LEMTA **LNCC**

Modèles à deux et trois échelles pour les phénomènes électro-chimio-hydro-mécaniques dans les milieux poreux déformables

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Summary

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1. A brief introduction to swelling clays

1.1. Structure of swelling clays

Mesoscopic view of a smectite (from D. Teissier)

1.2. General organization : three-scale medium

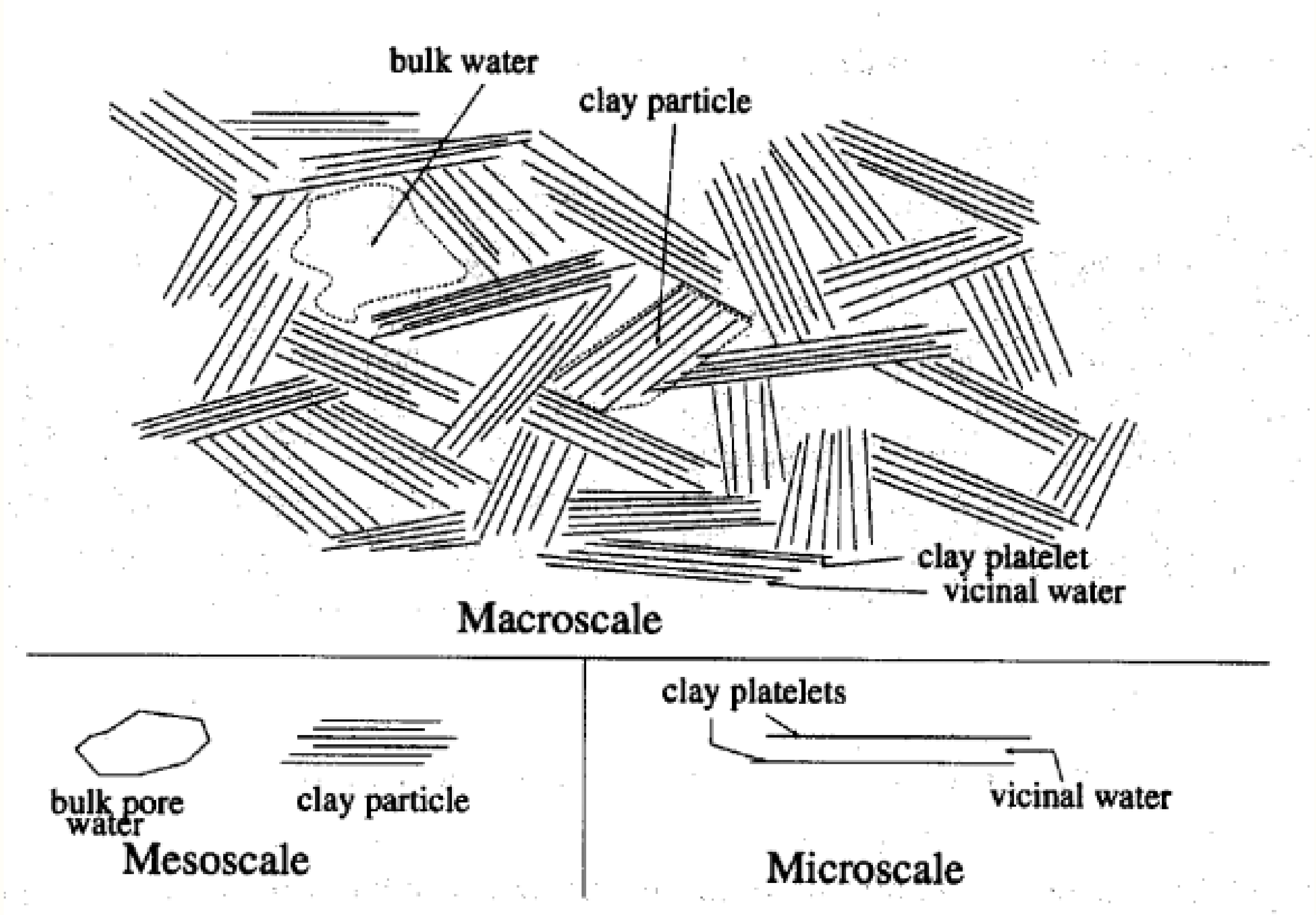


Fig. 1. Three-scale model for clay.

Clay microstructure

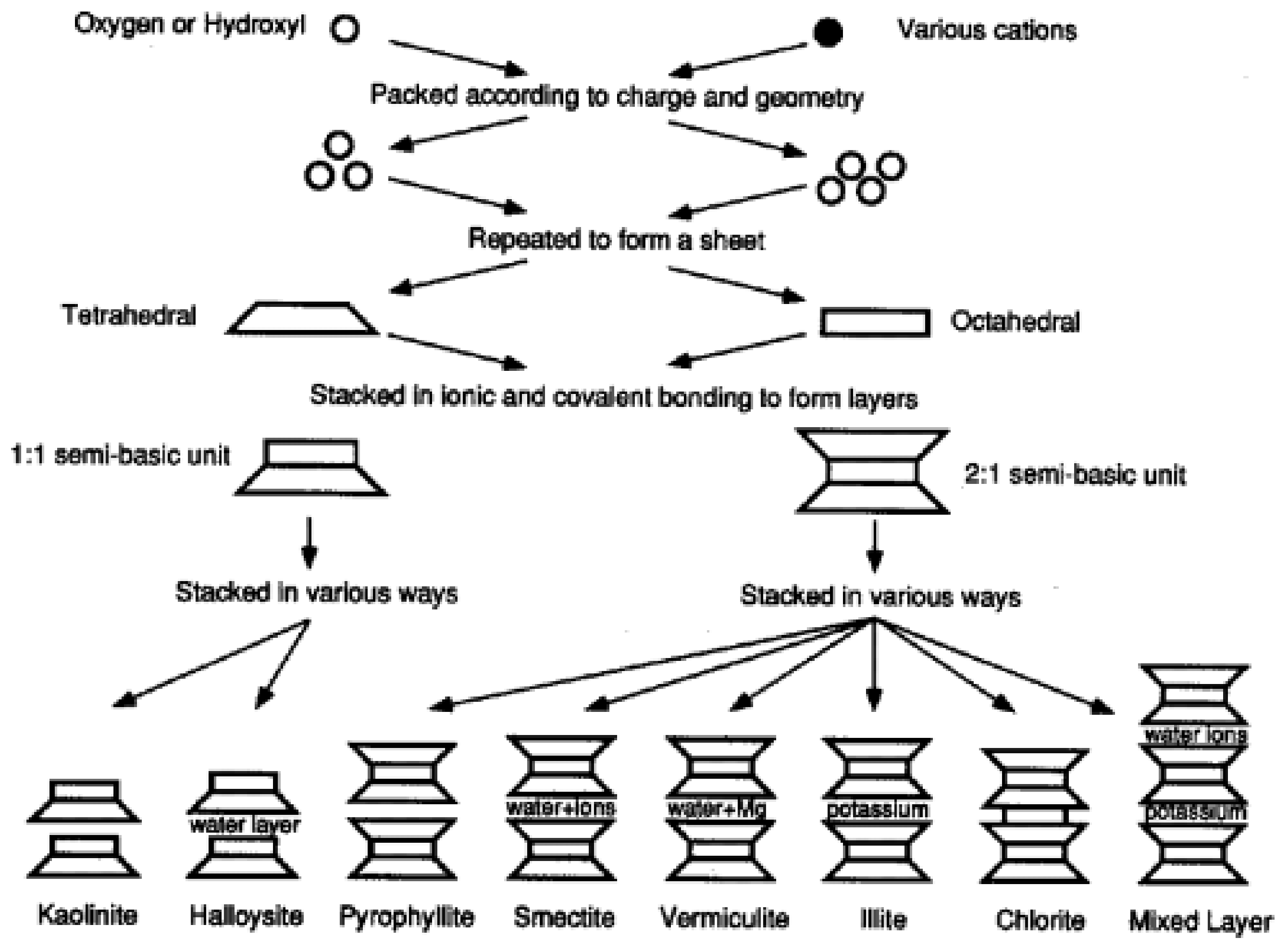


Figure 3.8 Synthesis pattern for the clay minerals.

- **Isomorphous Substitutions:** $\Rightarrow$ **Negative Surface Charge Density** ($\sigma < 0$)

2. From the microscale to the mesocale

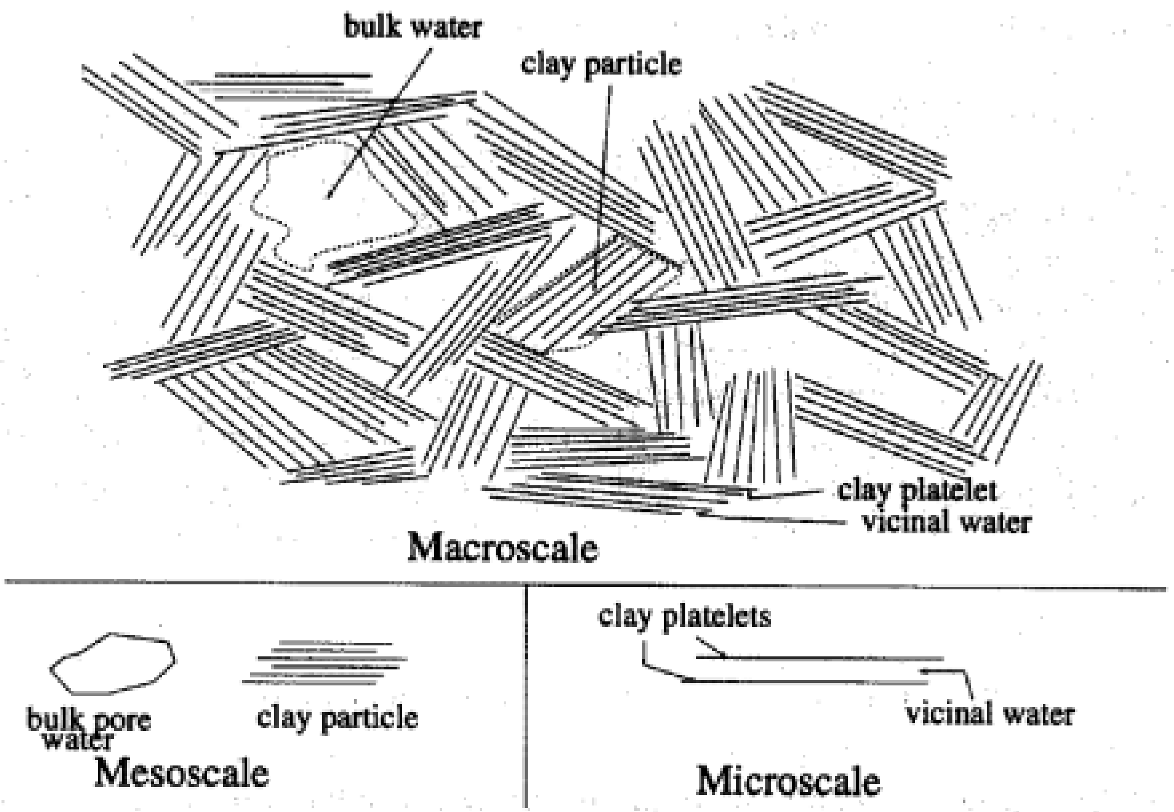


Fig. 1. Three-scale model for clay.

“Mesoscale” ⟵ **“Microscale”**

- **Porous medium:** **saturated by a Newtonian fluid with a monovalent salt: Na$^+$, Cl$^-$**
- **Osmotic swelling:** **electrostatic forces are predominant**
- **Solid phase:** **elastic**

Fluid velocity	**v**	**(Bulk) pressure**	$(p_b)p$		
Solid displacement	**u**				
Electric Potential or **Bulk Concentration**	Φ c_b	**Cations** **Double layer potential**	c^+ φ	**Anions** **Streaming potential**	c^- ψ_b

- **Change of variables** $\longrightarrow$ **Bulk equilibrium values:** c_b and ψ_b

$$\Phi = \varphi + \psi_b \qquad\qquad c^{\pm} = c_b \exp\left(\mp \frac{F\,\varphi}{R\,T}\right)$$

$$p_b = p - \underbrace{2\,R\,T\left(\frac{c^+ + c^-}{2} - c_b\right)}_{\textbf{Donnan pressure}} \quad = \quad p - 2\,R\,T\,c_b\left[\cosh\left(\frac{F\,\varphi}{R\,T}\right) - 1\right]$$

- **Scale separation: microscopic ℓ $(\boldsymbol{y})$; macroscopic L $(\boldsymbol{x})$; $\epsilon = \dfrac{\ell}{L} << 1$.**
- **Spatial derivative:** $\boldsymbol{\nabla} = \boldsymbol{\nabla}_x + \dfrac{1}{\epsilon}\boldsymbol{\nabla}_y$
- **Two-scale asymptotic expansion:** $\theta(\boldsymbol{x},\ \boldsymbol{y}, t) = \sum_{k=0}^{k=\infty} \epsilon^k\, \theta^k(\boldsymbol{x},\ \boldsymbol{y}, t)$
- **Bulk values:** c_b**,** ψ_b**,** p_b
  - **slow variables (independent of y)**
  - **continuous at the bulk interface**
- **Reference values:**
  - **macroscopic length scale :** L
  - θ_{ref}**:** $\theta^\star = \dfrac{\theta}{\theta_{ref}} = \mathcal{O}(1)$
  - **dimensionless equations**

2.1. Equations to be solved

- **Poisson equation in** Y_f

$$\boldsymbol{\epsilon^2}\,\nabla^2(\varphi + \psi_b) = -\frac{F(c^+ - c^-)}{\widetilde{\varepsilon}\,\widetilde{\varepsilon}_0}, \qquad c^\pm = c_b \exp(\mp\overline{\varphi}) \quad \text{and} \quad \overline{\varphi} = \frac{F\,\varphi}{R\,T}$$

$$\mathbf{E} = -\boldsymbol{\epsilon}\,\boldsymbol{\nabla}(\varphi + \psi_b)$$

- **Stokes equations in** Y_f

$$0 = \boldsymbol{\nabla}\,.\,\mathbf{v}$$

$$0 = -\boldsymbol{\nabla} p_b - 2\,R\,T\,(\cosh\overline{\varphi} - 1)\;\boldsymbol{\nabla} c_b + 2\,R\,T\,c_b\,\sinh\overline{\varphi}\,\boldsymbol{\nabla}\overline{\psi}_b + \boldsymbol{\epsilon^2}\mu_f\nabla^2\mathbf{v}$$

- **Ions transport** $^{(*)}$ **in** Y_f

$$\frac{\partial}{\partial t}\left[\exp\left(\mp\overline{\varphi}\right)c_b\right] + \boldsymbol{\epsilon^m}\,\boldsymbol{\nabla}\,.\,\left(\exp\left(\mp\overline{\varphi}\right)c_b\,\mathbf{v}\right) = \boldsymbol{\nabla}\,.\,\left[\mathcal{D}_\pm \exp\left(\mp\overline{\varphi}\right)\left(\boldsymbol{\nabla} c_b \pm c_b\boldsymbol{\nabla}\overline{\psi}_b\right)\right]$$

- **Solid deformation in** Y_s

$$\boldsymbol{\nabla}\,.\,\boldsymbol{\sigma}_s = 0 \qquad \boldsymbol{\sigma}_s = \boldsymbol{c}_s\,\boldsymbol{\mathcal{E}}(\mathbf{u})$$

$^{(*)}$ **Péclet number:** $\mathrm{Pe} = \dfrac{v_{ref}\,L}{\mathcal{D}_\pm} = \mathcal{O}\left(\boldsymbol{\epsilon^m}\right)$ **;** $m = 1$ **(diffusion) ;** $= 0$ **(+ convection)**

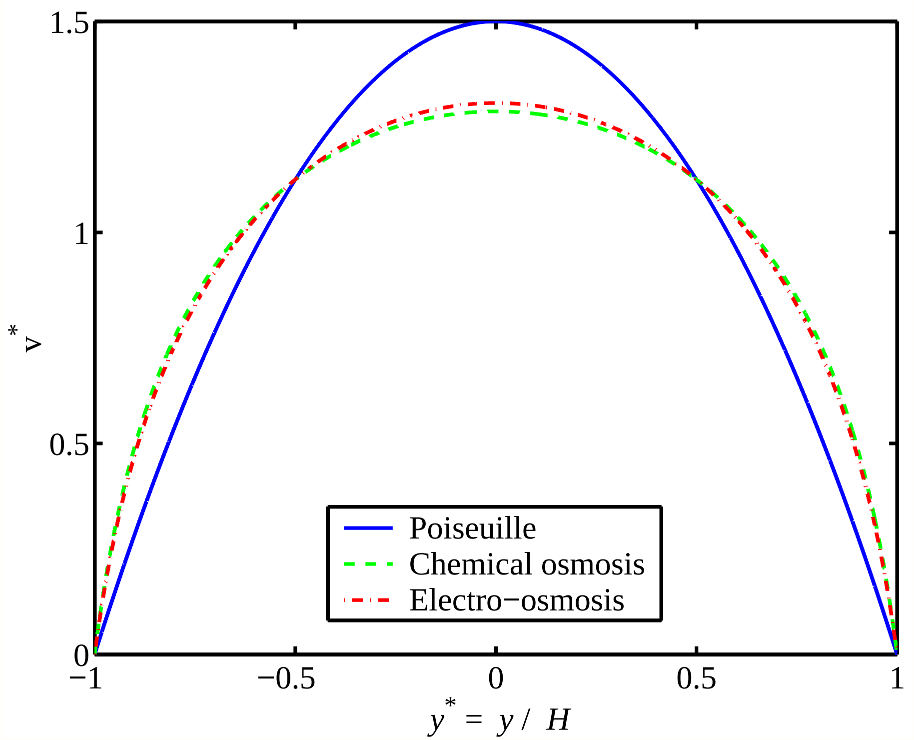
2.2. Homogenization procedure

Generalized Darcy's law

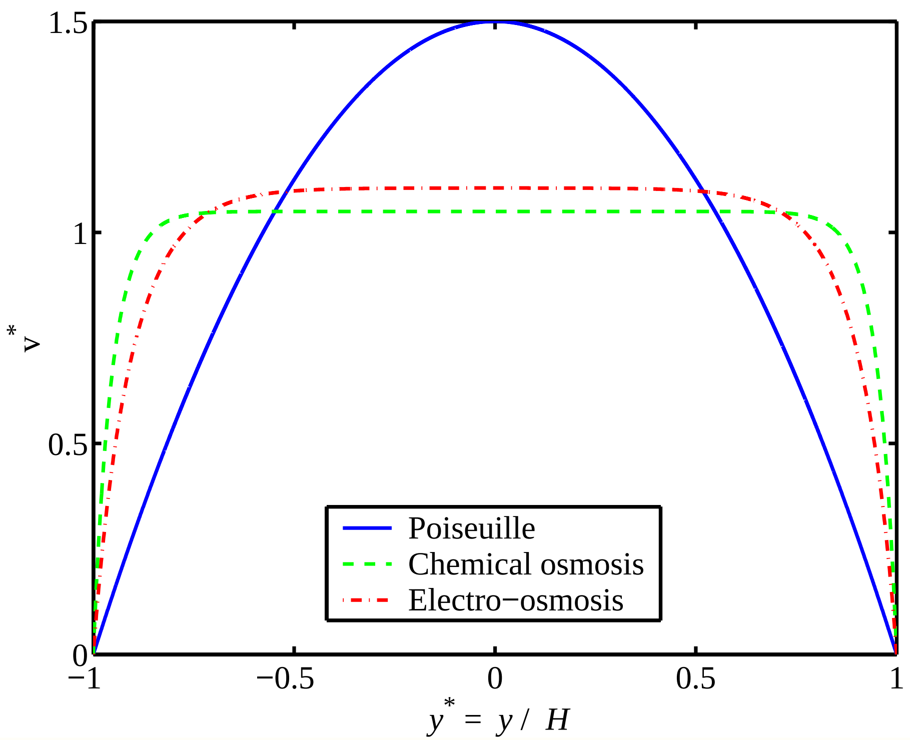
$$\begin{aligned}
\mathbf{v}_D^0 \equiv \left\langle \mathbf{v}^0 - \partial \mathbf{u}^0/\partial t \right\rangle &= \overbrace{\left\langle \mathbf{v}_p^0 - \partial \mathbf{u}^0/\partial t \right\rangle}^{\textbf{Darcy}} + \overbrace{\left\langle \mathbf{v}_c^0 \right\rangle}^{\textbf{chemical osmosis}} + \overbrace{\left\langle \mathbf{v}_e^0 \right\rangle}^{\textbf{electro-osmosis}} \\
&= -\boldsymbol{K}_P \boldsymbol{\nabla}_x p_b^0 - \boldsymbol{K}_C \boldsymbol{\nabla}_x c_b^0 - \boldsymbol{K}_E \boldsymbol{\nabla}_x \overline{\psi}_b^0
\end{aligned}$$

- **Closure problems to compute $\boldsymbol{K}_P$, $\boldsymbol{K}_C$, $\boldsymbol{K}_E$**

- **Example : 2 parallel plates separated by $2H$**
  - ∗ **Velocity profiles**
  - ∗ **Coefficients $\boldsymbol{K}_P$, $\boldsymbol{K}_C$, $\boldsymbol{K}_E$**

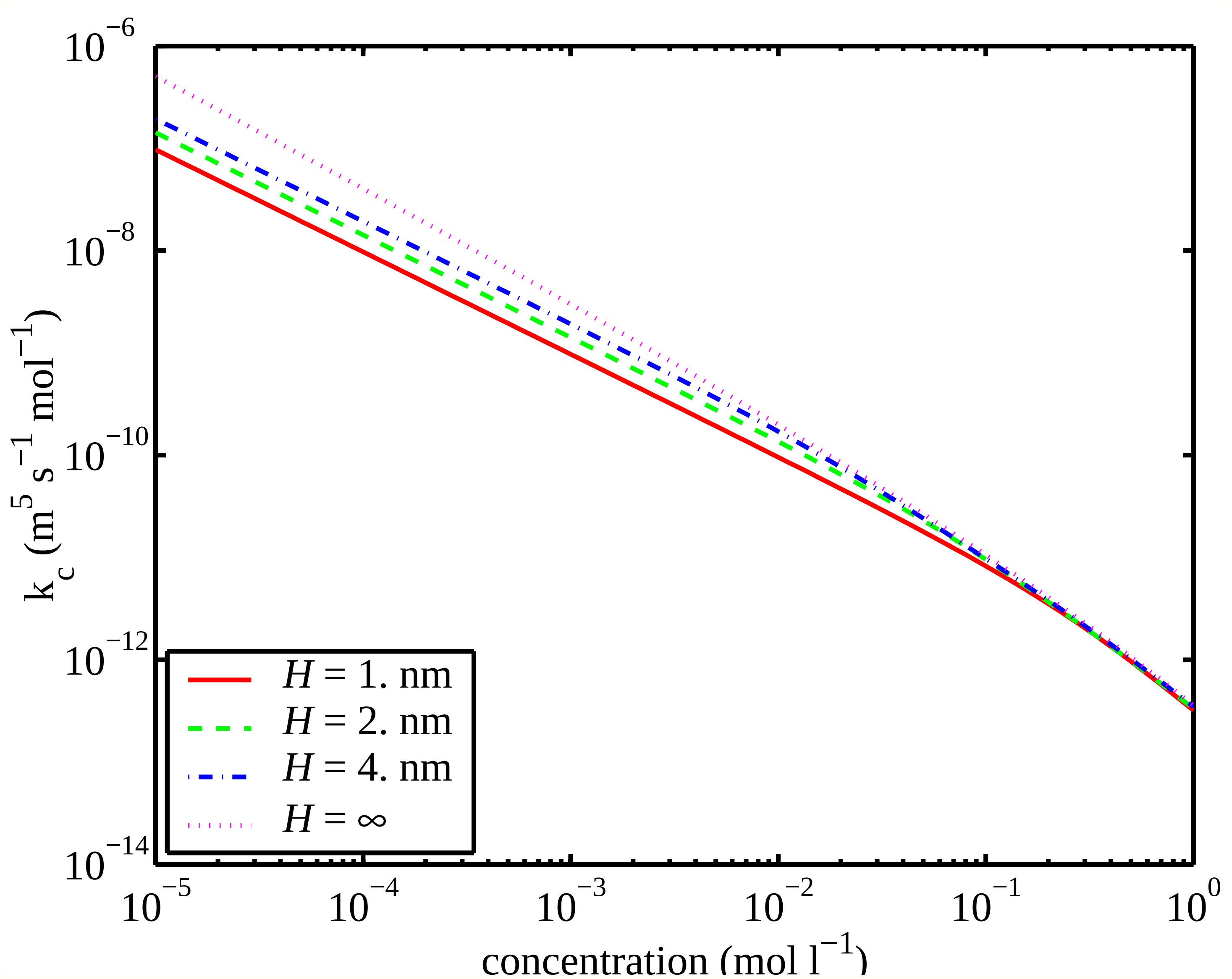


$$H/L_D = 1.$$

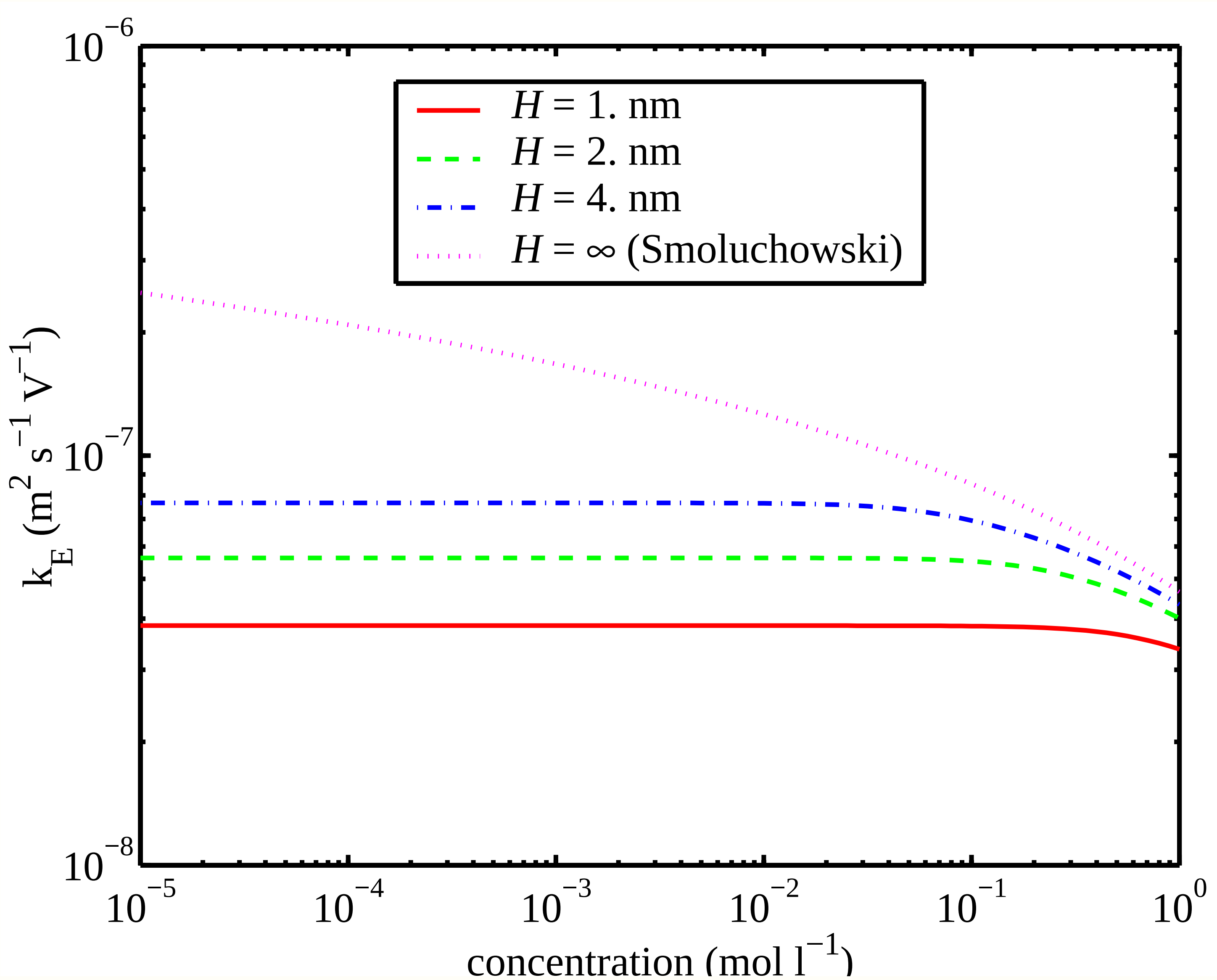


$$H/L_D = 10.$$

$$L_D = \sqrt{\frac{\varepsilon\,\varepsilon_0\,R\,T}{2\,F^2\,c_b}}\ :$$ **Debye's length**



Chemico-osmotic coefficient K_C



Electro-osmotic coefficient K_E

Ions transport

$$\frac{\partial}{\partial t}\left(\phi\, G^*_\pm\, c^0_b\right) + \boldsymbol{\nabla}_x \,.\, \boldsymbol{J}^0_\pm = 0$$

with $$\boldsymbol{J}^0_\pm \equiv G^*_\pm\, c^0_b\, \mathbf{v}^{*0}_\pm - \,\phi \left(\boldsymbol{D}^c_\pm \boldsymbol{\nabla}_x c^0_b \pm \boldsymbol{D}^e_\pm c^0_b\, \boldsymbol{\nabla}_x \overline{\psi}^0_b + \boldsymbol{D}^p_\pm \boldsymbol{\nabla}_x p^0_b\right)$$

- **Closure problems for $\boldsymbol{f}^\pm$ and $\boldsymbol{h}^\pm_{p,c,e}$**

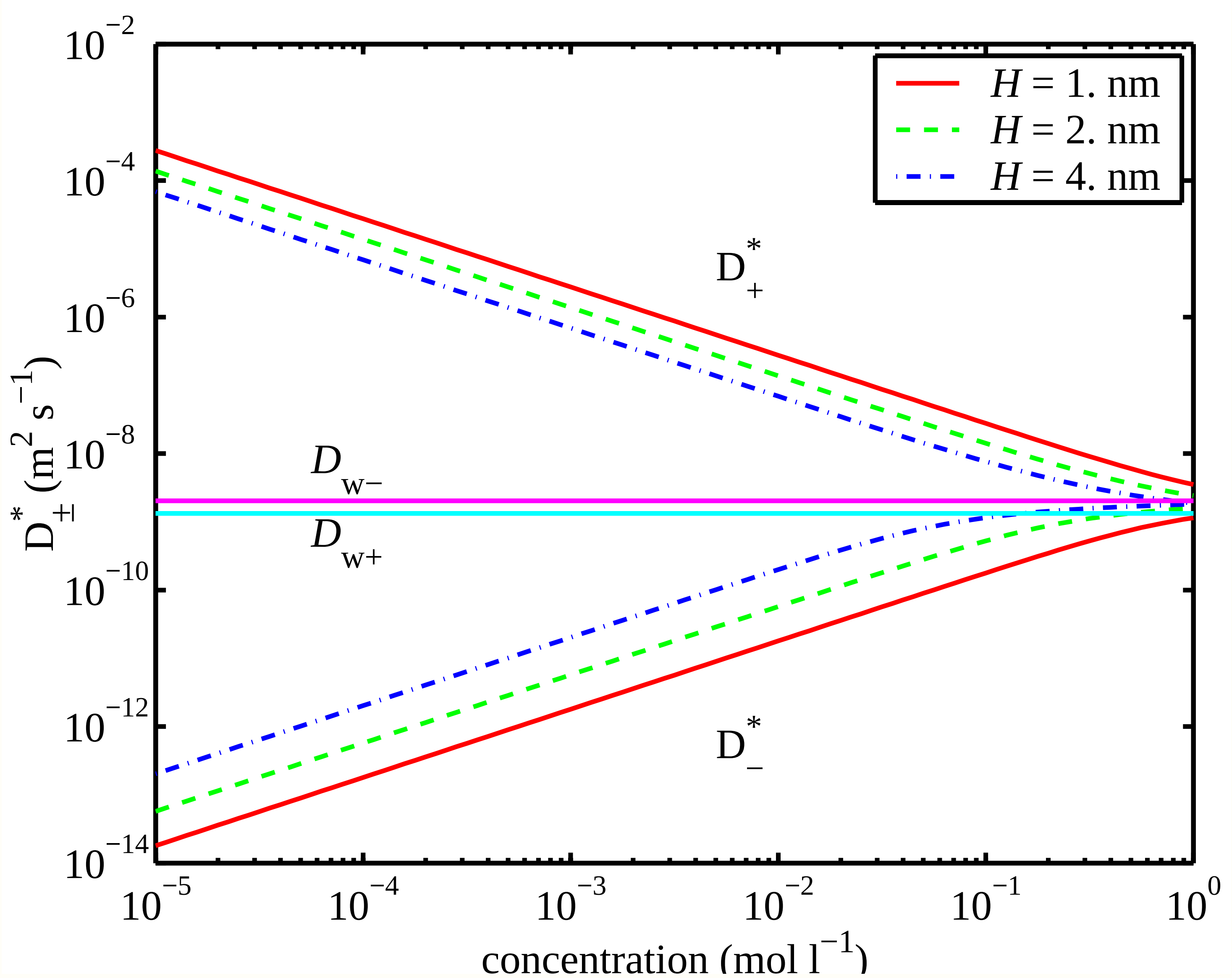
$$G^*_\pm = \left\langle \exp\left(\mp\overline{\varphi}^0\right)\right\rangle^f ; \quad G^*_\pm\, \mathbf{v}^{*0}_\pm = \left\langle \exp\left(\mp\overline{\varphi}^0\right) \mathbf{v}^0\right\rangle$$

$$\boldsymbol{D}^p_\pm = \mathcal{D}_\pm \left\langle \exp(\mp\overline{\varphi}^0) \boldsymbol{\nabla}_y \boldsymbol{h}^\pm_p \right\rangle^f ; \quad \boldsymbol{D}^{c,e}_\pm = \mathcal{D}_\pm \left\langle \exp\left(\mp\overline{\varphi}^0\right) \left(\boldsymbol{I} + \boldsymbol{\nabla}_y \boldsymbol{f}^\pm + \boldsymbol{\nabla}_y \boldsymbol{h}^\pm_{c,e}\right)\right\rangle^f$$

- **Example : two parallel plates distant of $2H$**

  $*\ D^c_\pm = D^e_\pm$

  $*\ D^p_\pm = 0$



Diffusion coefficient $D_\pm$

• Alternative formulation: Onsager's reciprocity relations

$$\boldsymbol{J}^0 \equiv \boldsymbol{J}^0_+ + \boldsymbol{J}^0_- \qquad \boldsymbol{I}^0_e \equiv F(\boldsymbol{J}^0_+ - \boldsymbol{J}^0_-) \qquad \boldsymbol{J}^0 = 2\, c^0_b\, \mathbf{v}^0_D + \boldsymbol{J}^0_d$$

∗ Onsager's reciprocity relations

$$\begin{pmatrix} \mathbf{v}^0_D \\ \boldsymbol{J}^0_d \\ \boldsymbol{I}^0_e \end{pmatrix} = -\begin{pmatrix} \boldsymbol{L}_{PP} & \boldsymbol{L}_{PC} & \boldsymbol{L}_{PE} \\ \boldsymbol{L}_{CP} & \boldsymbol{L}_{CC} & \boldsymbol{L}_{CE} \\ \boldsymbol{L}_{EP} & \boldsymbol{L}_{EC} & \boldsymbol{L}_{EE} \end{pmatrix} \begin{pmatrix} \boldsymbol{\nabla}_x p^0_b \\ RT\boldsymbol{\nabla}_x \ln c^0_b \\ \boldsymbol{\nabla}_x \psi^0_b \end{pmatrix}$$

∗ Symmetry of the coefficients ?

If the electro-chemical potentials do not fluctuate across the micropores:

$$\boldsymbol{L}_{PP} = \boldsymbol{L}^T_{PP} \qquad \boldsymbol{L}_{CC} = \boldsymbol{L}^T_{CC} \qquad \boldsymbol{L}_{EE} = \boldsymbol{L}^T_{EE}$$

$$\boldsymbol{L}_{PC} = \boldsymbol{L}^T_{CP} \qquad \boldsymbol{L}_{PE} = \boldsymbol{L}^T_{EP} \qquad \boldsymbol{L}_{CE} = \boldsymbol{L}^T_{EC}$$

Modified Terzaghi's decomposition

- **Order $\mathcal{O}(\epsilon^{\mathbf{0}})$: $\mathbf{u}^{\mathbf{0}}(\mathbf{x},\mathbf{t})$**
- **Order $\mathcal{O}(\epsilon)$:**

$$\mu_s \nabla_y^2\, \mathbf{u}^1 + (\lambda_s + \mu_s)\boldsymbol{\nabla}_y(\boldsymbol{\nabla}_y\,.\,\mathbf{u}^1) = 0 \qquad \text{in } Y_s$$

$$\begin{aligned}\left[\lambda_s \boldsymbol{\nabla}_y.\,\mathbf{u}^1\,\boldsymbol{I} + 2\,\mu_s \boldsymbol{\mathcal{E}}_y(\mathbf{u}^1)\right].\,\mathbf{n} \quad &= \quad -\left[p_b^0\,(\mathbf{x},t)\,\boldsymbol{I} + \boldsymbol{\Pi}^0\,(\mathbf{x},\mathbf{y},t)\right.\\ &\qquad \left. +\lambda_s \boldsymbol{\nabla}_x.\,\mathbf{u}^0 \boldsymbol{I} + 2\,\mu_s\,\boldsymbol{\mathcal{E}}_x(\mathbf{u}^0)\right].\,\mathbf{n} \qquad \text{on } \partial Y_{fs}\end{aligned}$$

- **on ∂Y_{se}: periodicity conditions**
- **Disjoining pressure $\boldsymbol{\pi}^0$**

$$\boldsymbol{\pi}^0 = \underbrace{-\int_0^{\varphi^0} F\,\left(c^{+\,0} - c^{-\,0}\right)\,\mathrm{d}\varphi\;\boldsymbol{I}}_{=R\,T(c^{+\,0}+c^{-\,0}-2\,c_b^0)} \quad \underbrace{-\frac{\widetilde{\varepsilon}\,\widetilde{\varepsilon}_0}{2}\left(2\,\mathbf{E}^0\,\mathbf{E}^0 - (E^0)^2\,\boldsymbol{I}\right)}_{\boldsymbol{\tau}_M^{\mathbf{0}}}$$

Donnan's pressure **Maxwell's tensor**

- **Closure for $\mathbf{u}^1$**

$$\mathbf{u}^1 = \boldsymbol{\zeta}(\mathbf{y})\, p_b^0(\mathbf{x},\, t) + \boldsymbol{\xi}(\mathbf{y}) \,:\, \boldsymbol{\mathcal{E}}_x(\mathbf{u}^0) + \mathbf{u}_\pi^1(\mathbf{x},\, \mathbf{y},\, t) + \hat{\mathbf{u}}^1(\mathbf{x},\, t)$$

- **ζ et ξ : Homogenization of the poroelasticity equations (Auriault and Sanchez-Palencia, 1977).**

- **$\mathbf{u}_\pi^1$ verifies on Y_s :**

$$\mu_s \nabla_y^2 \mathbf{u}_\pi^1 + (\lambda_s + \mu_s) \boldsymbol{\nabla}_y (\boldsymbol{\nabla}_y \,.\, \mathbf{u}_\pi^1) = 0$$

and on ∂Y_{fs} :

$$-\boldsymbol{\pi}^0 \,.\, \mathbf{n} = \left[\lambda_s \boldsymbol{\nabla}_y \,.\, \mathbf{u}_\pi^1\, \boldsymbol{I} + 2\, \mu_s\, \boldsymbol{\mathcal{E}}_y(\mathbf{u}_\pi^1)\right] \,.\, \mathbf{n}$$

with periodicity conditions on ∂Y_{se}

• Modified Biot's equations

∗ Overall stress tensor

$$\boldsymbol{\sigma}_T^0 = \phi\,\langle \boldsymbol{\sigma}_f^0 \rangle^f + (1-\phi)\,\langle \boldsymbol{\sigma}_s^0 \rangle^s$$

$$\boldsymbol{\nabla}_x \,\boldsymbol{.}\, \boldsymbol{\sigma}_T^0 = 0$$

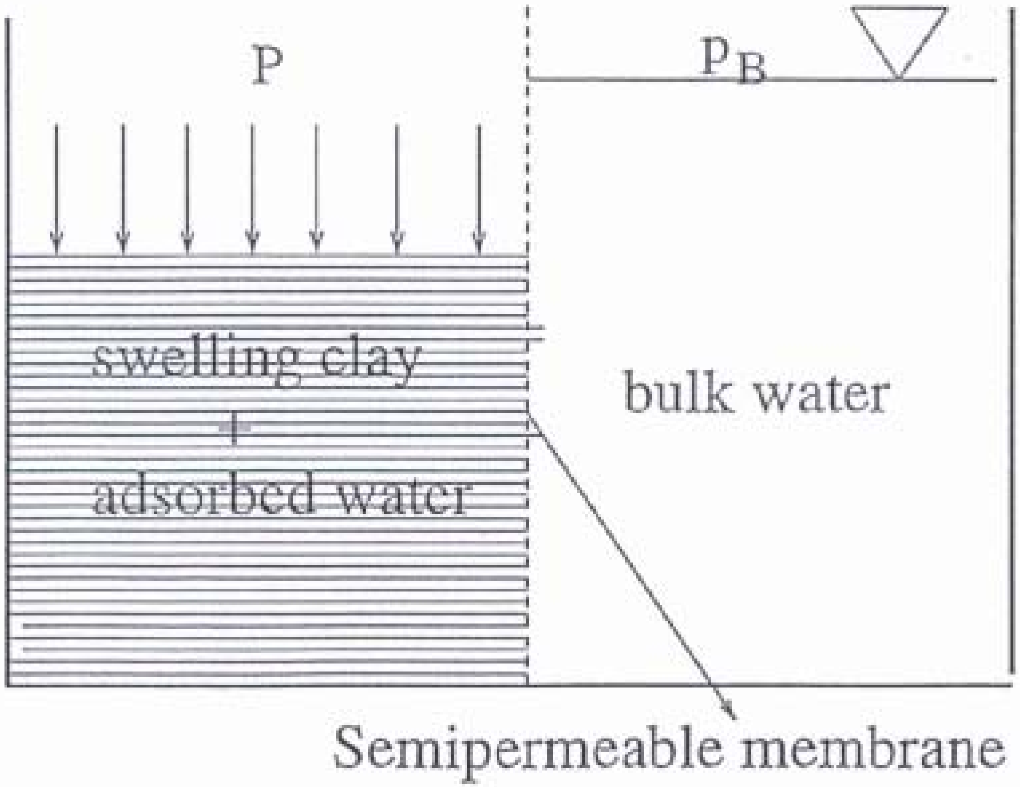
∗ Modified Terzaghi's principle

$$\boldsymbol{\sigma}_T^0 \quad = \quad -\underbrace{p_b^0\,(\phi\,\boldsymbol{I} - \langle \boldsymbol{c}_s \,\boldsymbol{.}\, \boldsymbol{\mathcal{E}}_y(\boldsymbol{\zeta})\rangle)}_{\textbf{pore pressure}} + \underbrace{\langle \boldsymbol{c}_s \,\boldsymbol{.}\, (\boldsymbol{I} + \boldsymbol{\mathcal{E}}_y(\boldsymbol{\xi}))\rangle \,\boldsymbol{.}\, \boldsymbol{\mathcal{E}}_x(\mathbf{u}^0)}_{\textbf{contact stresses}} \quad - \quad \underbrace{\boldsymbol{\Pi}^0}_{\textbf{electrochemical tensor}}$$

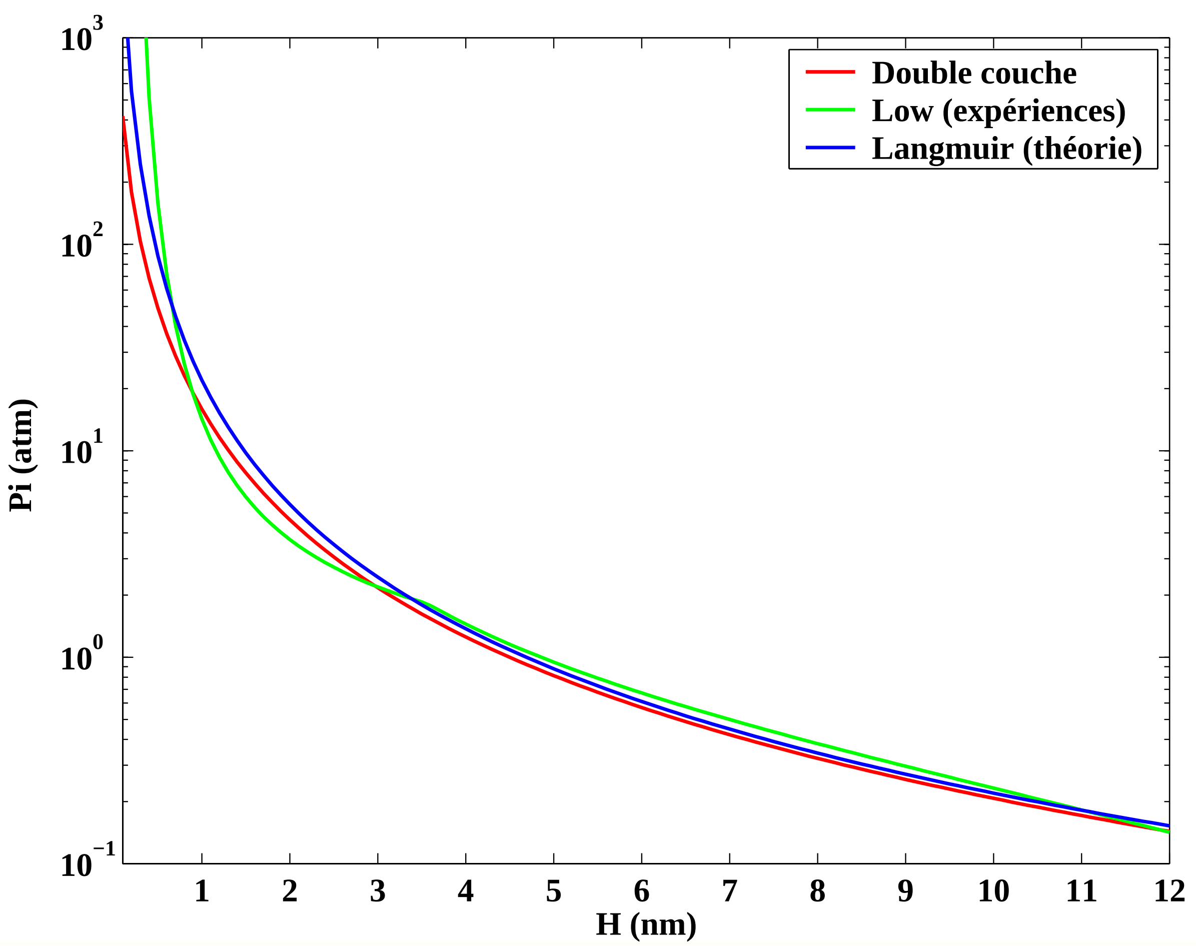
∗ Electro-chemical tensor

$$\boldsymbol{\Pi}^0 = \underbrace{-(1-\phi)\,\Big\langle \boldsymbol{c}_s \,.\, \boldsymbol{\mathcal{E}}_y(\mathbf{u}_\pi^1)\Big\rangle^s}_{\textbf{solid}} + \underbrace{\phi\langle \boldsymbol{\pi}^0\rangle^f}_{\textbf{fluid}}$$

- **Philip Low's experiment**
  - $*$ **Aligned clay particles without contact**
  - $*$ **No contact stress term in the macroscopic law**



$$\mathbf{\Pi} = (P - p_b)\, \boldsymbol{I}$$



$$C = 10^{-4} \text{ mole/l}$$

Langmuir's formula

$$\mathbf{\Pi} \simeq \frac{\pi^2}{2}\, \epsilon\, \epsilon_0 \left(\frac{R\,T}{F\,H}\right)^2$$

2.3. Equations at the mesoscale

- **Unknowns**

$$\boldsymbol{\sigma}_T^0,\ p_b^0,\ \mathbf{u}^0,\ \mathbf{v}_D^0,\ c_b^0,\ \psi_b^0,\ \phi$$

- **Two-scale model**

$$\left\{\begin{array}{ll}
\boldsymbol{\nabla}_x \,.\, \boldsymbol{\sigma}_T^0 = 0 & \textbf{Mechanical equilibrium} \\
\boldsymbol{\sigma}_T^0 = -\boldsymbol{\alpha}\, p_b^0 + \boldsymbol{C}_s\, \boldsymbol{\mathcal{E}}_x(\mathbf{u}^0) - \boldsymbol{\Pi}^0 & \textbf{Terzaghi's principle} \\
\mathbf{v}_D^0 = -\boldsymbol{K}_P \boldsymbol{\nabla}_x\, p_b^0 - \boldsymbol{K}_C \boldsymbol{\nabla}_x\, c_b^0 - \boldsymbol{K}_E \boldsymbol{\nabla}_x \psi_b^0 & \textbf{Darcy's law} \\
\boldsymbol{\nabla}_x . \mathbf{v}_D^0 + \boldsymbol{\alpha} : \dfrac{\partial}{\partial t} \boldsymbol{\mathcal{E}}_x(\mathbf{u}^0) = \beta \dfrac{\partial p_b^0}{\partial t} + \dfrac{\partial \gamma_\pi}{\partial t} & \textbf{Overall mass balance} \\
\dfrac{\partial}{\partial t}\left(\phi\, G_\pm^*\, c_b^0\right) + \boldsymbol{\nabla}_x \,.\, \Big[G_\pm^*\, c_b^0\, \mathbf{v}_*^{\pm 0} & \textbf{Ions conservation} \\
\qquad -\phi\, \left(\boldsymbol{D}_\pm^c \boldsymbol{\nabla}_x c_b^0 \pm \boldsymbol{D}_\pm^e c_b^0\, \boldsymbol{\nabla}_x \overline{\psi}_b^0 + \boldsymbol{D}_\pm^p \boldsymbol{\nabla}_x p_b^0 \right) \Big] = 0 & \\
\dfrac{\partial \phi}{\partial t} + \boldsymbol{\nabla}_x . \mathbf{v}_D^0 + \phi \boldsymbol{\nabla}_x . \dfrac{\partial \mathbf{u}^0}{\partial t} = 0 & \textbf{Fluid phase mass balance}
\end{array}\right.$$

3. From the mesocale to the macroscale

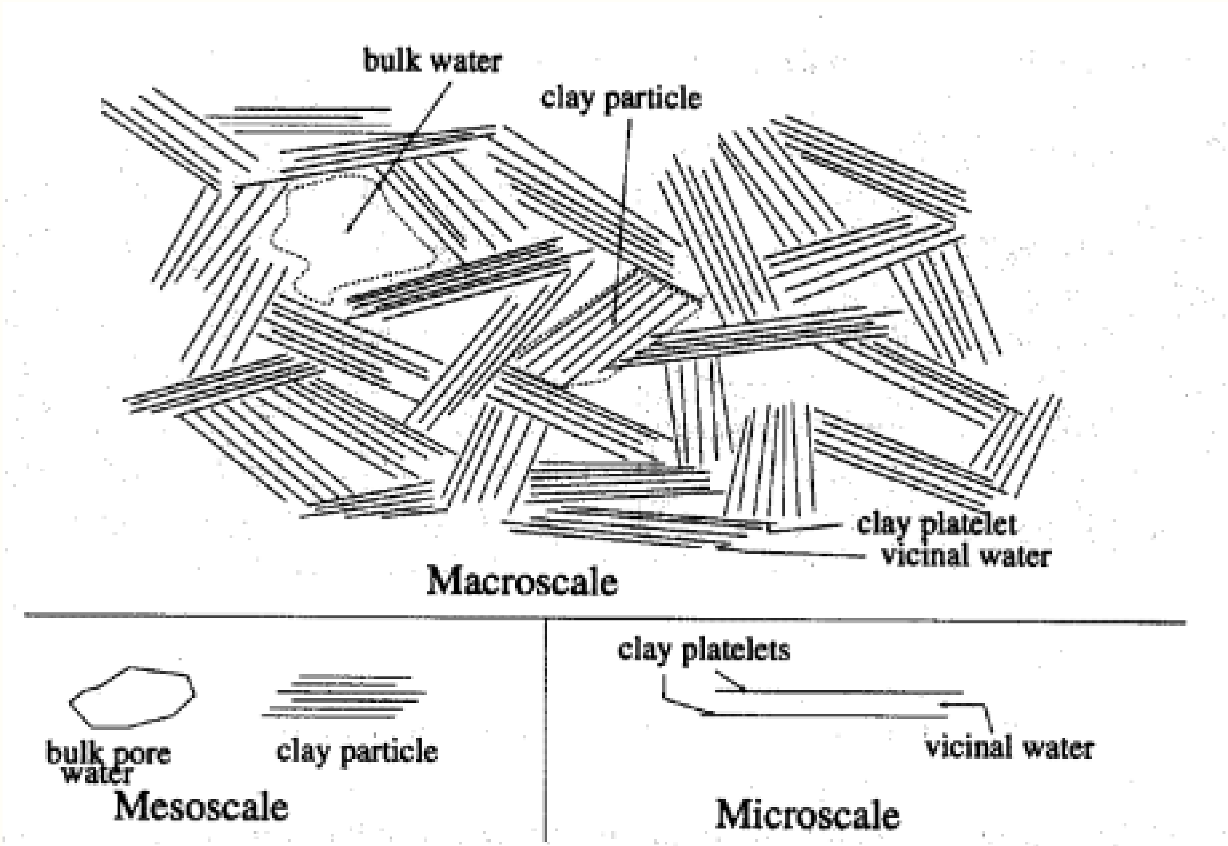


Fig. 1. Three-scale model for clay.

“Mesoscale” ⟶ **“Macroscale”**

3.1. Bulk (fissure) equations

- **Fluid flow**

$$\begin{aligned} \boldsymbol{\nabla}.\boldsymbol{\sigma}_f &= 0 \\ \boldsymbol{\sigma}_f &= -P_f\,\boldsymbol{I} + 2\,\mu_f\,\boldsymbol{\mathcal{E}}\,(\boldsymbol{V}_f) \qquad \textbf{in } \Omega_f \\ \boldsymbol{\nabla}.\boldsymbol{V}_f &= 0 \end{aligned}$$

- **Transport equations** $C_f^+ = C_f^- \equiv C_f$

$$\frac{\partial C_f}{\partial t} + \boldsymbol{\nabla}.\boldsymbol{J}_f = 0$$

$$\boldsymbol{\nabla}.\boldsymbol{I}_f = 0$$

$$\boldsymbol{J}_f = 2\,C_f\,\boldsymbol{V}_f - 2\left(D_f\boldsymbol{\nabla}C_f + \Delta_f\,C_f\boldsymbol{\nabla}\overline{\Psi}_f\right)$$

$$\boldsymbol{I}_f = -2\,F\left(\Delta_f\,\boldsymbol{\nabla}C_f + D_f\,C_f\boldsymbol{\nabla}\overline{\Psi}_f\right)$$

$$D_f = \frac{\mathcal{D}_{w+} + \mathcal{D}_{w-}}{2} \quad \text{and} \quad \Delta_f = \frac{\mathcal{D}_{w+} - \mathcal{D}_{w-}}{2}$$

- **Boundary conditions at the interface: on Γ_{fs}**
  - **Continuous interface conditions** $\left(\boldsymbol{V}_{fs} = \boldsymbol{V}_f - \dfrac{\partial \mathbf{u}}{\partial t}\right)$

$$
\begin{array}{ccc}
\textbf{Clay cluster} & & \textbf{Fissure} \\
p_b & = & P_f \\
c_b & = & C_f \\
\psi_b & = & \Psi_f \\
\mathbf{v}_D . \boldsymbol{N} & = & \boldsymbol{V}_{fs} . \boldsymbol{N} \\
\boldsymbol{J} . \boldsymbol{N} & = & \boldsymbol{J}_f . \boldsymbol{N} \\
\boldsymbol{I} . \boldsymbol{N} & = & \boldsymbol{I}_f . \boldsymbol{N} \\
\boldsymbol{\sigma}_T \, \boldsymbol{N} & = & \boldsymbol{\sigma}_f \, \boldsymbol{N}
\end{array}
$$

• Liquid slippage

Very small EDL near the wall ⟶ Tangential velocity slip

Clay cluster **Fissure**

$$
\begin{aligned}
(\mathbf{v}_D - \boldsymbol{V}_{fs}) \,.\, \boldsymbol{\tau} &= \boldsymbol{V}_{match} \,.\, \boldsymbol{\tau} \\
\boldsymbol{V}_{match} &= -K_E^{f\infty} \boldsymbol{\nabla} \Psi_f - K_C^{f\infty} \boldsymbol{\nabla} C_f \\
K_E^{f\infty} &= \frac{\widetilde{\varepsilon}\,\widetilde{\varepsilon}_0 \zeta}{\mu_f} \quad \text{(Smoluchovski)} \\
K_C^{f\infty} &= \frac{8RT\ell_D^2}{\mu_f} \ln\cosh\left(\frac{\overline{\zeta}}{4}\right)
\end{aligned}
$$

3.2. Dual porosity model

In the clay clusters:

$$\begin{pmatrix} \mathbf{v}_D^1 \\ \boldsymbol{J}_c^1 \\ \boldsymbol{I}_e^1 \end{pmatrix} = -\boldsymbol{\epsilon^2} \begin{pmatrix} \boldsymbol{L}_{PP} & \boldsymbol{L}_{PC} & \boldsymbol{L}_{PE} \\ \boldsymbol{L}_{CP} & \boldsymbol{L}_{CC} & \boldsymbol{L}_{CE} \\ \boldsymbol{L}_{EP} & \boldsymbol{L}_{EC} & \boldsymbol{L}_{EE} \end{pmatrix} \begin{pmatrix} \boldsymbol{\nabla}_y p_b^0 \\ RT\boldsymbol{\nabla}_y \ln c_b^0 \\ \boldsymbol{\nabla}_y \psi_b^0 \end{pmatrix}$$

Summary of the dual porosity model

$$
\left\{
\begin{array}{ll}
\nabla_x . \boldsymbol{\sigma}^0_L - \nabla_x P^0_f = 0 & \textbf{Overall momentum balance} \\
\boldsymbol{\sigma}^0_L = -\left\langle p^0_b \right\rangle_y \boldsymbol{I} + (1-\phi)\, \boldsymbol{C}_s\, \boldsymbol{\mathcal{E}}_x(\mathbf{u}^0) + \boldsymbol{C}_s \left\langle \boldsymbol{\mathcal{E}}_y(\mathbf{u}^1) \right\rangle_y - \left\langle \mathbf{\Pi}^0 \right\rangle_y & \\
\nabla_x . \dfrac{\partial \mathbf{u}^0}{\partial t} + \nabla_x . \boldsymbol{V}^0_{Df} = 0 & \textbf{Overall mass balance} \\
\boldsymbol{V}^0_{Df} = -\boldsymbol{K}^f_P\, \nabla_x P^0_f - \boldsymbol{K}^f_C\, \nabla_x C^0_f - \boldsymbol{K}^f_E\, \nabla_x \Psi^0_f & \textbf{Macroscopic Darcy's law} \\
\dfrac{\partial n_f}{\partial t} + (1-n_f)\, \nabla_x . \boldsymbol{V}^0_{Df} = -\left\langle \dfrac{1}{1-\phi^0} \dfrac{\partial \phi^0}{\partial t} \right\rangle_y & \textbf{Fluid phase mass balance} \\
2 \dfrac{\partial}{\partial t} \left(n_f\, C^0_f \right) + \nabla_x . \boldsymbol{J}^0_F = -\dfrac{\partial}{\partial t} \left\langle \phi^0\, G_c\, c^0_b \right\rangle_y & \textbf{Species overall mass balance} \\
\boldsymbol{J}^0_F = 2\, C^0_f\, \boldsymbol{V}^0_{Df} - 2\, \boldsymbol{D}^{eff}_f\, \nabla_x C^0_f & \\
\nabla_x . \boldsymbol{I}^0_F = 0 & \textbf{Macroscopic charge conservation} \\
\boldsymbol{I}^0_F = -2\, F \left(\boldsymbol{\Delta}^{eff}_f\, \nabla_x C^0_f + \boldsymbol{D}^{eff}_f\, C^0_f\, \nabla_x \overline{\Psi}^0_f \right) &
\end{array}
\right.
$$

and in the clay clusters

$$\left\{\begin{array}{l}
\boldsymbol{\nabla}_y.\left(\boldsymbol{C}_s\,\boldsymbol{\mathcal{E}}_y\left(\mathbf{u}^1\right)\right)-\boldsymbol{\nabla}_y p_b^0-\boldsymbol{\nabla}_y.\boldsymbol{\Pi}^0=0\\
\boldsymbol{\nabla}_y.\mathbf{v}_D^1+\boldsymbol{\nabla}_y.\dfrac{\partial\mathbf{u}^1}{\partial t}=-\boldsymbol{\nabla}_x.\dfrac{\partial\mathbf{u}^0}{\partial t}\\
\dfrac{\partial\phi^0}{\partial t}-\left(1-\phi^0\right)\boldsymbol{\nabla}_y.\dfrac{\partial\mathbf{u}^1}{\partial t}=\left(1-\phi^0\right)\boldsymbol{\nabla}_x.\dfrac{\partial\mathbf{u}^0}{\partial t}\\
\dfrac{\partial}{\partial t}\left(\phi^0\,G_c\,c_b^0\right)+\boldsymbol{\nabla}_y.\boldsymbol{J}^1+2\,\boldsymbol{\nabla}_y.\left(c_b^1\,\mathbf{v}_D^1\right)=0\\
\dfrac{\partial}{\partial t}\left(\phi^0\,G_s\,c_b^0\right)+\boldsymbol{\nabla}_y.\boldsymbol{I}^1=0\\
\mathbf{v}_D^1=-L_{PP}\,\boldsymbol{\nabla}_y p_b^0-L_{PC}\,\boldsymbol{\nabla}_y c_b^0-L_{PE}\,\boldsymbol{\nabla}_y\psi_b^0\\
\boldsymbol{J}^1=-L_{CP}\,\boldsymbol{\nabla}_y p_b^0-L_{CC}\,\boldsymbol{\nabla}_y c_b^0-L_{CE}\,\boldsymbol{\nabla}_y\psi_b^0\\
\boldsymbol{I}_D^1=-L_{EP}\,\boldsymbol{\nabla}_y p_b^0-L_{EC}\,\boldsymbol{\nabla}_y c_b^0-L_{EE}\,\boldsymbol{\nabla}_y\psi_b^0
\end{array}\right.$$

with the following boundary conditions

$$\left\{\begin{array}{l}
\left(-\boldsymbol{C}_s\,\boldsymbol{\mathcal{E}}_y(\mathbf{u}^1)+\boldsymbol{\Pi}^0\right)\boldsymbol{N}=\boldsymbol{C}_s\,\boldsymbol{\mathcal{E}}_x(\mathbf{u}^0)\boldsymbol{N}\\
p_b^0=P_f^0\qquad c_b^0=C_f^0\qquad \psi_b^0=\Psi_f^0
\end{array}\right.$$

3.3. Three-scale quasi-steady model

“uniform values assumed inside the clay clusters”

$$
\left\{
\begin{array}{l}
\boldsymbol{\nabla}_x . \boldsymbol{\sigma}_T^0 = 0 \\
\boldsymbol{\sigma}_T^0 = -P_f^0 \, \boldsymbol{I} + \boldsymbol{C}^{eff} \, \boldsymbol{\mathcal{E}}_x(\mathbf{u}^0) - \boldsymbol{\Pi}^{eff} \\
\boldsymbol{\nabla}_x . \dfrac{\partial \mathbf{u}^0}{\partial t} + \boldsymbol{\nabla}_x . \boldsymbol{V}_{Df}^0 = 0 \\
\boldsymbol{V}_{Df}^0 = -\boldsymbol{K}_P^f \, \boldsymbol{\nabla}_x P_f^0 - \boldsymbol{K}_C^f \, \boldsymbol{\nabla}_x C_f^0 - \boldsymbol{K}_E^f \, \boldsymbol{\nabla}_x \Psi_f^0 \\
\dfrac{\partial n_f}{\partial t} + (1 - n_f) \, \boldsymbol{\nabla}_x . \boldsymbol{V}_{Df}^0 + \boldsymbol{\alpha} : \dfrac{\partial}{\partial t} \boldsymbol{\mathcal{E}}_x(\mathbf{u}^0) = - \left\langle \boldsymbol{\nabla}_y . \dfrac{\partial \mathbf{u}_\pi^1}{\partial t} \right\rangle_y \\
\dfrac{\partial}{\partial t} \left(n_f \, C_f^0 \right) + \boldsymbol{\nabla}_x . \left(C_f^0 \, \boldsymbol{V}_{Df}^0 \right) - \boldsymbol{\nabla}_x . \left(\boldsymbol{D}_f^{eff} \boldsymbol{\nabla}_x C_f^0 \right) = - \dfrac{\partial \left(K_* \, C_f^0 \right)}{\partial t} \\
\boldsymbol{\nabla}_x . \boldsymbol{I}_F^0 = 0 \\
\boldsymbol{I}_F^0 = -2 \, F \left(\boldsymbol{\Delta}_f^{eff} \, \boldsymbol{\nabla}_x C_f^0 + \boldsymbol{D}_f^{eff} \, C_f^0 \, \boldsymbol{\nabla}_x \overline{\Psi}_f^0 \right)
\end{array}
\right.
$$

• Terzaghi’s decomposition in the quasi-steady approximation

$$\boldsymbol{\sigma}_T^0 = -P_f^0\,\boldsymbol{I} + \boldsymbol{C}^{eff}\,\boldsymbol{\mathcal{E}}_x(\mathbf{u}^0) - \boldsymbol{\Pi}^{eff}$$

• Closure

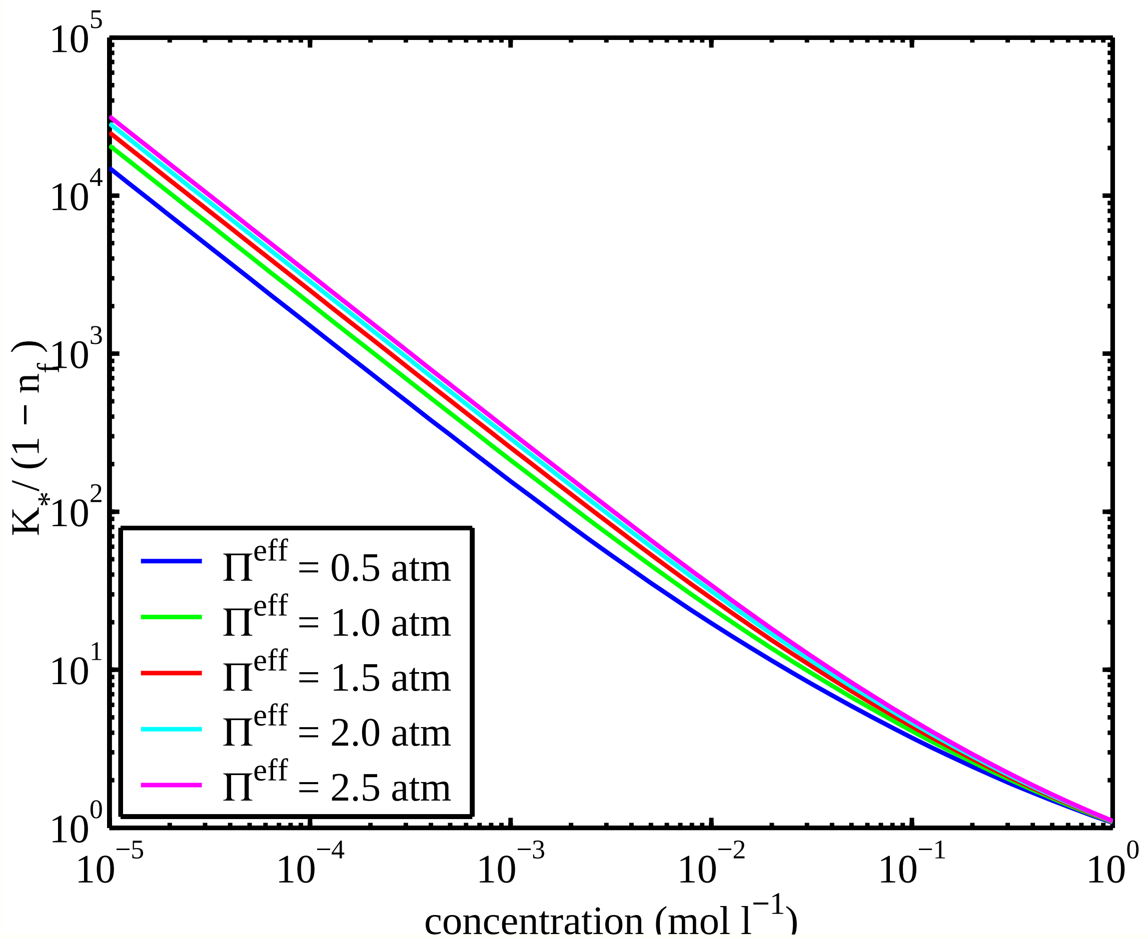
$$\left\{\begin{array}{rcccc} \boldsymbol{\nabla}_y.\,(\boldsymbol{C}_s\,\boldsymbol{\mathcal{E}}_y(\mathbf{u}^1)) - \boldsymbol{\nabla}_y.\boldsymbol{\Pi}^0 & = & 0 & \text{in} & Y_s \\ \boldsymbol{C}_s\left[\boldsymbol{\mathcal{E}}_x(\mathbf{u}^0)+\boldsymbol{\mathcal{E}}_y(\mathbf{u}^1)\right]\,\boldsymbol{N} & = & \boldsymbol{\Pi}^0\,\boldsymbol{N} & \text{on} & \partial Y_{fs} \end{array}\right.$$

$$\mathbf{u}^1(\boldsymbol{x},\boldsymbol{y},t) = \boldsymbol{\xi}(\boldsymbol{y})\,\boldsymbol{\mathcal{E}}_x\left(\mathbf{u}^0(\boldsymbol{x},t)\right) + \mathbf{u}^1_\pi(\boldsymbol{x},\boldsymbol{y},t) + \widehat{\mathbf{u}}(\boldsymbol{x},t)$$

$$\begin{array}{rcl|rcl|ll} \boldsymbol{\nabla}_y.\,(\boldsymbol{C}_s\,\boldsymbol{\mathcal{E}}_y\,(\boldsymbol{\xi})) & = & 0 & \boldsymbol{\nabla}_y.\,\left(\boldsymbol{C}_s\,\boldsymbol{\mathcal{E}}_y(\mathbf{u}^1_\pi)\right) & = & \boldsymbol{\nabla}_y.\boldsymbol{\Pi}^0 & \text{in} & Y_s \\ (\boldsymbol{C}_s\,\boldsymbol{\mathcal{E}}_y\,(\boldsymbol{\xi}))\,\boldsymbol{N} & = & -\boldsymbol{C}_s\,(\boldsymbol{I}\otimes\boldsymbol{I})\,\boldsymbol{N} & \boldsymbol{C}_s\,\boldsymbol{\mathcal{E}}_y(\mathbf{u}^1_\pi)\boldsymbol{N} & = & \boldsymbol{\Pi}^0\,\boldsymbol{N} & \text{on} & \partial Y_{fs} \end{array}$$

• Homogenized properties

$$\boldsymbol{C}^{eff} \equiv \left\langle \boldsymbol{C}_s\left[\boldsymbol{I}\otimes\boldsymbol{I} + \boldsymbol{\mathcal{E}}_y(\boldsymbol{\xi})\right]\right\rangle_y \qquad \text{and} \qquad \boldsymbol{\Pi}^{eff} \equiv \left\langle \boldsymbol{\Pi}^0 - \boldsymbol{C}_s\,\boldsymbol{\mathcal{E}}_y\left(\mathbf{u}^1_\pi\right)\right\rangle_y$$



Blocks made of parallel arrangement of clay particles

4. Conclusions

$\ast$ **Complete theory for the two–scale problem.**

$\ast$ **The physics of the model can be extended at the microscale: hydratation forces, Van der Walls forces, couplings with molecular dynamics. . .**

$\ast$ **New three-scale solution for the saturated case.**

$\ast$ **Extension needed for the non-saturated case: couplings between disjoining pressure and capillary pressure.**

$\ast$ **Applications : engineered barriers (nuclear waste); clay liner (waste); stability of wells; electro-osmosis; biomechanics. . .**