Colloids transport in porous media: analysis and applications.

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What are colloids?

Colloid aggregation is important in:
- Cheese production
- Colloid filtration
- Carbon transport in seawater
- Nanoparticles engineering
- Water treatment

Our goal: see the effects of aggregation on colloidal transport in porous media.
Soret effect: the heat makes the particles move
Dufour effect: the particles carry the heat
Model assumptions

Figure: View of a “real” (a) and a “model” (b) aggregate

Figure: Each aggregate is uniquely identified by the number of monomers it’s composed of.
Assuming presently a well-mixed solution, we have:

\[ \frac{du_k}{dt} = R(u) := \frac{1}{2} \sum_{i+j=k} \alpha_{ij} \beta_{ij} u_i u_j - u_k \sum_{i=1}^{N} \alpha_{ij} \beta_{ki} u_i - b_k u_k + \sum_{i=k}^{N} d_{ki} b_i u_i \]

- \( u_k \) – concentration of species composed of \( k \) monomers
- \( a_k \) – the effective diameter for \( u_k \)
- \( \beta_{ij} = \beta_{ij}(a_i, a_j) \) – aggregation rate
- \( \alpha_{ij} = \alpha_{ij}(a_i, a_j) \) – collision efficiency
- \( b_k \) – breakage coefficient
- \( d_{ki} \) – breakage distribution
Figure: Microstructure of $\Omega^\varepsilon$ (isotropic case on the left, anisotropic case on the right). $Y_{ij}$ is the periodic cell.
Microscopic model equations

System for $P_\varepsilon$:

\[
\partial_t \theta_\varepsilon + \nabla \cdot (-\kappa_\varepsilon \nabla \theta_\varepsilon) - \tau_\varepsilon \sum_{i=1}^{N} \nabla^\delta u_\varepsilon^i \cdot \nabla \theta_\varepsilon = 0, \quad \text{in } \Omega_\varepsilon,
\]

\[
\partial_t u_\varepsilon^i + \nabla \cdot (-d_\varepsilon^i \nabla u_\varepsilon^i) - f_\varepsilon^i \nabla^\delta \theta_\varepsilon \cdot \nabla u_\varepsilon^i = R_i(u_\varepsilon), \quad \text{in } \Omega_\varepsilon,
\]

\[
\partial_t v_\varepsilon^i = a_\varepsilon^i u_\varepsilon^i - b_\varepsilon^i v_\varepsilon^i, \quad \text{on } (0, T) \times \Gamma_\varepsilon,
\]

with boundary conditions:

\[
- \kappa_\varepsilon \nabla \theta_\varepsilon \cdot n = 0, \quad \text{on } (0, T) \times \Gamma_\varepsilon,
\]

\[
- d_\varepsilon^i \nabla u_\varepsilon^i \cdot n = \varepsilon (a_\varepsilon^i u_\varepsilon^i - b_\varepsilon^i v_\varepsilon^i), \quad \text{on } (0, T) \times \Gamma_\varepsilon,
\]

\[
\theta_\varepsilon(x, 0) = \theta_\varepsilon(x, 1) \quad x \in [0, 1],
\]

\[
\theta_\varepsilon(0, y) = \theta_\varepsilon(1, y) \quad y \in [0, 1],
\]

\[
u_\varepsilon^i(x, 0) = u_\varepsilon^i(x, 1) \quad x \in [0, 1], i \in \{1, \ldots, N\}
\]

\[
u_\varepsilon^i(0, y) = u_\varepsilon^i(1, y) \quad y \in [0, 1], i \in \{1, \ldots, N\}
\]
Model challenges

\[
\partial_t \theta^\varepsilon + \nabla \cdot (-\kappa^\varepsilon \nabla \theta^\varepsilon) - \tau^\varepsilon \sum_{i=1}^{N} \nabla \delta u_i^\varepsilon \cdot \nabla \theta^\varepsilon = 0, \quad \text{in } \Omega^\varepsilon,
\]

\[
\partial_t u_i^\varepsilon + \nabla \cdot (-d_i^\varepsilon \nabla u_i^\varepsilon) - f_i^\varepsilon \nabla \delta \theta^\varepsilon \cdot \nabla u_i^\varepsilon = R_i(u^\varepsilon), \quad \text{in } \Omega^\varepsilon,
\]

\[
\partial_t v_i^\varepsilon = a_i^\varepsilon u_i^\varepsilon - b_i^\varepsilon v_i^\varepsilon, \quad \text{on } (0, T) \times \Gamma^\varepsilon,
\]

with boundary conditions:

\[
- \kappa^\varepsilon \nabla \theta^\varepsilon \cdot n = 0, \quad \text{on } (0, T) \times \Gamma^\varepsilon,
\]

\[
- d_i^\varepsilon \nabla u_i^\varepsilon \cdot n = \varepsilon(a_i^\varepsilon u_i^\varepsilon - b_i^\varepsilon v_i^\varepsilon), \quad \text{on } (0, T) \times \Gamma^\varepsilon.
\]

- Non-linear cross-diffusion terms with a gradient
- Non-linear coupling via the aggregation reaction
- PDE-ODE coupling via the deposition condition
\[ \frac{\partial \theta^\varepsilon}{\partial t} + \nabla \cdot (-\kappa^\varepsilon \nabla \theta^\varepsilon) - \tau^\varepsilon \sum_{i=1}^{N} \nabla \delta u_i^\varepsilon \cdot \nabla \theta^\varepsilon = 0, \quad \text{in } \Omega^\varepsilon, \]

\[ \frac{\partial u_i^\varepsilon}{\partial t} + \nabla \cdot (-d_i^\varepsilon \nabla u_i^\varepsilon) - f_i^\varepsilon \nabla \delta \theta^\varepsilon \cdot \nabla u_i^\varepsilon = R_i(u^\varepsilon), \quad \text{in } \Omega^\varepsilon, \]

\[ \frac{\partial v_i^\varepsilon}{\partial t} = a_i^\varepsilon u_i^\varepsilon - b_i^\varepsilon v_i^\varepsilon, \quad \text{on } (0, T) \times \Gamma^\varepsilon, \]

with boundary conditions:

\[ - \kappa^\varepsilon \nabla \theta^\varepsilon \cdot n = 0, \quad \text{on } (0, T) \times \Gamma^\varepsilon, \]

\[ - d_i^\varepsilon \nabla u_i^\varepsilon \cdot n = \varepsilon(a_i^\varepsilon u_i^\varepsilon - b_i^\varepsilon v_i^\varepsilon), \quad \text{on } (0, T) \times \Gamma^\varepsilon. \]

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Model challenges

\[ \partial_t \theta^\epsilon + \nabla \cdot (-\kappa^\epsilon \nabla \theta^\epsilon) - \tau^\epsilon \sum_{i=1}^N \nabla \delta u_i^\epsilon \cdot \nabla \theta^\epsilon = 0, \quad \text{in } \Omega^\epsilon, \]

\[ \partial_t u_i^\epsilon + \nabla \cdot (-d_i^\epsilon \nabla u_i^\epsilon) - f_i^\epsilon \nabla \delta \theta^\epsilon \cdot \nabla u_i^\epsilon = R_i(u^\epsilon), \quad \text{in } \Omega^\epsilon, \]

\[ \partial_t v_i^\epsilon = a_i^\epsilon u_i^\epsilon - b_i^\epsilon v_i^\epsilon, \quad \text{on } (0, T) \times \Gamma^\epsilon, \]

with boundary conditions:

\[ -\kappa^\epsilon \nabla \theta^\epsilon \cdot n = 0, \quad \text{on } (0, T) \times \Gamma^\epsilon, \]

\[ -d_i^\epsilon \nabla u_i^\epsilon \cdot n = \epsilon(a_i^\epsilon u_i^\epsilon - b_i^\epsilon v_i^\epsilon), \quad \text{on } (0, T) \times \Gamma^\epsilon. \]

- Non-linear cross-diffusion terms with a gradient
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For $P_\epsilon$, under the assumptions:

- Positivity of initial data
- $d_i^\epsilon > d_i^{\epsilon,0} > 0$, $\kappa^\epsilon > \kappa^{\epsilon,0} > 0$
- $a_i^\epsilon > 0$, $b_i^\epsilon > 0$

we show (for weak solutions):

- Existence
- Uniqueness
- Positivity
- Boundedness

Proof idea:

- Galerkin method is used to prove existence of two auxiliary problems
- Banach fixed point theorem is used to prove the existence and uniqueness of the full problem
**Definition (Two-scale convergence)**

Let \((u^\varepsilon) \in L^2(0, T; L^2(\Omega)), \Omega \subset \mathbb{R}^n.\)

\((u^\varepsilon)\) two-scale converges to a unique function

\(u_0(t, x, y) \in L^2((0, T) \times \Omega \times Y) \iff \forall \phi \in C_0^\infty((0, T) \times \Omega, C_\#^\infty(Y)):\)

\[
\lim_{\varepsilon \to 0} \int_0^T \int_\Omega u^\varepsilon \phi(t, x, \frac{x}{\varepsilon}) dxdt = \frac{1}{|Y|} \int_0^T \int_\Omega \int_Y u_0(t, x, y) \phi(t, x, y) dydxdt
\]

Denote as \(u^\varepsilon \xrightarrow{2} u_0.\)
Two-scale compactness

Theorem (Two-scale compactness on domains)

(i) From each bounded sequence \((u^\varepsilon)\) in \(L^2(0, T; L^2(\Omega))\), a subsequence may be extracted which two-scale converges to \(u_0(t, x, y) \in L^2((0, T) \times \Omega^\varepsilon \times Y)\).

(ii) Let \((u^\varepsilon)\) be a bounded sequence in \(H^1(0, T, H^1(\Omega))\), then there exists \(\tilde{u} \in L^2((0, T) \times H^1_\#(Y))\) such that up to a subsequence \((u^\varepsilon)\) two-scale converges to \(u_0 \in L^2(0, T; L^2(\Omega))\) and \(\nabla u^\varepsilon \rightharpoonup \nabla_x u_0 + \nabla_y \tilde{u}\).
Lemma

With positive initial data and coercive and bounded diffusion and heat conduction coefficients, the following holds:

(i) \( u_i \rightharpoonup u_i \) and \( \theta^\varepsilon \rightharpoonup \theta \) in \( L^2(0, T; H^1(\Omega)) \),

(ii) \( u_i^* \rightharpoonup u_i \) and \( \theta^\varepsilon^* \rightharpoonup \theta \) in \( L^\infty((0, T) \times \Omega) \),

(iii) \( \partial_t u_i \rightharpoonup \partial_t u_i \) and \( \partial_t \theta^\varepsilon \rightharpoonup \partial_t \theta \) in \( L^2(0, T; H^1(\Omega)) \),

(iv) \( u_i \rightarrow u_i \) and \( \theta^\varepsilon \rightarrow \theta \) strongly in \( L^2(0, T; H^\beta(\Omega^\varepsilon)) \) for \( \frac{1}{2} < \beta < 1 \) and \( \sqrt{\varepsilon} \| u_i - u_i \|_{L^2((0, T) \times \Omega^\varepsilon)} \rightarrow 0 \) as \( \varepsilon \rightarrow 0 \),

(v) \( u_i \overset{2}{\rightarrow} u_i, \nabla u_i \overset{2}{\rightarrow} \nabla_x u_i + \nabla_y u_i^1 \) where \( u_i^1 \in L^2((0, T) \times \Omega^\varepsilon; H^1_\#(Y)) \),

(vi) \( \theta^\varepsilon \overset{2}{\rightarrow} \theta, \nabla \theta^\varepsilon \overset{2}{\rightarrow} \nabla_x \theta + \nabla_y \theta^1 \) where \( \theta^1 \in L^2((0, T) \times \Omega^\varepsilon; H^1_\#(Y)) \),

(vii) \( v_i \overset{2}{\rightarrow} v_i \in L^\infty((0, T) \times \Omega^\varepsilon \times (0, T) \times \Gamma^\varepsilon) \) and \( \partial_t v_i \overset{2}{\rightarrow} \partial_t v_i \in L^2((0, T) \times \Omega^\varepsilon \times (0, T) \times \Gamma^\varepsilon) \).
\[ \partial_t u_i + \nabla \cdot ( -d_i \nabla u_i ) = R_i(u) \quad \text{in } \Omega, \quad (1) \]

\[ \partial_t v_i = a_i u_i - b_i v_i \quad \text{on } \Gamma, \quad (2) \]

with the boundary conditions

\[ -d_i \nabla u_i \cdot n = a_i u_i - b_i v_i \quad \text{on } \Gamma, \quad (3) \]

\[ -d_i \nabla u_i \cdot n = 0 \quad \text{on } \Gamma_N, \quad (4) \]

\[ u_i(t, x) = u_D(t, x) \quad \text{on } \Gamma_D, \quad (5) \]

and the initial conditions

\[ u_i(0, x) = u_i^0(x) \quad \text{in } \Omega, \quad (6) \]

\[ v_i(0, x) = v_i^0(x) \quad \text{on } \Gamma. \quad (7) \]
Nondimensionalized system

After rescaling, we obtain this system:

\[
\begin{align*}
\partial_t u_i + \nabla \cdot (-d_i \nabla u_i) &= \Lambda R_i(u) & \text{in } \Omega, \\
\partial_t v_i &= Bi(a_i u_i - b_i v_i) & \text{on } \Gamma,
\end{align*}
\]

with the boundary conditions

\[
\begin{align*}
-d_i \nabla u_i \cdot n &= \varepsilon (a_i u_i - b_i v_i) & \text{on } \Gamma, \\
-d_i \nabla u_i \cdot n &= 0 & \text{on } \Gamma_N, \\
u_i(t, x) &= \frac{u_D(t, x)}{u_0} & \text{on } \Gamma_D,
\end{align*}
\]

and the initial conditions

\[
\begin{align*}
u_i(0, x) &= \frac{u_i^0(x)}{u_0} & \text{in } \Omega, \\
v_i(0, x) &= \frac{v_i^0(x)}{v_0} & \text{on } \Gamma.
\end{align*}
\]
Rigorous homogenization result

The final upscaled system:

\[
\begin{align*}
\partial_t u_i - \nabla \cdot (\bar{D}_i \nabla u_i) + A_i u_i - B_i v_i &= \Lambda R_i(u) \quad \text{in } \Omega, \\
\partial_t v_i &= A_i u_i - B_i v_i \quad \text{in } \Omega
\end{align*}
\]

(15)

(16)

with effective parameters:

\[
\bar{D}_{ijk} = \int_Y d_i^\varepsilon(y)(\delta_{jk} + \nabla_y w_i)dy \quad i \in \{1, \ldots, N\}
\]

(17)

\[
A_i := B_i \int_{\Gamma^\varepsilon} a_i^\varepsilon(y) d\sigma(y) \quad i \in \{1, \ldots, N\}
\]

(18)

\[
B_i := B_i \int_{\Gamma^\varepsilon} b_i^\varepsilon(y) d\sigma(y) \quad i \in \{1, \ldots, N\}
\]

(19)

where \(w_j(y)\) solve the cell problem:

\[
\nabla_y \cdot (d_i^\varepsilon(y) \nabla w_j) = -(\nabla d_i^\varepsilon(y))_j \quad j \in \{1, \ldots, d\}, y \in Y
\]

(20)
**Figure**: Solutions to the cell problems that correspond to isotropic periodic geometry.

The resulting effective diffusion tensor:

\[ D = \begin{bmatrix} 0.75 & 0.171476 \\ 0.171476 & 0.75 \end{bmatrix} \]
Cell problem solution: anisotropic case

Figure: Solutions to the cell problems that correspond to anisotropic periodic geometry.

The resulting effective diffusion tensor:

\[
D = \begin{bmatrix}
0.817467 & 0.0786338 \\
0.214942 & 0.817467
\end{bmatrix}
\]
A model with a blocking function for the deposition

\[ \partial_t n = -v_p \cdot \nabla n + D_h \Delta n - \frac{f}{\pi a_p^2} \partial_t \theta, \]  
(21)

\[ \partial_t \theta = \pi a_p^2 k n B(\theta), \]  
(22)

with the boundary conditions

\[ n(t, 0) = \begin{cases} n_0 & t \in [0, t_0] \\ 0 & t > t_0 \end{cases}, \]  
(23)

\[ \frac{\partial n}{\partial \nu}(t, L) = 0, \]  
(24)

and initial conditions

\[ n(0, x) = 0, \]  
(25)

\[ \theta(0, x) = 0. \]  
(26)
Figure: Simulation comparison for a single species system versus an aggregating system. The straight line is the breakthrough curve for the colloidal mass for the problem without aggregation. The dashed line is the breakthrough curve for the colloidal mass for the problem with aggregation. It is obtained by summing mass-wise the breakthrough curves for the monomers $u_1$ and dimers $u_2$. 

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Simulation for the Langmuirian blocking function

Figure: The effect of the Langmuirian dynamic blocking function $B(\theta) = 1 - \beta \theta$ on the deposition (right) versus no blocking function (left). $u_1$ and $u_2$ are the breakthrough curves, while $v_1$ and $v_2$ are the concentrations of the deposited species.
Simulation for the RSA blocking function

![Diagram](image)

**Figure**: The effect of the RSA dynamic blocking function

\[
B(\theta) = 1 - 4\theta_\infty \beta \theta + 3.308(\theta_\infty \beta \theta)^2 + 1.4069(\theta_\infty \beta \theta)^3
\]

on the deposition (right) versus no blocking function (left). \(u_1\) and \(u_2\) are the breakthrough curves, while \(v_1\) and \(v_2\) are the concentrations of the deposited species.
Simulation of the aggregation effects on deposition - 2

Figure: The effect of aggregation rates on the breakthrough curves. On the left, the default rate of aggregation is used, on the right - it's doubled. A change of aggregation rate can be achieved by varying the concentration of salt in the suspension, according to DLVO theory.

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PBE for colloids

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Implementation details

- **cell problem solver (FEM):**
  deal.II - a numeric library for parallel computations

- **spatial discretization (FEM):**
  DUNE - a numeric library for parallel computations
  [http://www.dune-project.org/](http://www.dune-project.org/)

- **time discretization:**
  CVODE library from the SUNDIALS package

- Fully coupled or operator splitting
- Code is 2D/3D
Multiscale FEM

General idea:

\[ L_\varepsilon u_\varepsilon = f \quad \text{in } \Omega \]
\[ u_\varepsilon = 0 \quad \text{on } \partial \Omega \]

Approximate \( u_\varepsilon \) with \( u_h \in V^h = \text{span}\{\phi_K^i : K \in K^h\} \) s.t.:

\[ L_\varepsilon \phi_i^j = 0 \quad \text{in } K \in K^h \]
\[ a(u_h, v) = f(v) \quad \forall v \in V^h \]

Error estimate:

\[ \|u_\varepsilon - u_h\|_{1,\Omega} \leq C_1 h \|f\|_{0,\Omega} + C_2 \sqrt{\frac{\varepsilon}{h}} \]
Outlook

- Multiscale Finite Element method implementation for the system
- Pore clogging due to deposition
- Corrector estimates for the cross-diffusion problem
- MSFEM estimates and implementation for the cross-diffusion problem
Thank you for your attention.