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**Diffusion, Convection, Adsorption and Reaction of Chemicals
in Porous Media.**

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Outline

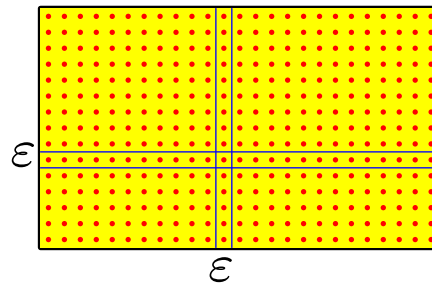
- I** The model on the microscale.
- II** The model on the macroscale.
- III** Towards a justification of the macro model.
Micro to Macro?

I. The geometry on the microscale

porous
medium

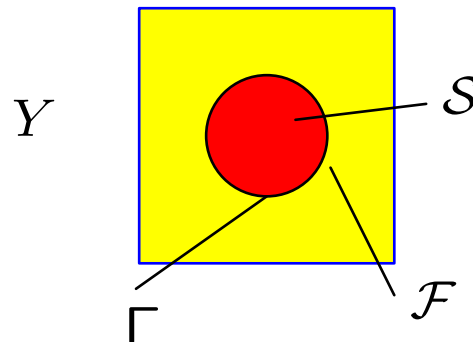


fluid part
solid part
surface



$$\begin{aligned}\mathcal{F}_\varepsilon &= \Omega \cap \varepsilon \mathcal{F}_\#, \\ \mathcal{S}_\varepsilon &= \Omega \cap \varepsilon \mathcal{S}_\#, \\ \Gamma_\varepsilon &= \Omega \cap \varepsilon \Gamma_\#.\end{aligned}$$

unit cell



$$\begin{aligned}\mathcal{F}_\# &= \mathcal{F} + \mathbb{Z}^n, \\ \mathcal{S}_\# &= \mathcal{S} + \mathbb{Z}^n, \\ \Gamma_\# &= \Gamma + \mathbb{Z}^n,\end{aligned}$$

The microscopic model.

A chemical substance

is transported by and diffuses in a fluid,
is adsorbed at the pore surface,
reacts at the pore surface.

The unknowns.

- $v_\varepsilon : \mathcal{F}_\varepsilon \rightarrow \mathbb{R}^n$ velocity field of the fluid,
- $p_\varepsilon : \mathcal{F}_\varepsilon \rightarrow \mathbb{R}$ pressure in the fluid,
- $u_\varepsilon : (0, T) \times \mathcal{F}_\varepsilon \rightarrow \mathbb{R}$ concentration of the chemical substance in the fluid,
- $U_\varepsilon : (0, T) \times \Gamma_\varepsilon \rightarrow \mathbb{R}$ concentration of the chemical substance on the surface.

The sets of equations.

- Steady Stokes equation for the fluid $[v_\varepsilon, p_\varepsilon]$,
- Diffusion, convection (and reaction) of the substance in the fluid $[u_\varepsilon, v_\varepsilon]$,
- Adsorption at the surface $[u_\varepsilon, U_\varepsilon]$,
- Reaction (and surface diffusion) on the surface $[U_\varepsilon, u_\varepsilon]$.

Steady Stokes equation (S_ε).

$$\begin{aligned}\varepsilon^2 \Delta v_\varepsilon &= \nabla p_\varepsilon && \text{in } \mathcal{F}_\varepsilon, \\ \nabla \cdot v_\varepsilon &= 0 && \text{in } \mathcal{F}_\varepsilon, \\ v_\varepsilon \cdot \nu_\varepsilon &= 0 && \text{on } \Gamma_\varepsilon,\end{aligned}$$

where

ν_ε denotes the outer normal of \mathcal{F}_ε on Γ_ε ,

and where we add

a boundary condition on $\partial\Omega$.

Diffusion, Convection in the fluid (DC_ε).

$$\partial_t u_\varepsilon = \nabla \cdot (a_\varepsilon \nabla u_\varepsilon - v_\varepsilon u_\varepsilon) \quad \text{in } \mathcal{F}_\varepsilon,$$

where the **diffusion coefficient**

$$a_\varepsilon : \mathcal{F}_\varepsilon \rightarrow \mathbb{R},$$

is given by

$$a_\varepsilon(x) = a\left(\frac{x}{\varepsilon}\right),$$

with an Y -periodic function $a : \mathbb{R}^n \rightarrow \mathbb{R}$,

and where we add a boundary condition on $\partial\Omega$ and an initial condition at $t = 0$.

Adsorption at the surface (A_ε).

$$-a_\varepsilon(x) \nabla u_\varepsilon(t, x) \cdot \nu_\varepsilon(x) = \varepsilon b_\varepsilon(x, U_\varepsilon(t, x), u_\varepsilon(t, x)),$$

where a **linear adsorption rate**

$$b_\varepsilon : \Gamma_\varepsilon \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R},$$

is given by

$$b_\varepsilon(x, \dots) = b\left(\frac{x}{\varepsilon}, \dots\right),$$

with $b : \mathbb{R}^n \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ being Y -periodic in the first argument.

Reaction on the surface (R_ε).

$$\partial_t U_\varepsilon(t, x) = b_\varepsilon(x, U_\varepsilon(t, x), u_\varepsilon(t, x)) + r_\varepsilon(x, U_\varepsilon(t, x)),$$

where a **linear reaction rate**

$$r_\varepsilon : \Gamma_\varepsilon \times \mathbb{R} \rightarrow \mathbb{R},$$

is given by

$$r_\varepsilon(x, \cdot) = r\left(\frac{x}{\varepsilon}, \cdot\right),$$

with $r : \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}$ being Y -periodic in the first argument, and where we add an initial condition at $t = 0$.

Summary: The microscopic model.

$$\begin{aligned} (S_\varepsilon) \quad \varepsilon^2 \Delta v_\varepsilon &= \nabla p_\varepsilon, \\ \nabla \cdot v_\varepsilon &= 0, \\ v_\varepsilon \cdot \nu_\varepsilon &= 0, \end{aligned}$$

$$(DC_\varepsilon) \quad \partial_t u_\varepsilon = \nabla \cdot (a_\varepsilon \nabla u_\varepsilon - v_\varepsilon u_\varepsilon),$$

$$(A_\varepsilon) \quad 0 = a_\varepsilon(x) \nabla u_\varepsilon(t, x) \cdot \nu_\varepsilon(x) + \varepsilon b_\varepsilon(x, U_\varepsilon(t, x), u_\varepsilon(t, x)),$$

$$(R_\varepsilon) \quad \partial_t U_\varepsilon(t, x) = b_\varepsilon(x, U_\varepsilon(t, x), u_\varepsilon(t, x)) + r_\varepsilon(x, U_\varepsilon(t, x))$$

II. The macroscopic model.

The unknowns.

- $v : \Omega \rightarrow \mathbb{R}^n$ velocity field of the fluid,
- $p : \Omega \rightarrow \mathbb{R}$ pressure in the fluid,
- $u : (0, T) \times \Omega \rightarrow \mathbb{R}$ concentration of the *fluid chemical substance*,
- $U : (0, T) \times \Omega \times \Gamma \rightarrow \mathbb{R}$ concentration of the *adsorbed chemical substance*

Note: $U = U(t, x, y)$

The sets of equations.

- Darcy law for the fluid $[v, p]$,
- Diffusion, convection equation with a sink $[u, v, U]$,
- Reaction equation $[U, u]$.

Darcy-like law (S)

for the velocity v and the pressure p in the fluid.

$$\begin{aligned}v &= -K\nabla p, \\ \nabla \cdot v &= 0,\end{aligned}$$

in Ω , where

$K : \Omega \rightarrow \mathbb{R}^{n \times n}$, the permeability matrix,

is determined by the data \mathcal{S} and can be calculated from a *local* problem.

Diffusion-Convection equation with a sink (DC).

For the concentration u of the chemical substance in the fluid we obtain

$$|\mathcal{F}|\partial_t u = \nabla \cdot (A\nabla u - vu) - Q,$$

in Ω , where

$A : \Omega \rightarrow \mathbb{R}^{n \times n}$, the **effective diffusivity**,

is determined by \mathcal{S} , a and can be obtained from a *local* problem;
the **sink term** $Q : (0, T) \times \Omega \rightarrow \mathbb{R}$ is given by

$$Q(t, x) = \int_{\Gamma} b(y, u(t, x), U(t, x, y)) d\mathcal{H}^{n-1}(y).$$

Reaction equation (R).

For the concentration U of the adsorbed chemical substance we obtain

$$\partial_t U(t, x, y) = b(y, u(t, x), U(t, x, y)) + r(y, U(t, x, y)),$$

for $t \in (0, T)$, $x \in \Omega$, $y \in \Gamma$. Recalling

$$\begin{aligned} |\mathcal{F}|u_t &= \nabla \cdot (A\nabla u - vu) - Q, \\ Q(t, x) &= \int_{\Gamma} b(y, u(t, x), U(t, x, y)) d\mathcal{H}^{n-1}(y), \end{aligned}$$

we find a kind of **mass balance equation**,

$$\partial_t \left(|\mathcal{F}|u + \int_{\Gamma} U d\mathcal{H}^{n-1} \right) = \nabla \cdot (A\nabla u - vu) + \int_{\Gamma} r(u, U) d\mathcal{H}^{n-1}.$$

The local problems.

The permeability matrix K is given by

$$K_{ij} = \int_{\mathcal{F}} w_i(y) \cdot e_j \, dy,$$

where $w_i : \mathcal{F} \rightarrow \mathbb{R}^n$, and $\pi_i : \mathcal{F} \rightarrow \mathbb{R}$, $i = 1, \dots, n$ solve

$$\begin{aligned} \nabla \pi_i - \Delta w_i &= e_i, & \text{in } \mathcal{F}, \\ \nabla \cdot w_i &= 0 & \text{in } \mathcal{F}, \\ w_i &= 0 & \text{on } \Gamma. \end{aligned}$$

The effective diffusivity matrix A is given by

$$A_{ij} = \int_{\mathcal{F}} a(y) (\delta_{ij} + \partial_{y_j} \eta_i(y)) \, dy,$$

where $\eta_i : \mathcal{F} \rightarrow \mathbb{R}$, $i = 1, \dots, n$ solves the local problem

$$\begin{aligned} \nabla \cdot (a(\nabla \eta_i + e_i)) &= 0 & \text{in } \mathcal{F}, \\ \nu \cdot (\nabla \eta_i + e_i) &= 0 & \text{on } \Gamma. \end{aligned}$$

Summary: The macroscopic model.

$$v = -K\nabla p, \quad (S)$$

$$\nabla \cdot v = 0,$$

$$|\mathcal{F}|\partial_t u = \nabla \cdot (A\nabla u - vu) - Q, \quad (DC)$$

$$Q(t, x) = \int_{\Gamma} b(y, u(t, x), U(t, x, y)) d\mathcal{H}^{n-1}(y),$$

$$\partial_t U(t, x, y) = b(y, u(t, x), U(t, x, y)) + r(y, U(t, x, y)), \quad (R)$$

III Justification of the Macro model.

The goal:

For $\varepsilon > 0$ let $v_\varepsilon, p_\varepsilon, u_\varepsilon, U_\varepsilon$ be a solution of the micro model. Then we have

$$v_\varepsilon \rightarrow v, \quad p_\varepsilon \rightarrow p, \quad u_\varepsilon \rightarrow u, \quad U_\varepsilon \rightarrow U$$

in a suitable sense and v, p, u, U is a solution of the macro model.

Parts of the program:

- Weak formulation of the problems,
- Compactness of the solutions of the micro model,
- Convergence in the weak formulation.

Weak formulation of (DC_ε) .

For all $\zeta \in C_c^\infty((0, T) \times \Omega)$ holds

$$\begin{aligned} \int_0^T \int_\Omega \zeta_t \chi_\varepsilon u_\varepsilon &= \int_0^T \int_\Omega \nabla \eta \cdot \chi_\varepsilon (a_\varepsilon \nabla u_\varepsilon - u_\varepsilon v_\varepsilon) - \int_0^T \int_{\Gamma_\varepsilon} \eta \nu \cdot a_\varepsilon \nabla u_\varepsilon \\ &= \int_0^T \int_\Omega \nabla \eta \cdot \chi_\varepsilon (a_\varepsilon \nabla u_\varepsilon - u_\varepsilon v_\varepsilon) + \int_0^T \int_{\Gamma_\varepsilon} \eta \varepsilon b_\varepsilon(\cdot, u_\varepsilon, U_\varepsilon), \end{aligned}$$

with $\chi_\varepsilon(x) = \chi(x/\varepsilon)$ and

$$\chi(y) = \begin{cases} 1 & \text{if } y \in \mathcal{F}, \\ 0 & \text{if } y \in Y \setminus \mathcal{F}. \end{cases}$$

Compactness of the solutions.

We obtain for a subsequence $\varepsilon \rightarrow 0$

$$\begin{aligned} \mathcal{X}_\varepsilon v_\varepsilon &\rightarrow v && \text{weakly in } L^2(\Omega), \\ u_\varepsilon &\rightarrow u && \text{strongly in } L^2((0, T) \times \Omega), \\ \nabla u_\varepsilon &\rightarrow \nabla u && \text{weakly in } L^2((0, T) \times \Omega), \\ &\dots && \end{aligned}$$

Moreover we assume

$$\begin{aligned} u_\varepsilon(t, x) &\approx u(t, x) && \text{on } \Gamma_\varepsilon, \\ U_\varepsilon(t, x) &\approx U(t, x, x/\varepsilon) && \text{on } \Gamma_\varepsilon. \end{aligned}$$

Why do we get $|\mathcal{F}|\partial_t u$ in (DC)?

$$\int_0^T \int_{\Omega} \zeta_t \mathcal{X}_{\varepsilon} u_{\varepsilon} \rightarrow |\mathcal{F}| \int_0^T \int_{\Omega} \zeta_t u,$$

since for all $\zeta \in L^1(\Omega)$

$$\int_{\Omega} \mathcal{X}_{\varepsilon} \zeta \rightarrow \int_{\Omega} |\mathcal{F}| \zeta.$$

To understand this observe for continuous ζ that

$$\begin{aligned} \int_{\Omega} \mathcal{X}_{\varepsilon} \zeta &\geq \sum_{i=1}^{N(\varepsilon)} (\inf_{Y_i} \zeta) \int_{Y_i} \mathcal{X}_{\varepsilon} = \sum_i (\inf_{Y_i} \zeta) \varepsilon^n \int_Y \mathcal{X} \\ &= \sum_i (\inf_{Y_i} \zeta) |Y_i| |\mathcal{F}| \rightarrow |\mathcal{F}| \int_{\Omega} \zeta. \end{aligned}$$

Why do we obtain this sink term?

$$\int_0^T \int_{\Gamma_\varepsilon} \eta \varepsilon b_\varepsilon(\cdot, u_\varepsilon, U_\varepsilon) \rightarrow \int_0^T \int_\Omega \eta \left(\int_\Gamma b(\cdot, u, U) dy \right) dx dt.$$

Assume b_ε to be linear in $u_\varepsilon, U_\varepsilon$, consider the U -term

$$\int_0^T \int_{\Gamma_\varepsilon} \eta(t, x) \varepsilon b^1\left(\frac{x}{\varepsilon}\right) U\left(t, x, \frac{x}{\varepsilon}\right) \rightarrow \int_0^T \int_\Omega \eta \left(\int_\Gamma b^1(y) U(\cdot, \cdot, y) d\mathcal{H}^{n-1}(y) \right),$$

or even

$$\int_{\Gamma_\varepsilon} \varepsilon \zeta\left(x, \frac{x}{\varepsilon}\right) d\mathcal{H}^{n-1}(x) \rightarrow \int_\Omega \left(\int_\Gamma \zeta(x, y) d\mathcal{H}^{n-1}(y) \right) dx.$$

$$\begin{aligned}
\int_{\Gamma_\varepsilon} \varepsilon \zeta\left(x, \frac{x}{\varepsilon}\right) d\mathcal{H}^{n-1}(x) &= \sum_i \int_{\Gamma_\varepsilon \cap Y_i} \varepsilon \zeta\left(x, \frac{x}{\varepsilon}\right) d\mathcal{H}^{n-1}(x) \\
&\geq \sum_i \int_{\Gamma_\varepsilon \cap Y_i} \varepsilon \left[\inf_{x \in Y_i} \zeta\left(x, \frac{x}{\varepsilon}\right) \right] d\mathcal{H}^{n-1}(x) \\
&= \int_\Gamma \varepsilon^n \sum_i \left[\inf_{x \in Y_i} \zeta(x, y) \right] d\mathcal{H}^{n-1}(y) \\
&= \int_\Gamma \sum_i |Y_i| \left[\inf_{x \in Y_i} \zeta(x, y) \right] d\mathcal{H}^{n-1}(y) \\
&\rightarrow \int_\Gamma \int_\Omega \zeta(x, y) dx d\mathcal{H}^{n-1}(y) \\
&= \int_\Omega \int_\Gamma \zeta(x, y) d\mathcal{H}^{n-1}(y) dx.
\end{aligned}$$