Swelling Porous Media: Developing a Multiscale Model of Overburden Pressure as a Function of Water Content in Montmorillonite-Bearing Clayey Soils

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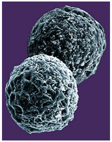
Outline

Outline

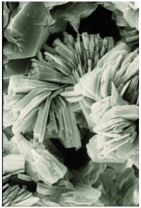
Examples of Swelling Porous Media

Swelling Porous Media: Examples



Drug delivery polymers

R. Langer, Massachusetts Institute of Technology, Cambridge, MA



Clay

Rye Bread

Outline

Obtaining Macroscale Governing Equations

Homogenization or Averaging (Auriault, Whitaker):

Microscale Balance Laws Const. Eqns	Avg/Homogenize $---------->$	Macroscale Balance Laws Const. Eqns

Mixture Theory (Bowen):

Postulate Balance Laws at Macroscale	Exploit Entropy Ineq. $-------->$	Macroscale Const. Eqns

Hybrid Mixture Theory (Hassanizadeh and Gray):

Microscale Balance Laws	Volume Average $---------->$	Macroscale Balance Laws
	Exploit Entropy Ineq. $---------->$	Macroscale Const. Eqns

Exploiting Entropy Inequality for a Fluid

Conservation of Linear Momentum

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) - \nabla \cdot \mathbf{t} - \rho \mathbf{g} = 0$$

Need constitutive equation for stress, $\mathbf{t}$.
Assume a set of independent variables upon which all constitutive variables depend:

$$T, \ \rho, \ (\nabla \mathbf{v})_{\mathrm{sym}} = \mathbf{d}$$

Exploiting entropy inequality gives

Exploiting Entropy Inequality

Exploiting entropy inequality, linearizing about equilibrium ($\nabla \boldsymbol{v} = \boldsymbol{0}$):

$$\boldsymbol{t} = (-\overline{p} + \lambda \mathrm{tr}(\boldsymbol{d}))\boldsymbol{I} + 2\boldsymbol{\nu} : \boldsymbol{d}, \qquad \overline{p} = \rho^2 \frac{\partial \Psi}{\partial \rho}$$

where Ψ is the Helmholtz potential.
It is generally *assumed* that

$$-\frac{1}{3}\mathrm{tr}(\boldsymbol{t}) = p = \overline{p} = \rho^2 \frac{\partial \Psi}{\partial \rho}$$

Substitute in Conservation of Linear Momentum: N-S Eqns:

$$\rho \frac{D\boldsymbol{v}}{Dt} + \nabla p - \nabla(\lambda \nabla \cdot \boldsymbol{v}) - \nabla \cdot \left(\mu \frac{1}{2}(\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T \right) - \rho \boldsymbol{g} = \boldsymbol{0}$$

It's often assumed that $\lambda = -\frac{2}{3}\mu$

Outline

Macroscale Balance Laws

Volume Fraction = $\varepsilon^\alpha = \frac{|\delta V_\alpha|}{|\delta V|}$, $\qquad \varepsilon^l + \varepsilon^s = 1$

Conservation of Mass ($\alpha = l, s$)

$$\frac{D^\alpha(\varepsilon^\alpha \rho^\alpha)}{Dt} + \varepsilon^\alpha \rho^\alpha \nabla \cdot \boldsymbol{v}^\alpha = \sum_{\beta \neq \alpha} \widehat{e}^\alpha_\beta$$

Conservation of Momentum ($\alpha = l, s$)

$$\varepsilon^\alpha \rho^\alpha \frac{D^\alpha \boldsymbol{v}^\alpha}{Dt} - \nabla \cdot (\varepsilon^\alpha \boldsymbol{t}^\alpha) - \varepsilon^\alpha \rho^\alpha \boldsymbol{g}^\alpha = \sum_{\beta \neq \alpha} \widehat{\boldsymbol{T}}^\alpha_\beta$$

Conservation of energy ($\alpha = l, s$)
(similarly)

Assumptions on Behavior of Material

Assume:

- Two phases - liquid and solid
- Phases may be charged
- Multiple constituents for each phase

It is assumed that the consititutive variables depend on:

$$\varepsilon^l,\ \rho^{l_j},\ \rho^{s_j},\ T,\ \boldsymbol{E}^s,\ \boldsymbol{v}^{l,s},\ \boldsymbol{u}^{l_j},\ \boldsymbol{\mathcal{E}},$$
$$\nabla\varepsilon^l,\ \nabla\rho^{\alpha_j},\ \nabla T,\ \nabla\boldsymbol{E}^s,\ \boldsymbol{d}^l,\ \nabla\boldsymbol{u}^{l_j},$$

ε^l = void fraction

ρ^{l_j} = density of constituent j in liquid phase

(mass l_j / volume of liquid)

T = temperature

$\boldsymbol{v}^{l,s}$ = relative velocities: $\boldsymbol{v}^l - \boldsymbol{v}^s$

$\boldsymbol{u}^{l_j}$ = diffusive velocity: $\boldsymbol{v}^{l_j} - \boldsymbol{v}^l$

$\boldsymbol{\mathcal{E}}$ = electric field

$\boldsymbol{E}^s$ = macroscale strain of solid phase

Closure issue: $\dot{\varepsilon}^l$ is a constitutive variable.

Three Pressures

As a result of having volume fraction, ε^l, as an independent variable:

$$p^l = -\frac{1}{3}\mathrm{tr}(\boldsymbol{t}^l) \qquad \overline{p}^l = (\rho^l)^2 \left.\frac{\partial \Psi^l}{\partial \rho^l}\right|_{\varepsilon^l} \qquad \pi^l = \varepsilon^l \rho^l \left.\frac{\partial \Psi^l}{\partial \varepsilon^l}\right|_{\rho^l}$$

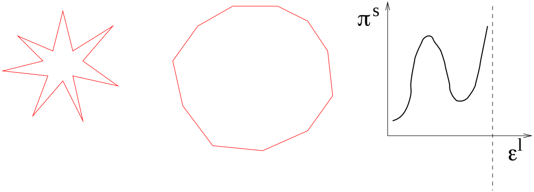
$$p^s = -\frac{1}{3}\mathrm{tr}(\boldsymbol{t}^s) \qquad \overline{p}^s = (\rho^s)^2 \left.\frac{\partial \Psi^s}{\partial \rho^s}\right|_{\varepsilon^s} \qquad \pi^s = \varepsilon^s \rho^s \left.\frac{\partial \Psi^s}{\partial \varepsilon^s}\right|_{\rho^s}$$

where we can show mathematically (no assumptions)

$$p^\alpha = \overline{p}^\alpha + \pi^\alpha, \qquad \alpha = l, s$$

Three Pressures

What is $\pi^s = \varepsilon^s \rho^s \left.\frac{\partial \Psi^s}{\partial \varepsilon^s}\right|_{\rho^s, \rho^l}$? Represents how the solid energy changes when changing porosity without changing the densities of liquid or solid. Configurational pressure



Three Pressures

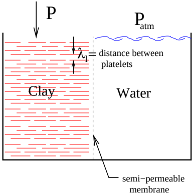
What is $\pi^l = \varepsilon^l \rho^l \left. \frac{\partial \Psi^l}{\partial \varepsilon^l} \right|_{\rho^s, \rho^l}$? Represents how the liquid energy changes as the volume fraction changes

Non-swelling porous media, $\pi^l = 0$: we recover $p^l = \overline{p}^l$.

Swelling porous media, π^l can be measured using a reverse osmotic experiment:

$$P = \pi^l = \exp\left(\frac{\alpha}{\lambda}\right) - 1$$

α is a function of cation exchange and specific surface area



P.F. Low, *Soil Science Society of America Journal*, 44(4), 1980
P.F. Low, *Soil Science Society of America Journal*, 45, 1981

P.F. Low, *Progr Colloid & Polym Sci*, 95, 1994

Three Pressures

Consequences

- Low's empirical results can be derived by balancing the *macroscale* Gibbs (chemical) potential across the boundary.
- The boundary condition between vicinal water and bulk water is *not* a balance of pressures. *It is a balance of chemical potentials.*
- DLVO theory was originally derived for gas particles and has been applied to vicinal liquid in swelling clay at the *microscale*. According to Mitchel and Soga (2005), a double layer model cannot "explain the swelling of pure clay accurately."

Darcy's Law

Conservation of Linear Momentum for liquid phase

$$\varepsilon^l \rho^l \frac{D^l \boldsymbol{v}^l}{Dt} - \nabla \cdot (\varepsilon^l \boldsymbol{t}^l) - \varepsilon^l \rho^l \boldsymbol{g} = \sum_{\beta \neq \alpha} \widehat{\boldsymbol{T}}_s^l$$

Constitutive results from exploiting entropy inequality (linearizing)

$$\boldsymbol{t}^l = -p^l + \mu \boldsymbol{d}^l$$

$$\widehat{\boldsymbol{T}}_s^l = p^l \nabla \varepsilon^l - (\varepsilon^l)^2 \boldsymbol{R} \cdot \boldsymbol{v}^{l,s}$$

Neglect gravity, inertial term, and viscous term:

$$\boldsymbol{R} \cdot \boldsymbol{v}^{l,s} = -\varepsilon^l \nabla p^l - \pi^l \nabla \varepsilon^l$$

Flow can be inhibited by swelling.

Outline

1. Swelling Porous Media
2. Modeling Approach - HMT
3. Macroscale Equations
4. **Generalized Terzaghi Stress Principle**
5. Overburden Pressure vs Water Content for Clayey Soils

What is Terzaghi Stress Principle with π^l and π^s?

By adding the conservation of momentum we have that the total or applied stress, $\boldsymbol{t}$,

$$\boldsymbol{t} = \varepsilon^l \boldsymbol{t}^l + \varepsilon^s \boldsymbol{t}^s$$

$$p = \varepsilon^l p^l + \varepsilon^s p^s \qquad \text{where} \quad p^l = -\frac{1}{3}\mathrm{tr}\boldsymbol{t}^l, \quad p^s = -\frac{1}{3}\mathrm{tr}\boldsymbol{t}^s$$

Experimentally we have (for nonswelling porous media)
Terzaghi Stress Principle:

$$\boldsymbol{t}_{\mathrm{eff}} = \boldsymbol{t} + \alpha p^l \boldsymbol{I} \qquad p_{\mathrm{eff}} = p - \alpha p^l$$

When $\alpha = 1$ it can be shown that the max. microscale shear stress is proportional to the Terzaghi effective pressure, p_{eff}
(Schreyer et al., 2021)

What is Terzaghi Stress Principle with π^l and π^s?

Using $\overline{p}^l = \overline{p}^s$ at equilibrium (result from exploiting entropy inequality) we get

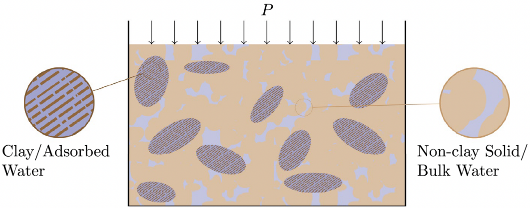
$$\begin{aligned} p_{\text{eff}} &= p - p^l \\ &= (\varepsilon^l p^l + \varepsilon^s p^s) - (\varepsilon^l + \varepsilon^s) p^l \\ &= \varepsilon^l(\overline{p}^l + \pi^l) + \varepsilon^s(\overline{p}^s + \pi^s) - \varepsilon^l(\overline{p}^l + \pi^l) - \varepsilon^s(\overline{p}^l + \pi^l) \\ &= \varepsilon^s(\pi^s - \pi^l) \end{aligned}$$

So this theory says that the effective pressure is completely determined by the swelling pressure and configurational pressure (see also, Ehlers 2018 for multiphase flow where saturation is used instead of volume fraction).

W. Ehlers, *Geomechanics for Energy and the Environment* (15), 2018

Outline

Generalized Terzaghi Stress Principle

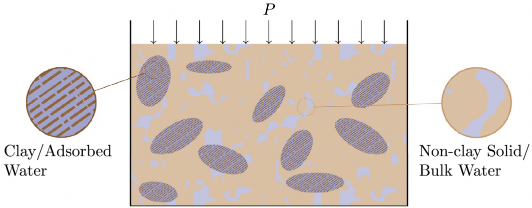


For soils containing swelling clays, we want an equation that reduces to Terzaghi's when there is no swelling clays and reduces to Low's relationship when it is all swelling clay.

This is a 3-scale problem:

- microscale Distinguish between the vicinal (adsorbed) fluid and clay platelets
- mesoscale Disitinguish between the clay particles and the bulk fluid
- macroscale Cannot distinguish between the phases.

Generalized Terzaghi Stress Principle



Four phases:

- A_l vicinal fluid
- A_s clay minerals that adsorb fluid
- B_l nonabsorbed fluid
- B_s non-clay solids

Generalized Terzaghi Stress Principle

Results from HMT:

$$
\begin{aligned}
\pi^\alpha_\beta &= \sum_\delta \varepsilon^\delta \rho^\delta \left.\frac{\partial \psi^\delta}{\partial \varepsilon^\alpha}\right|_{\varepsilon^\gamma, \rho^\zeta} \\
\overline{p}^\alpha_\beta &= -\sum_\delta \varepsilon^\delta \rho^\delta \left.\frac{\partial \psi^\delta}{\partial \varepsilon^\alpha}\right|_{\varepsilon^\beta, \varepsilon^\zeta \rho^\zeta} \\
& \quad \gamma \neq \alpha, \beta, \qquad \alpha, \zeta = A_l, A_s, B_l, B_s \\
p^\alpha &= -\frac{1}{3}\mathrm{tr}\boldsymbol{t}^\alpha = (\rho^\alpha)^2 \frac{\partial \psi^\alpha}{\partial \rho^\alpha}
\end{aligned}
$$

In words: $\pi^{A_l}_{B_l}$ is the change in energy as water moves between A_l and B_l while volume fraction of solid phases are fixed and all densities stay fixed.

π^α_β is the swelling pressure above the bulk phase pressure so we can use Low's exponential relationship (almost).

Generalized Terzaghi Stress Principle

Results from HMT: Equivalent 3 pressure relationships:

$$p^\alpha - p^\beta = \pi^\alpha_\beta + \overline{p}^\alpha_\beta$$

$$\sum_\beta \varepsilon^\beta \rho^\beta \frac{\partial \psi^\beta}{\partial \varepsilon^\alpha} - p^\alpha + p^{B_s} = 0 \qquad \Rightarrow$$

$$\overline{p}^\alpha_{B_s} = 0 \quad \text{at equil}$$

And using the fact that the total pressure is the weighted sum of the 4 pressures:

$$p = \varepsilon^{A_l} p^{A_l} + \varepsilon^{A_s} p^{A_s} + \varepsilon^{B_l} p^{B_l} + \varepsilon^{B_s} p^{B_s}$$

We get...

Generalized Terzaghi Stress Principle

Effective pressure and total pressure expressions are

$$p_{\text{eff}} = \varepsilon^{A_s}\pi^{A_s}_{A_l} + \varepsilon^{B_s}\pi^{B_s}_{B_l}$$
$$p = (\varepsilon^{A_s} + \varepsilon^{A_l})\pi^{A_l}_{B_l} + p^{B_l} + p_{\text{eff}}$$

where the terms in blue act as the effective fluid pore pressure.
How do we use this generalized Terzaghi Stress Principle? This is the art of modeling! Make some educated assumptions!

Generalized Terzaghi Stress Principle

Assume

1. p^{B_l}, bulk fluid pressure, and p, overburden pressure, mass fractions of A_s and B_s, and total water content are measurable
2. adsorbed and bulk water have the same density, $\rho^{A_l} = \rho^{B_l}$ (see Low for the magnitude of this approximation)
3. Low's exponential relationship is still valid for $\pi_{B_l}^{A_l}$
4. effective pressure, p_{eff} is linear in strain
5. solid components are incompressible, $V^{A_s} = V_0^{A_s}$ and $V^{B_s} = V_0^{B_s}$

After a fair bit of algebra:

$$p = P_{\text{atm}} \frac{\omega^A + f^c \frac{\rho^l}{\rho^{A_s}}}{\omega + \frac{\rho^l}{\rho^s}} \left(\exp\left(\frac{\alpha f^c}{\omega^A} \right) - 1 \right) + p^{B_l} - K \frac{\omega - \omega_0}{\omega_0 + \frac{\rho^l}{\rho^s}}$$

Generalized Terzaghi Stress Principle

$$p = P_{\text{atm}} \frac{\omega^A + f^c \frac{\rho^l}{\rho^{As}}}{\omega + \frac{\rho^l}{\rho^s}} \left(\exp\left(\frac{\alpha f^c}{\omega^A} \right) - 1 \right) + p^{B_l} - K \frac{\omega - \omega_0}{\omega_0 + \frac{\rho^l}{\rho^s}}$$

= Low's relationship + bulk liquid pressure (=p_{atm} under drained conditions) + bulk linear elasticity where

- ω^A ratio of mass of adsorbed water to mass of total solid
- ω ratio of mass of total water to mass of total solid
- f^c ratio of mass of clay to mass of total solid
- K bulk modulus of elasticity for effective pressure, assumed constant
- α is from Low's exponential relationship and is a fn of cation exchange capacity and specific surface area

Generalized Terzaghi Stress Principle

What to do with adsorbed (vicinal) water content?

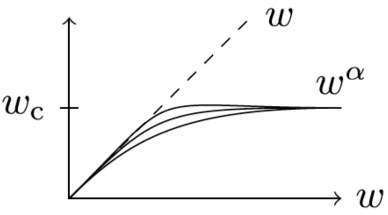


Figure: Adsorbed water content, $\omega^\alpha = \omega^A$, as a function of total water

For results, we assumed piecewise linear

R. Whithead, L.Schreyer, I. Akin, Geotechnical and Geological Engineering, 42, 3843-3856
doi.org/10.1007/s10706-024-02761-0, 2024

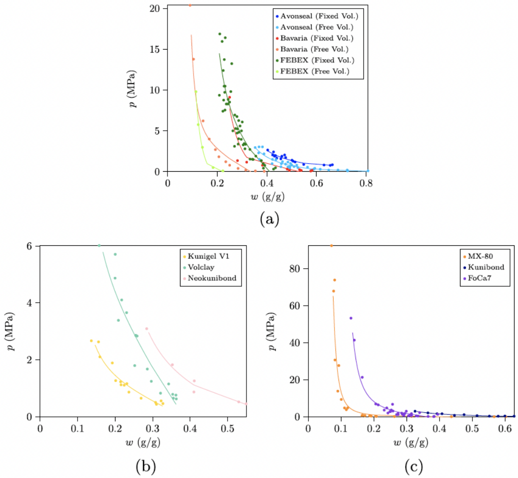
Generalized Terzaghi Stress Principle

We now have an equation with 4 empirical constants:

- f^c mass fraction of clay
- ω_c from ω vs ω^A function
- ω_0 initial water content,
- K bulk modulus of elasticity for effective pressure

$$p = P_{\text{atm}} \frac{\omega^A(\omega, \omega_c) + f^c \frac{\rho^l}{\rho^{A_s}}}{\omega + \frac{\rho^l}{\rho^s}} \left(\exp\left(\frac{\alpha \pi f^c}{4\omega^A(\omega, \omega_c)} \right) - 1 \right) + p^{B_l} - K \frac{\omega - \omega_0}{\omega_0 + \frac{\rho^l}{\rho^s}}$$

Generalized Terzaghi Stress Principle for Clayey soils - results



Conclusions

- When modeling swelling porous media, swelling pressure is a key process to incorporate.
- The proposed model is designed to capture the behavior of soils ranging from low pressure (dominated by skeletal deformation), to high pressure limits where adsorbed water pressure dominates.
- The assumption that the bulk modulus is constant can be relaxed to be piecewise constant as is done for modeling plasticity [e.g. Schreyer et al., 2021]
- Comparison with machine learning models: coefficients have physical interpretation, allowing for predictions for clayey solid not used in the training set.
- Other physics models have fewer parameters, but are designed for the low moisture content regime only.

THANK YOU

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