross-coefficients Q^r_{ij} are common for (6) and (7), and $B^{rs} = B^{sr}$.

Assume that a change in the applied stress $d\sigma_{ij}$ compresses the components of the pore fluid is proportional to their molar fractions and, therefore, (7), $Q^p_{ij} = x^p$. From the Gibbs–Dumen equation it follows that $\sum_p Q^p_{ij} d\mu^p = V_{\text{soln}} dp$ and only changes in the pore pressure are required for solving (6). Assume that a rock is isotropic with the shear modulus G, the Skempton parameter B, and the drained and undrained Poisson ratios ν, ν_u, respectively. Then equation (6) takes the following form:

$$2G de_{ij} = d\sigma_{ij} - \frac{\nu}{1+\nu} d\sigma_{kk} \delta_{ij} + \frac{3(\nu_u - \nu)}{B(1+\nu)(1+\nu_u)} p \delta_{ij}. \tag{8}$$

The chemical potentials μ^i in (7) cannot be reduced to a simple pore pressure p. However, in a two-component porous liquid, it is convenient to use the pressure p and the molar fraction x^s, rather than the chemical potentials μ^s, μ^w, respectively. Thus, for some constant α there are:

$$dm^s = \frac{3x^s(\nu_u - \nu)}{2GB(1+\nu)(1+\nu_u)V_{\text{soln}}} [d\sigma_{kk} + 3B^{-1} dp] + \frac{\alpha}{V_s} dx^s,$$

$$dm^w = \frac{3(1 - x^s)(\nu_u - \nu)}{2GB(1+\nu)(1+\nu_u)V_{\text{soln}}} [d\sigma_{kk} + 3B^{-1} dp] - \frac{\alpha}{V_w} dx^s.$$

If the pore volume (per unit reference volume) is ϕ_0, the number of moles of a solvent and a solute is as follows

$$m^w = (1 - x^s) \frac{\phi_0}{V_{\text{soln}}}, \qquad m^s = x^s \frac{\phi_0}{V_{\text{soln}}}$$

and, hence

$$\alpha = \frac{\phi_0 V_w V_s}{V^2_{\text{soln}}}.$$

Using the conservation laws

$$\frac{\partial m^s}{\partial t} + \nabla f_s = 0, \qquad \frac{\partial m^w}{\partial t} + \nabla f_w = 0,$$

we obtain

$$\frac{3x^s(\nu_u-\nu)}{2GB(1+\nu)(1+\nu_u)V_{\text{soln}}}\left[\frac{\partial\sigma_{kk}}{\partial t}+\frac{3}{B}\frac{\partial p}{\partial t}\right]+\frac{\alpha}{V_s}\frac{\partial x^s}{\partial t}$$
$$=\lambda k\nabla x^s\nabla p+\lambda D\Delta x^s, \tag{9}$$

and

$$\frac{3(1-x^s)(\nu_u-\nu)}{2GB(1+\nu)(1+\nu_u)V_{\text{soln}}}\left[\frac{\partial\sigma_{kk}}{\partial t}+\frac{3}{B}\frac{\partial p}{\partial t}\right]-\frac{\alpha}{V_w}\frac{\partial x^s}{\partial t}$$
$$=k\nabla(1-x^s)\nabla p-[(1-\lambda)RTk+\lambda DV_s]V_w^{-1}\Delta x^s. \tag{10}$$

Following [1], we further assume that changes x^s are sufficiently small, and we can neglect changes in coefficients in (9) and (10). After simple transformations, we obtain a system of diffusion equations:

$$\frac{\partial\Phi}{\partial t}=A\nabla^2\Phi+H\nabla^2x^s,\qquad \frac{\partial x^s}{\partial t}=C\nabla^2\Phi+E\nabla^2x^s, \tag{11}$$

where

$$\begin{aligned}
\Phi&=\sigma_{kk}+\frac{3p}{B},\\
A&=\frac{2GB^2k(1-\nu)(1+\nu_u)^2}{9(1-\nu_u)(\nu_u-\nu)V_{\text{soln}}}[\gamma V_sx_0^s+V_w(1-x_0^s)],\\
H&=\frac{2GB(1+\nu)(1+\nu_u)(\gamma-1)RTk}{3(\nu_u-\nu)},\\
C&=\frac{(\gamma-1)Bk(1-\nu)(1+\nu_u)V_sV_wx_0^s(1-x_0^s)}{3(1-\nu_u)(1+\nu)\alpha V_{\text{soln}}},\\
E&=\frac{V_s}{\alpha V_{\text{soln}}}[\gamma DV_{so\ln}+(1-\gamma)RTkx_0^s].
\end{aligned}$$

As is shown in [4–7], the coefficients ν and k can be associated with the porosity:

$$\nu=\frac{\tilde\lambda}{2(\tilde\lambda+G)},\quad \tilde\lambda=\lambda-(\alpha\rho^2)^{-1}K^2,\quad K=\lambda+\frac{2}{3}G,\quad k=\frac{\mu}{\chi\rho\rho_l},$$

where μ is the water viscosity, χ is the friction coefficient, $\rho=\rho_l+\rho_s$, $\rho_s=\rho_s^f(1-d_0)$ and $\rho_l=\rho_l^fd_0$, d_0 is the porosity, ρ_s^f and ρ_l^f are the physical densities of the elastic porous body and the liquid, respectively, λ, G, $\alpha\rho^2$ are the elastic parameters of the porous medium [8]. The elastic parameters K, G, $\alpha\rho^2$ are expressed in terms of the velocity of the propagation of the transverse wave c_s and two velocities of the longitudinal waves c_{p_1}, c_{p_2} [9,10].

4. Modeling the swelling process around the wellbore

We now apply the results of the previous paragraph to a two-dimensional plane strain analysis of a cylindrical wellbore of radius b surrounded by a porous rock. We assume that the pore pressure and the mole fraction of a solute within the rock are initially p^{∞} and x^s_{∞}. The stress at infinity is uniform, with the components $\sigma_{zz} = \sigma^{\infty}_{zz}$ and $\sigma_{rr} = \sigma_{\theta\theta} = \sigma^{\infty}_{rr}$. After drilling (at the time instant $t = 0$), the boundary conditions at the wellbore (at $r = b$) take the form

$$p = -\sigma_{rr} = p_{\text{mud}}, \quad x^s = x^s_{\text{mud}},$$

where p_{mud} is the pressure of the drilling fluid within the wellbore, and x^s_{mud} is the mole fraction of solute within the drilling fluid.

Next, following [11,12] consider the behavior of a rock at infinity as initial state, and measure all the stresses, pressures and concentrations relative to those at infinity, so that the boundary conditions in the well at $r = b$ have the form [1]:

$$\begin{aligned} p = p_w &= p_{\text{mud}} - p^{\infty}, \\ \sigma_{rr} = \sigma^w_{rr} &= -p_{\text{mud}} - \sigma^{\infty}_{rr}, \\ x^s = x^s_w &= x^s_{\text{mud}} - x^s_{\infty}, \end{aligned} \tag{12}$$

Consequently, the process of diffusion of deformation is controlled by the system of equations (11). Applying the Fourier transform with respect to time to both parts of system (11) we obtain

$$i\omega\hat{\Phi} = A\nabla^2\hat{\Phi} + H\nabla^2\hat{x}^s, \qquad i\omega\hat{x}^s = C\nabla^2\hat{\Phi} + E\nabla^2\hat{x}^s, \tag{13}$$

where

$$\hat{v}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} v \, dt.$$

The bounded solution of system (13) is the following:

$$\hat{\Phi} + \lambda_i \hat{x}^s = B_i(\omega) H_0^{(1)}(q_i r), \quad i = 1, 2,$$

where $q_i = \sqrt{i\omega/k_i}$, $H_0^{(1)}$ is the Hankel function, $B_i(\omega)$ are unknown functions, and the coefficients λ_i and k_i are determined by formulas (2)–(5).

Using the boundary conditions (12) when $r = b$, we obtain

$$B_i(\omega) = \left[\frac{3(1+\nu)(1-\nu_u)}{B(1-\nu)(1+\nu_u)} p_w + \lambda_i x^s_w \right] \Big/ H_0^{(1)}(q_i b), \quad i = 1, 2.$$

Then the bounded solution takes the following form:

$$\begin{aligned}
\hat{x}^s &= \frac{B_1(\omega)H_0^{(1)}(q_1 r) - B_2(\omega)H_0^{(1)}(q_2 r)}{\lambda_1 - \lambda_2},\\
\hat{\Phi} &= \frac{\lambda_2 B_1(\omega)H_0^{(1)}(q_1 r) - \lambda_1 B_2(\omega)H_0^{(1)}(q_2 r)}{\lambda_2 - \lambda_1},\\
\hat{p} &= \frac{B(1-\nu)(1+\nu_u)}{3(1+\nu)(1-\nu_u)}\hat{\Phi}.
\end{aligned}$$

Since there are no deformations in the direction z and, therefore, by virtue of (8),

$$\hat{\sigma}_{zz} = \frac{\nu\hat{\Phi}}{1+\nu} - \frac{3\nu_u \hat{p}}{B(1+\nu_u)} = \frac{(\nu-\nu_u)}{(1+\nu)(1-\nu_u)}\hat{\Phi}.$$

From the equilibrium equation it follows that

$$\sigma_{kk} = -\frac{6(\nu_u - \nu)}{B(1-\nu)(1+\nu_u)}p. \tag{14}$$

From (8) and (14), we find that the radial displacement $u(r,t)$ satisfies

$$2G\frac{\partial}{\partial r}(ur) = \frac{r(\nu_u-\nu)}{(1+\nu)(1-\nu_u)}\Phi,$$

and, hence

$$2G\hat{u}r = C_2(\omega) + \frac{r(\nu_u-\nu)}{(1+\nu)(1-\nu_u)(\lambda_2-\lambda_1)} \times \left[\frac{\lambda_1 B_2(\omega)H_1^{(1)}(q_2 r)}{q_2} - \frac{\lambda_2 B_1(\omega)H_1^{(1)}(q_1 r)}{q_1}\right],$$

where $C_2(s)$ is a constant of integration. The radial stress is defined as

$$\hat{\sigma}_{rr} = \frac{b^2}{r^2}\sigma_{rr}^w + \frac{(\nu_u-\nu)}{(1+\nu)(1-\nu_u)(\lambda_2-\lambda_1)} \times \left[\lambda_2 B_1(\omega)\left(\frac{H_1^{(1)}(q_1 r)}{q_1 r} - \frac{bH_1^{(1)}(q_1 b)}{q_1 r^2}\right) - \lambda_1 B_2(\omega)\left(\frac{H_1^{(1)}(q_2 r)}{q_2 r} - \frac{bH_1^{(1)}(q_2 b)}{q_2 r^2}\right)\right],$$

where, taking into account the stress boundary condition in the wellbore, it is possible to determine the constant

$$C_2(\omega) = -b^2\sigma_{rr}^w + \frac{(\nu_u-\nu)b}{(1+\nu)(1-\nu_u)(\lambda_2-\lambda_1)} \times \left[\lambda_2 B_1(\omega)\frac{H_1^{(1)}(q_1 b)}{q_1} - \lambda_1 B_2(\omega)\frac{H_1^{(1)}(q_2 b)}{q_2}\right].$$

The tangential stress is determined by the formula

$$\hat{\sigma}_{\theta\theta} = -\frac{b^2}{r^2}\sigma^w_{rr} + \frac{\nu_u - \nu}{(1+\nu)(1-\nu_u)(\lambda_2 - \lambda_1)} \times$$
$$\Bigg[\lambda_1 B_2(\omega)\bigg(\frac{H_1^{(1)}(q_2 r)}{q_2 r} - \frac{bH_1^{(1)}(q_2 b)}{q_2 r^2} + H_0^{(1)}(q_2 r)\bigg) -$$
$$\lambda_2 B_1(\omega)\bigg(\frac{H_1^{(1)}(q_1 r)}{q_1 r} - \frac{bH_1^{(1)}(q_1 b)}{q_1 r^2} + H_0^{(1)}(q_1 r)\bigg)\Bigg].$$

Hence, the deviator stress tensor is calculated by the formula

$$\hat{\sigma}_{rr} - \hat{\sigma}_{\theta\theta} = \frac{2b^2}{r^2}\sigma^w_{rr} + \frac{\nu_u - \nu}{(1+\nu)(1-\nu_u)(\lambda_2 - \lambda_1)} \times$$
$$\Bigg[\lambda_2 B_1(\omega)\bigg(\frac{2H_1^{(1)}(q_1 r)}{q_1 r} - \frac{2bH_1^{(1)}(q_1 b)}{q_1 r^2} + H_0^{(1)}(q_1 r)\bigg) -$$
$$\lambda_1 B_2(\omega)\bigg(\frac{2H_1^{(1)}(q_2 r)}{q_2 r} - \frac{2bH_1^{(1)}(q_2 b)}{q_2 r^2} + H_0^{(1)}(q_2 r)\bigg)\Bigg].$$

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