Crystal Precipitation and Dissolution in a Porous Medium: Evolving Microstructure & Perforated Solid Matrix

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Evolving Microstructure & Perforated Solid Matrix

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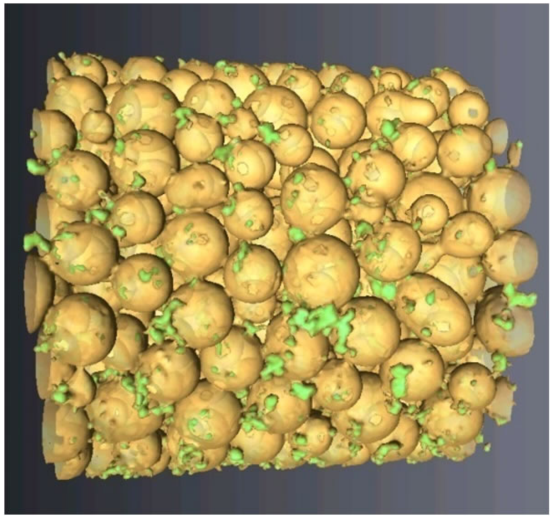
Evolving Microstructure

- Typically we are interested in the *flow of a fluid* as well as the *transport of substances* distributed in the fluid: DARCY equations, tranport equations
- Sometimes, reactions of the substances are able to *change hydrodynamical properties* of the porous media: minerals, electrically charged particles, biofilms



Oregon State University, Wildenschild Research Group, Iltis, Armstrong, Jansik.

- Strong coupling: flow → transport → porous medium → flow, transport
- Applications: Filter systems, biobarriers (MEOR), ...

Perforated Solid Matrix

- Some porous media do not have a throughout homogeneous structure of the void spaces.
- Inclusions of the solid material may be of different size, e.g. carbonate rocks.
- We take this into account and hence consider fluid flow and solute transport in a porous medium, where the *solid matrix is assumed to be perforated*, i.e. each solid grain is porous.
- The fluid flow within the perforated solid matrix is given by Darcy's law, but by the Stokes equations in the large cavities (pore space). Therefore, a *Darcy-Stokes system at the pore-scale* describes the fluid flow through the porous medium.
- In case of *high flow rates or large microporosities*, the flow within the permeable grain is not negligible and hence affects solute transport (and reactions) in the porous medium significantly [Landa-Marbán et al. '18].

From Pore-scale to an Effective Model

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Pore-scale Model

We consider the following pore-scale model for the description of flow and transport in a porous medium $\Omega_\varepsilon(t)$ with microporous solid matrix, which is evolving due to heterogeneous reactions at the solid–liquid interface $\Gamma_{\varepsilon,I}$.

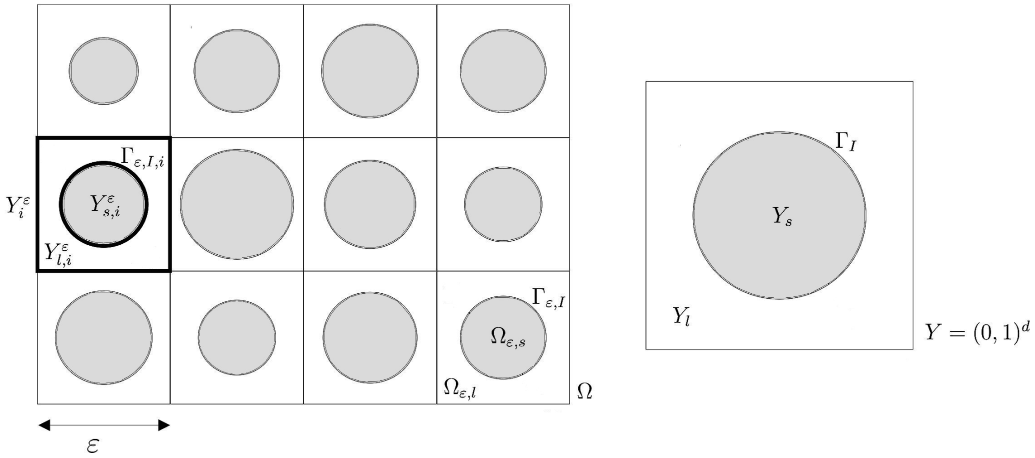

Figure: Periodic representation of a porous medium Ω with perforated solid matrix (gray) and the unit cell Y.

Pore-scale Model

We consider the following pore-scale model for the description of flow and transport in a porous medium $\Omega_\varepsilon(t)$ with microporous solid matrix, which is evolving due to heterogeneous reactions at the solid–liquid interface $\Gamma_{\varepsilon,l}$.

The fluid in the pore space is incompressible and described by the **Stokes equations**:

$$\begin{cases} \mu\varepsilon^2 \Delta v_\ell^\varepsilon = \nabla p_\ell^\varepsilon & \text{in } \Omega_{\varepsilon,\ell}(t) \\ \nabla \cdot v_\ell^\varepsilon = 0 & \text{in } \Omega_{\varepsilon,\ell}(t)\,, \end{cases}$$

where v_ℓ^ε and p_ℓ^ε are the velocity and the pressure of the fluid, respectively.

The small viscosity of order ε^2 physically balances the friction of the fluid on the interface, [Hornung, Allaire ’97].

The fluid flow within the perforated solid matrix is described via **Darcy’s law**, cf. [1]:

$$\begin{cases} v_s^\varepsilon = -\frac{1}{\mu} K(\theta_s^\varepsilon) \nabla p_s^\varepsilon & \text{in } \Omega_{\varepsilon,s}(t) \\ \nabla \cdot v_s^\varepsilon = -B \partial_t \theta_s^\varepsilon & \text{in } \Omega_{\varepsilon,s}(t)\,. \end{cases}$$

Also here v_s^ε and p_s^ε denote the velocity and the pressure, respectively, of the fluid contained in the grains. Furthermore, K and θ_s^ε describe the changeable permeability tensor and inner porosity of the microporous matrix, respectively.

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[1]: R. Schulz, P. Knabner: *Derivation and analysis of an effective model for biofilm growth in evolving porous media*, Math. Meth. Appl. Sci. 40 (8), 2930–2948, (2017).

Furthermore, we consider the **Beavers-Joseph interface condition**, continuity of mass flux, and continuity of normal stress at the solid-liquid interface $\Gamma_{\varepsilon,I}(t)$, cf. [2]:

$$\begin{cases} (v_\ell^\varepsilon - v_s^\varepsilon)\cdot\nu_I \;=\; \varepsilon B(1-\theta_s^\varepsilon)v_n^\varepsilon & \text{on } \Gamma_{\varepsilon,I}(t) \\ \frac{\alpha}{\varepsilon\sqrt{K(\theta_s^\varepsilon)}} v_\ell^\varepsilon\cdot\tau \;=\; \nu_I\cdot\nabla v_\ell^\varepsilon\tau & \text{on } \Gamma_{\varepsilon,I}(t) \\ p_\ell^\varepsilon - p_s^\varepsilon \;=\; \mu\varepsilon^2\nu_I\cdot\nabla v_\ell^\varepsilon\nu_I & \text{on } \Gamma_{\varepsilon,I}(t) \end{cases}$$

with the normal velocity of the interface v_n^ε and the dimensionless slip coefficient α. The unit normal ν_I is defined to point into the solids and the tangential vector τ with length 1 being orthogonal to ν_I.

Let c_ℓ^ε denote the solute concentration in the liquid phase. On the other hand, c_s^ε is the solute concentration distributed in the fluid contained in the grains. Therefore, the transport of solutes is given by the following equations:

$$\begin{cases} \partial_t c_\ell^\varepsilon - \nabla\cdot\left(D\nabla c_\ell^\varepsilon - c_\ell^\varepsilon v_\ell^\varepsilon\right) \;=\; 0 & \text{in } \Omega_{\varepsilon,\ell}(t)\times(0,T) \\ \partial_t(\theta_s^\varepsilon c_s^\varepsilon) - \nabla\cdot\left(D_s(\theta_s^\varepsilon)\nabla c_s^\varepsilon - c_s^\varepsilon v_s^\varepsilon\right) \;=\; -\sigma(\theta_s^\varepsilon) f_s(c_s^\varepsilon,\theta_s^\varepsilon)\rho & \text{in } \Omega_{\varepsilon,s}(t)\times(0,T) \end{cases}$$

Here $\sigma(\theta_s^\varepsilon(x,t))$ denotes the specific surface of a single “microscopic grain”. The solid part of the grains is assumed to have constant density $\rho > 0$.

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[2]: T. Arbogast, H.L. Lehr: *Homogenization of a Darcy-Stokes system modeling vuggy porous media*, Comput. Geosci. 10 (3), 291–302, (2006).

We also have the rate of **precipitation/dissolution** f_s in the inner of the grain, which is assumed to be given via $f_s(c_s^\varepsilon, \theta_s^\varepsilon) := k(r(c_s^\varepsilon) - \omega_s)$ with a constant k, a function r for the precipitation and the dissolution rate $\omega_s \in H(\theta_{s,\max} - \theta_s^\varepsilon)$ with the set-valued Heaviside graph:

$$H(\psi) := \begin{cases} \{0\} & , \psi < 0 \\ [0,1] & , \psi = 0 \\ \{1\} & , \psi > 0 \, . \end{cases}$$

It is reasonable to define the dissolution rate as follows:

$$\omega_s(\theta_s^\varepsilon) := \begin{cases} 1 & , \theta_s^\varepsilon < \theta_{s,\max} \\ \min\{r(c_s^\varepsilon), 1\} & , \theta_s^\varepsilon = \theta_{s,\max} \, , \end{cases}$$

where $\theta_{s,\max} \in (0,1)$ denotes the solid porosity in such a way that a crystalline layer is absent.

The porosity θ_s^ε of the perforated solid matrix is assumed to satisfy the following ordinary differential equation, cf. [3]:

$$\partial_t \theta_s^\varepsilon = -\sigma(\theta_s^\varepsilon) f_s(c_s^\varepsilon, \theta_s^\varepsilon) \, .$$

Throughout this talk, at initial time $t = 0$ each single solid grain is perforated uniformly, i.e. $\theta_s^\varepsilon(x_1, 0) = \theta_s^\varepsilon(x_2, 0)$ if $x_1, x_2 \in \Omega_{\varepsilon,s,i,j}(t)$ for some i, j.

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[3]: R. Schulz, N. Ray, F. Frank, H. Mahato, P. Knabner: *Strong solvability up to clogging of an effective diffusion-precipitation model in an evolving porous medium*, Eur. J. Appl. Math. 28 (2), 179–207, (2017).

We still need appropriate boundary conditions describing the **interchange of solutes** across the interface $\Gamma_{\varepsilon,l}(t)$:

$$\left(D\nabla c_\ell^\varepsilon - c_\ell^\varepsilon v_\ell^\varepsilon - D_s(\theta_s^\varepsilon)\nabla c_s^\varepsilon + c_s^\varepsilon v_s^\varepsilon\right)\cdot \nu_l = \varepsilon v_n^\varepsilon\left((1-\theta_s^\varepsilon)\rho + \theta_s^\varepsilon c_s^\varepsilon - c_\ell^\varepsilon\right) \quad \text{on } \Gamma_{\varepsilon,l}(t)\ .$$

These conditions ensure mass conservation at $\Gamma_{\varepsilon,l}$. Furthermore, we assume the solute concentration to be continuous across the interface $\Gamma_{\varepsilon,l}$, hence the right-hand side simplifies to

$$\varepsilon v_n^\varepsilon(1-\theta_s^\varepsilon)(\rho - c_\ell^\varepsilon)\ .$$

The **normal velocity** v_n^ε of the interface $\Gamma_{\varepsilon,l}$ is caused by precipitation and dissolution on $\Gamma_{\varepsilon,l}$, such that we have

$$v_n^\varepsilon = -k(r(c_\ell^\varepsilon) - \omega) \qquad \text{on } \Gamma_{\varepsilon,l}(t)$$

with $\omega \in H(\mathrm{dist}\,(x, \Omega_{\varepsilon,s}(t)))$ and the Euclidian distance function dist. Similar to ω_s we define $\omega = 1$ whenever crystalline layer is present. Otherwise, we set $\omega = \min\{r(c_\ell^\varepsilon), 1\}$.

To locate the interface $\Gamma_{\varepsilon,l}$, we use the **level-set framework**:

The moving interface $\Gamma_{\varepsilon,l}$ can be described as the zero set of an appropriate level-set function $L^\varepsilon : \Omega_T \to \mathbb{R}$:

$$\Gamma_{\varepsilon,l}(t) = \{\xi \in \Omega \,|\, L^\varepsilon(\xi, t) = 0\} \,,$$

where $\Omega_T := \Omega \times (0, T)$. Thus the liquid phase and the complementary perforated solid phase are characterized via:

$$\Omega_{\varepsilon,\ell}(t) = \{\xi \in \Omega \,|\, L^\varepsilon(\xi, t) < 0\} \quad \text{and} \quad \Omega_{\varepsilon,s}(t) = \{\xi \in \Omega \,|\, L^\varepsilon(\xi, t) > 0\} \,.$$

The level-set function L^ε satisfies the hyperbolic differential equation

$$\partial_t L^\varepsilon + v_n^\varepsilon |\nabla L^\varepsilon| = 0 \qquad \text{in } \Omega_T \,.$$

We are choosing an initial data L_0^ε corresponding to L^ε such that $\Gamma_{\varepsilon,l}(0)$ is nothing, but the zero set of L_0^ε.

To derive an effective model which approximates the original problem of the pore-scale we make use of the **periodic homogenization method**. We assume that all variable functions can be represented with the formal asymptotic expansion with respect to the small scale parameter ε, e.g.

$$v_\ell^\varepsilon(x,t) = v_\ell^0(x,\tfrac{x}{\varepsilon},t) + \varepsilon v_\ell^1(x,\tfrac{x}{\varepsilon},t) + \varepsilon^2 v_\ell^2(x,\tfrac{x}{\varepsilon},t) + \dots$$

Defining the vector $y := \frac{x}{\varepsilon}$ the functions v_ℓ^k, $k = 0, 1, 2, \dots$, depend on the two space variables

x: “macroscopic” variable locating of the microstructure

y: “microscopic” variable describing the oscillations inside the microstructure

As a consequence, the expansion of the gradient and the Laplacian read

$$\nabla = \nabla_x + \varepsilon^{-1}\nabla_y \qquad \text{and} \qquad \Delta = \Delta_x + 2\varepsilon^{-1}\nabla_x \cdot \nabla_y + \varepsilon^{-2}\Delta_y\,,$$

respectively.

Applying the formal expansion on the level-set equation we obtain

$$\partial_t L^0 + v_n^0|\nabla_y L^0| = 0 \qquad \text{in } \Omega \times Y \times (0,T)\,,$$

where the scalar v_n^0 denotes the ε^0-ordered terms of an approriate extension of v_n^ε.

Owing to the assumption on θ_s^ε at initial time, the initial data $\theta_s^0(.,0)$ is independent of y. Thus, we obtain that $\theta^0_{s\,(x,t)}$ does not depend on y likewise.

Also $v^0_{n\,(x,t)}$ is independent of y (due to $c^0_{\ell\,(x,t)}$). The coarea formula of geometric measure theory yields

$$\partial_t \big| Y^0_{\ell\,(x,t)} \big| = \int_{\Gamma^0_{l\,(x,t)}} v^0_{n\,(x,y,t)}\, d\sigma_y = \big| \Gamma^0_{l\,(x,t)} \big| \cdot v^0_{n\,(x,t)} \qquad \text{in } \Omega_T \, ,$$

which is nothing but the change of the liquid phase volume fraction $\theta = \big| Y^0_\ell \big|$ in time within the domain Ω. Let us denote the volume fraction of the entire void space (including microscopic perforations of the solid) or *porosity* by

$$\vartheta_{(x,t)} := \theta_{(x,t)} + \int_{Y^0_{s\,(x,t)}} \theta^0_{s\,(x,t)}\, dy = \big(\theta + (1-\theta)\theta^0_s \big)_{\,(x,t)} \, .$$

Since v^0_n is independent of y, the normal velocity is constant along the interface in a unit cell. This enables us to characterize the geometrical setting of the surfaces $\Gamma^0_{l\,(x,t)}$ via $\theta_{(x,t)}$. In this case, the hyperbolic level-set equation reduces to an ODE for θ, cf. [1,3,4]:

$$\partial_t \theta \;=\; -|\Gamma^0_l(\theta)|\, k \left(r(c^0) - \omega^0 \right) \;\text{ in } \Omega_T \, .$$

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[4]: T. L. van Noorden: *Crystal precipitation and dissolution in a porous medium: effective equations and numerical experiments*, Multiscale Model. Simul. 7, 1220–1236, (2009).

Derivation of the DARCY (macro)-equations

ε^{-1}: p^0 independent of y: $\quad p^0{}_{(x,t)} = p^0_{\ell\,(x,t)} = p^0_{s\,(x,t)}$.

ε^0: DARCYs law: $q_{(x,t)} \left(:= \int_{Y^0_{\ell\,(x,t)}} v^0_{\ell\,(x,y,t)}\, dy + \int_{Y^0_{s\,(x,t)}} v^0_{s\,(x,y,t)}\, dy \right) = -\frac{1}{\mu}\mathbb{K}_{(x,t)} \nabla_x p^0{}_{(x,t)}$

with the permeabilty tensor

$$[\mathbb{K}]_{i,j\,(x,t)} := \int_{Y^0_{\ell\,(x,t)}} (\omega_{\ell,j})_{i(x,y,t)}\, dy + \int_{Y^0_{s\,(x,t)}} (\omega_{s,j})_{i(x,y,t)}\, dy \,,$$

where $(\omega_{k,j}, \pi_{k,j}) : Y^0_{k\,(x,t)} \to \mathbb{R}^d \times \mathbb{R}$, $k \in \{\ell, s\}$, solves the cell problem

$$(\mathrm{C1}) \left\{ \begin{array}{rcll} -\Delta_y \omega_{\ell,j} + \nabla_y \pi_{\ell,j} & = & e_j & \text{in } Y^0_{\ell\,(x,t)} \\ \nabla_y \cdot \omega_{\ell,j} & = & 0 & \text{in } Y^0_{\ell\,(x,t)} \\ (K(\theta^0_s))^{-1}\omega_{s,j} + \nabla_y \pi_{s,j} & = & e_j & \text{in } Y^0_{s\,(x,t)} \\ \nabla_y \cdot \omega_{s,j} & = & 0 & \text{in } Y^0_{s\,(x,t)} \\ \left(\omega_{\ell,j} - \omega_{s,j}\right) \cdot \nu^0_I & = & 0 & \text{on } \Gamma^0_{I\,(x,t)} \\ \frac{\alpha}{\sqrt{K(\theta^0_s)}}\omega_{\ell,j} \cdot \tau^0 & = & \nu^0_I \cdot \nabla_y \omega_{\ell,j} \tau^0 & \text{on } \Gamma^0_{I\,(x,t)} \\ \pi_{\ell,j} - \pi_{s,j} & = & \mu \nu^0_I \cdot \nabla_y \omega_{\ell,j} \nu^0_I & \text{on } \Gamma^0_{I\,(x,t)} \\ \multicolumn{4}{l}{\omega_{\ell,j} \text{ and } \pi_{\ell,j} \text{ are } Y\text{-periodic}\,,} \end{array} \right.$$

See [2].

$$\nabla_x \cdot q_{(x,t)} = -B \int_{Y^0_{s\,(x,t)}} \partial_t \theta^0_s - B \int_{\Gamma^0_{I\,(x,t)}} (1 - \theta^0_s) v^0_n \, d\sigma_y = -B \partial_t \vartheta_{(x,t)} \,,$$

i.e. the change of the porosity $\vartheta_{(x,t)}$ induces fluid flow.

Derivation of the upscaled transport equation

ε^{-2}: c^0 independent of y, i.e. $c^0{}_{(x,t)} = c^0_{\ell}{}_{(x,t)} = c^0_{s}{}_{(x,t)}$, since

$$\begin{cases} -D\Delta_y c^0_\ell = 0 & \text{in } Y^0_{\ell}{}_{(x,t)} \\ -D_s(\theta^0_{s}{}_{(x,t)})\Delta_y c^0_s = 0 & \text{in } Y^0_{s}{}_{(x,t)} \\ D\nabla_y c^0_\ell \cdot \nu_I = D_s(\theta^0_{s}{}_{(x,t)})\nabla_y c^0_s \cdot \nu_I & \text{on } \Gamma^0_{I}{}_{(x,t)} \\ c^0_\ell \text{ is } Y\text{-periodic.} \end{cases}$$

ε^{-1}: The terms of order ε^{-1} describing the transport lead to

$$c^1_{\ell}{}_{(x,y,t)} = \nabla_x c^0{}_{(x,t)} \cdot \eta_{\ell(x,y,t)} \quad \text{and} \quad c^1_{s}{}_{(x,y,t)} = \nabla_x c^0{}_{(x,t)} \cdot \eta_{s(x,y,t)} \,,$$

where $(\eta_\ell, \eta_s) := (\eta_{\ell,j}, \eta_{s,j})_{j=1}^{d}$, $j = 1, ..., d$, solves the following PDEs in the unit cell:

$$\text{(C2)} \begin{cases} -D\Delta_y \eta_{\ell,j} = 0 & \text{in } Y^0_{\ell}{}_{(x,t)} \\ -D_s(\theta^0_{s}{}_{(x,t)})\Delta_y \eta_{s,j} = 0 & \text{in } Y^0_{s}{}_{(x,t)} \\ \left(D\nabla_y \eta_{\ell,j} - D_s(\theta^0_s)\nabla_y \eta_{s,j}\right) \cdot \nu^0_I = -(D - D_s(\theta^0_s))e_j \cdot \nu^0_I & \text{on } \Gamma^0_{I}{}_{(x,t)} \\ \eta_{\ell,j} = \eta_{s,j} & \text{on } \Gamma^0_{I}{}_{(x,t)} \\ \eta_{\ell,j} \text{ is } Y\text{-periodic}\,. \end{cases}$$

ε^0: Integrating over the equation corresponding to the ε^0-terms gives

$$\partial_t \left(\vartheta c^0\right) = \nabla_x \cdot \left(\mathbb{D}\nabla_x c^0 - qc^0\right) + \rho\partial_t\vartheta \,.$$

Effective Model

Darcy's law:

$$\begin{aligned} q &= -\tfrac{1}{\mu}\mathbb{K}\nabla_x p^0 && \text{in } \Omega_T \\ \nabla_x \cdot q &= -B\partial_t\vartheta && \text{in } \Omega_T \end{aligned}$$

Transport equation:

$$\partial_t\left(\vartheta c^0\right) = \nabla_x \cdot \left(\mathbb{D}\nabla_x c^0 - qc^0\right) + \rho\partial_t\vartheta \quad \text{in } \Omega_T$$

Evolution of the microstructure:

$$\begin{aligned} \partial_t\theta &= -|\Gamma_l^0(\theta)|k\left(r(c^0) - \omega^0\right) && \text{in } \Omega_T \\ \partial_t\theta_s^0 &= -\sigma(\theta_s^0)\,k\left(r(c^0) - \omega_s^0\right) && \text{in } \Omega_T \end{aligned}$$

with $\vartheta = \theta + (1-\theta)\theta_s^0$.

The dissolution rate ω_s^0 is defined by $\omega_s^0(\theta,\theta_s^0) := \begin{cases} 1 & ,\ \theta_s^0 < \theta_{s,\max} \\ \min\{r(c^0), 1\} & ,\ \theta_s^0 = \theta_{s,\max} \end{cases}$,

where $\theta_{s,\max(x,t)} = 0$ if $\theta_{(x,t)} < \theta_{\mathrm{clean}(x,t)}$ otherwise $\theta_{s,\max(x,t)} > 0$.

The effective parameters, depending on θ, θ_s^0 and containing the essential information of the microscale, are given by the solutions of the cell problems (C1), (C2):

$$[\mathbb{K}]_{i,j\,(x,t)} := \int_{Y_\ell^0(x,t)} (\omega_{\ell,j})_{i(x,y,t)}\,dy + \int_{Y_s^0(x,t)} (\omega_{s,j})_{i(x,y,t)}\,dy\,,$$

$$[\mathbb{D}]_{i,j\,(x,t)} := D\int_{Y_\ell^0(x,t)} \left(\delta_{i,j} + \partial_{y_i}\eta_{\ell,j}\right)_{(x,y,t)} dy + D_s(\theta_s^0)\int_{Y_s^0(x,t)} \left(\delta_{i,j} + \partial_{y_i}\eta_{s,j}\right)_{(x,y,t)} dy\,.$$

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[5]: Schulz R.: *Crystal precipitation and dissolution in a porous medium: Evolving microstructure and perforated solid matrix*, Special Topics Rev. Porous Media, accepted.

Computational Illustration

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Computational Illustration

In the following we illustrate the impact of the porous matrix on the permeability. We first compare the cell problems' solution for the Stokes regime with those of the Stokes-Darcy regime (C1). A representative porous matrix (quadratic inclusion) $Y_s = [\frac{1}{4}, \frac{3}{4}] \times [\frac{1}{4}, \frac{3}{4}]$ is considered. Here, different values of permeability ranging from $K = 10^{-1}$ to $= 10^{-7}$ are considered in the Darcy region. Grids of fineness 2^{-6} are used for the discretization.

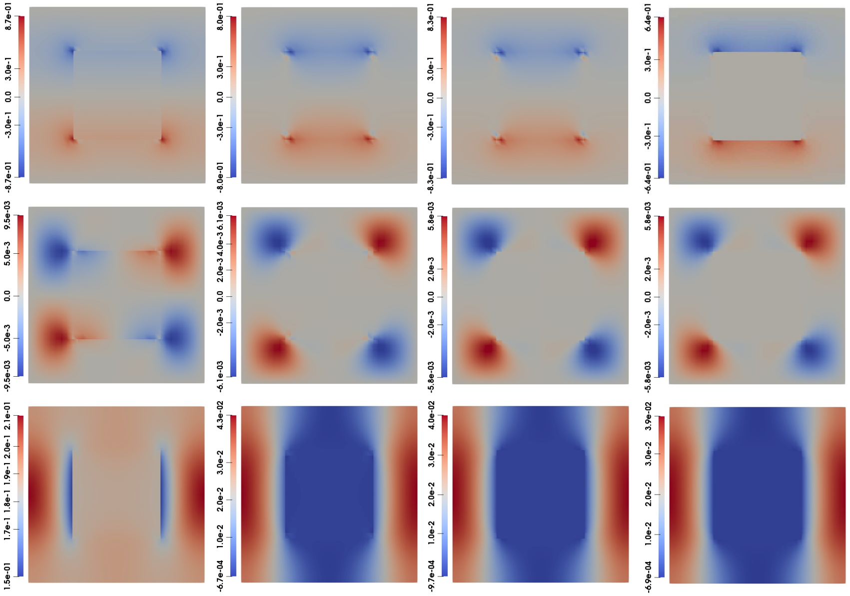

Figure: Cell problems' solutions π (*top*), ω_1 (*middle*) and ω_2 (*bottom*) for Stokes-Darcy regime (C1) with right hand side e_2 and $K = 10^{-1}$ (*left*), $K = 10^{-4}$ (*2nd column*), $K = 10^{-7}$ (*3rd column*) and Stokes flow (*right*).

We compare the impact on the permeability values:

- For the Stokes regime, we calculate $\mathbb{K} = 0.0131$.
- The table shows the different permeability $\mathbb{K}$ for the Stokes-Darcy regime ranging from 0.795 to 0.0134.

K	10^0	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}
$\mathbb{K}$	0.795	0.189	0.0436	0.0196	0.0149	0.0138	0.0135	0.0134	0.0134

- It is evident that the impact of the Darcy regime is negligible for small values of K in the porous matrix.]

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[6]: Schulz R., Ray N., Zech S., Rupp A., Knabner P.: *Beyond Kozeny-Carman: Predicting the permeability in porous media*, submitted.

Advective Biofilms

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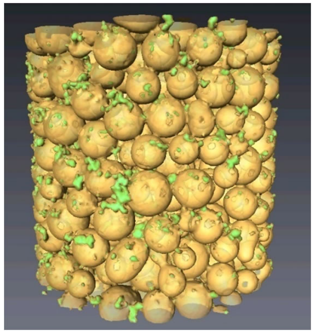

Oregon State University, Wildenschild Research Group, Iltis, Armstrong, Jansik.

- The increase of a biomass on the surface of the solid matrix changes the porosity and impede the flow through the pores.
- Such microorganims can be used for forming biobarriers which restrict the flow of ground water, e.g. to control the propagation of contaminants.
- In filter systems biofilms lead to an unwanted decrease in efficiency (*biofouling*).
- *Biofilms form fluid channels significantly supporting the transport of nutrients.* This advective transport within the biomass facilitates also the “deepest” bacteria to get nutrients in an adequate time.

Pore-scale Model

- In this sense, a biofilm itself should be considered as a porous medium, with the fluid channels as “pores” and immobile bacteria or EPS as “organic grains”.

We consider the following pore-scale model for the description of transport within a porous medium $\Omega_\varepsilon(t)$, which is evolving due to de-/attachment at the solid–liquid interface $\Gamma_{\varepsilon,I}$.

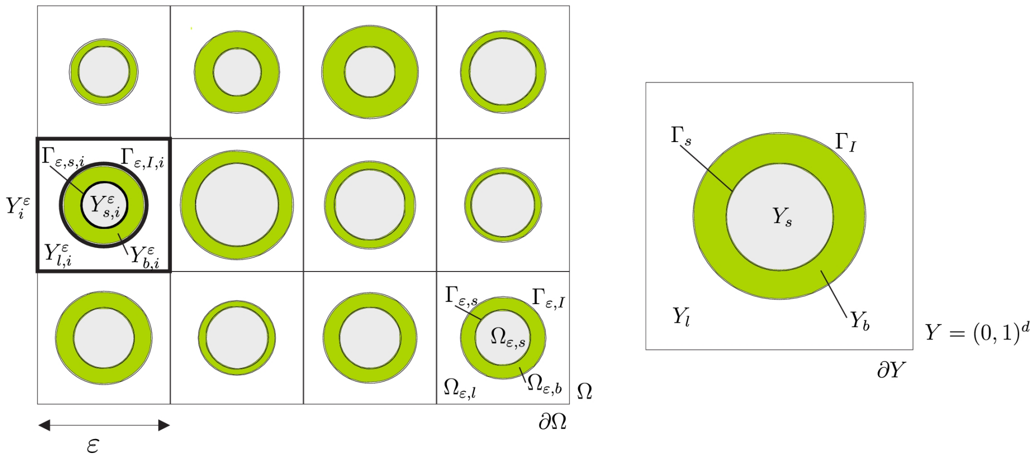

Figure: Periodic representation of a porous medium Ω and the unit cell Y, where each solid grain (gray) is surrounded by a biofilm (green).

Effective Model

Darcy's law:

$$\begin{aligned} q &= -\tfrac{1}{\mu}\mathbb{K}\nabla_x p^0 && \text{in } \Omega_T \\ \nabla_x \cdot q &= -B\,\partial_t\theta && \text{in } \Omega_T \end{aligned}$$

Transport equations:

$$\begin{aligned} \partial_t\left((\theta+\theta_b(\theta_s-\theta))m^0\right) &= \nabla_x \cdot (\mathbb{D}_m\nabla_x m^0 - qm^0) + (\theta+\theta_b(\theta_s-\theta)) \\ &\quad \times \left(YR_{\mathrm{mon}}(n^0, m^0) - km\right) + \tilde{R}_{\mathrm{DA}} && \text{in } \Omega_T \\ \partial_t(\theta_s n^0) &= \nabla_x \cdot (\mathbb{D}_n\nabla_x n^0 - qn^0) - (\theta+\theta_b(\theta_s-\theta)) \\ &\quad \times R_{\mathrm{mon}}(n^0, m^0) - (1-\theta_b)(\theta_s-\theta)R_{\mathrm{mon},b}(n^0) && \text{in } \Omega_T \end{aligned}$$

Change of porosity:

$$\partial_t\theta = \frac{1}{\rho_b}\tilde{R}_{\mathrm{DA}} + (\theta_s-\theta)\left(k_b - \frac{Y}{\rho_b}R_{\mathrm{mon},b}(n^0)\right) \quad \text{in } \Omega_T\,.$$

On basis of the asymptotic expansion method the effective parameters are given by the following solutions of cell problems, which contains the essential informations of the microscale:

$$\begin{aligned} [\mathbb{K}]_{i,j\,(x,t)} &:= \int_{Y_\ell^0(x,t)} (\omega_{\ell,j})_{i\,(x,y,t)}\,dy + \int_{Y_s^0(x,t)} (\omega_{s,j})_{i\,(x,y,t)}\,dy\,, \\ [\mathbb{D}_m]_{i,j\,(x,t)} &:= D\int_{Y_\ell^0(x,t)} (\delta_{i,j} + \partial_{y_i}\beta_{\ell,j})_{\,(x,y,t)}\,dy + D_{m,b}\int_{Y_b^0(x,t)} (\delta_{i,j} + \partial_{y_i}\beta_{b,j})_{\,(x,y,t)}\,dy\,, \\ [\mathbb{D}_n]_{i,j\,(x,t)} &:= D\int_{Y_\ell^0(x,t)} (\delta_{i,j} + \partial_{y_i}\eta_{\ell,j})_{\,(x,y,t)}\,dy + D_{n,b}\int_{Y_b^0(x,t)} (\delta_{i,j} + \partial_{y_i}\eta_{b,j})_{\,(x,y,t)}\,dy\,. \end{aligned}$$

The effective diffusion parameter $\mathbb{D}_n$ corresponding to the nutrients is given via the functions $\eta_{\ell,j(x,\cdot,t)} : Y^0_{\ell\,(x,t)} \to \mathbb{R}$ and $\eta_{b,j(x,\cdot,t)} : Y^0_{b\,(x,t)} \to \mathbb{R}$ solving the cell problem

$$\text{(C2)} \begin{cases} -\Delta_y \eta_{\ell,j} &= 0 & \text{in } Y^0_{\ell\,(x,t)} \\ -\Delta_y \eta_{b,j} &= 0 & \text{in } Y^0_{b\,(x,t)} \\ (D\nabla_y \eta_{\ell,j} - D_{n,b}\nabla_y \eta_{b,j}) \cdot \nu^0_l &= -(D - D_{n,b})e_j \cdot \nu^0_l & \text{on } \Gamma^0_{l\,(x,t)} \\ \eta_{\ell,j} &= \eta_{b,j} & \text{on } \Gamma^0_{l\,(x,t)} \\ \nabla_y \eta_{b,j} \cdot \nu^0_s &= -e_j \cdot \nu^0_s & \text{on } \Gamma^0_{s(x)} \\ \eta_{\ell,j} \text{ is } Y\text{-periodic}\,. \end{cases}$$

The functions $(\beta_\ell, \beta_b) := (\beta_{\ell,j}, \beta_{b,j})_{j=1}^d$ also solve componentwisely a system of PDEs similar to (C2). In contrast to the above PDEs the boundary condition $(\text{C2})_3$ Γ^0_l slightly changes by replacing $D_{n,b}$ with $D_{m,b}$.

Furthermore, the permeability tensor $\mathbb{K}$ is determined by the functions $(\omega_{k,j}, \pi_{k,j}) : Y^0_{k\,(x,t)} \to \mathbb{R}^d \times \mathbb{R}$, $k \in \{\ell, s\}$ solving the cell problem (C1) with an additional boundary condition on $\Gamma^0_{s(x)}$: $-\nabla_y \pi_{s,j} \cdot \nu^0_s = e_j \cdot \nu^0_s$.

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[7]: R. Schulz: *Biofilm modeling in evolving porous media with Beavers-Joseph condition*, Z. Angew. Math. Mech., 2018;e201800123. https://doi.org/10.1002/zamm.201800123, (2019).

Thank you for your attention!