HOMOGENIZATION OF REACTIVE TRANSPORT IN POROUS MEDIA

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Work partially supported by the GDR MOMAS CNRS-2439

Dedicated to Alain Bourgeat

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-I- INTRODUCTION

We consider a periodic porous medium: fluid part Ω_f, solid part $\mathbb{R}^n \setminus \Omega_f$.

convection diffusion of a single solute:

$$\frac{\partial c^*}{\partial t^*} + b^* \cdot \nabla_{x^*} c^* - \operatorname{div}_{x^*}(D^* \nabla_{x^*} c^*) = 0 \quad \text{in} \ \ \Omega_f \times (0, T^*),$$

with a linear adsorption process on the pore boundaries:

$$-D^* \nabla_{x^*} c^* \cdot n = \frac{\partial \hat{c}^*}{\partial t^*} = k^*(c^* - \frac{\hat{c}^*}{K^*}) \quad \text{on} \ \ \partial\Omega_f \times (0, T^*),$$

The incompressible fluid velocity $b^*(x^*, t^*)$ is assumed to be known.

The unknowns are the concentrations c^* in the fluid and $\hat{c}^*$ on the solid boundary.

Scaling

We adimensionalize the equations as follows:

- ✗ Characteristic lengthscale L_R and timescale T_R.
- ✗ Period $\ell << L_R$: we introduce a small parameter $\epsilon = \frac{\ell}{L_R}$.
- ✗ Characteristic velocity b_R.
- ✗ Characteristic concentrations c_R and $\hat{c}_R$.
- ✗ Characteristic diffusivity D_R.
- ✗ Characteristic adsorption rate k_R and adsorption equilibrium constant K_R.

New adimensionalized variables and constants:

$$x = \frac{x^*}{L_R},\ t = \frac{t^*}{T_R},\ b_\epsilon(x,t) = \frac{b^*(x^*,t^*)}{b_R},\ D = \frac{D^*}{D_R},\ k = \frac{k^*}{k_R},\ K = \frac{K^*}{K_R}$$

Scaling (continued)

New unknowns:

$$u_\epsilon = \frac{c^*}{c_R},\ v_\epsilon = \frac{\hat{c}}{\hat{c}_R}$$

and dimensionless equations

$$\frac{\partial u_\epsilon}{\partial t} + \frac{V_R T_R}{L_R} b_\epsilon \cdot \nabla_x u_\epsilon - \frac{D_R T_R}{L_R^2}\,\mathrm{div}_x(D\nabla_x u_\epsilon) = 0 \quad \text{in } \Omega_\epsilon \times (0,T)$$

and

$$-\frac{DD_R}{L_R} c_R \nabla_x u_\epsilon \cdot n = \frac{\hat{c}_R}{T_R}\frac{\partial v_\epsilon}{\partial t} = k_R k(c_R u_\epsilon - \frac{\hat{c}_R v_\epsilon}{KK_R}) \quad \text{on } \partial\Omega_\epsilon \times (0,T).$$

Péclet number: $\mathbf{Pe} = \frac{L_R b_R}{D_R} = \frac{T_{diff}}{T_{advec}}$

Damkohler number: $\mathbf{Da} = \frac{L_R k_R}{D_R} = \frac{T_{diff}}{T_{react}}$

We choose a diffusion timescale, i.e., we assume $T_R = \frac{L_R^2}{D_R} = T_{diff}$.

Scaling (continued)

$$\frac{\partial u_\epsilon}{\partial t} + \mathbf{Pe}\, b_\epsilon \cdot \nabla_x u_\epsilon - \operatorname{div}_x(D\nabla_x u_\epsilon) = 0 \quad \text{in } \ \Omega_\epsilon \times (0,T)$$

and

$$-D\nabla_x u_\epsilon \cdot n = \frac{\hat{c}_R}{c_R L_R}\frac{\partial v_\epsilon}{\partial t} = \mathbf{Da}\, k(u_\epsilon - \frac{\hat{c}_R v_\epsilon}{c_R K K_R}) \quad \text{on } \ \partial\Omega_\epsilon \times (0,T).$$

We assume

$$\mathbf{Pe} = \epsilon^{-1}, \quad \mathbf{Da} = \epsilon^{-1}, \quad \frac{\hat{c}_R}{c_R L_R} = \frac{T_{adsorp}}{T_{react}} = \epsilon, \quad \frac{\hat{c}_R}{c_R K_R} = \frac{T_{adsorp}}{T_{desorp}} = 1$$

Scaling (continued)

$$\begin{cases} \dfrac{\partial u_\epsilon}{\partial t} + \dfrac{1}{\epsilon} b_\epsilon \cdot \nabla_x u_\epsilon - \operatorname{div}_x (D_\epsilon \nabla_x u_\epsilon) = 0 & \text{in } \Omega_\epsilon \times (0,T) \\ u_\epsilon(x,0) = u^0(x), \quad x \in \Omega_\epsilon, \\ -D_\epsilon \nabla_x u_\epsilon \cdot n = \epsilon \dfrac{\partial v_\epsilon}{\partial t} = \dfrac{k}{\epsilon}\left(u_\epsilon - \dfrac{v_\epsilon}{K}\right) & \text{on } \partial\Omega_\epsilon \times (0,T) \\ v_\epsilon(x,0) = v^0(x), \quad x \in \partial\Omega_\epsilon \end{cases}$$

Assumptions:

- ✗ Unit cell $Y = (0,1)^n = Y^* \cup \mathcal{O}$ with fluid part Y^*
- ✗ Stationary incompressible periodic flow $b_\epsilon(x) = b\left(\dfrac{x}{\epsilon}\right)$ with $\operatorname{div}_y b = 0$ in Y^* and $b \cdot n = 0$ on $\partial\mathcal{O}$ (not a necessary assumption, see Allaire-Raphael 2007)
- ✗ Periodic symmetric coercive diffusion $D_\epsilon(x) = D\left(\dfrac{x}{\epsilon}\right)$

Goal of homogenization

Find the effective diffusion tensor.

This is the so-called problem of **Taylor dispersion** (1953).

Many previous works, including Adler, Auriault, van Duijn, Knabner, Mauri, Mikelic, Quintard, Rosier, Rubinstein, etc.

-II- MAIN RESULT

Theorem. The solution (u_ϵ, v_ϵ) satisfies

$$u_\epsilon(t,x) \approx u_0\left(t, x - \frac{b^*}{\epsilon}t\right) \quad \text{and} \quad v_\epsilon(t,x) \approx K u_0\left(t, x - \frac{b^*}{\epsilon}t\right)$$

with the effective drift

$$b^* = (|Y^*| + |\partial\mathcal{O}|_{n-1}K)^{-1} \int_{Y^*} b(y)dy$$

and u_0 the solution of the homogenized problem

$$\begin{cases} \dfrac{\partial u_0}{\partial t} - \operatorname{div}(A^* \nabla u_0) = 0 & \text{in } \mathbb{R}^n \times (0,T) \\ u_0(t=0,x) = \dfrac{|Y^*|u^0(x) + |\partial\mathcal{O}|_{n-1}v^0(x)}{|Y^*| + K|\partial\mathcal{O}|_{n-1}} & \text{in } \mathbb{R}^n \end{cases}$$

Precise convergence

$$u_\epsilon(t,x) = u_0\left(t, x - \frac{b^*}{\epsilon}t\right) + r_\epsilon^u(t,x) \quad \text{and} \quad v_\epsilon(t,x) = K u_0\left(t, x - \frac{b^*}{\epsilon}t\right) + r_\epsilon^v(t,x)$$

with

$$\lim_{\epsilon \to 0} \int_0^T \int_{\mathbb{R}^n} \left| r_\epsilon^{u,v}(t,x) \right|^2 dt\, dx = 0,$$

Homogenized coefficients

The homogenized diffusion tensor is

$$A^* = \left(|Y^*| + K|\partial\mathcal{O}|_{n-1}\right)^{-1}\left(A_1^* + A_2^*\right)$$

$$\text{with } A_1^* = \frac{K^2}{k}|\partial\mathcal{O}|_{n-1} b^* \otimes b^* \quad \text{and} \quad A_2^* = \int_{Y^*} D(\mathbf{I} + \nabla_y w(y))(\mathbf{I} + \nabla_y w(y))^T dy$$

where the components $w_i(y)$, $1 \leq i \leq n$, of $w(y)$ are solutions of the cell problem

$$\begin{cases} b(y) \cdot \nabla_y w_i - \operatorname{div_y}\left(D(y)\left(\nabla_y w_i + e_i\right)\right) = (b^* - b(y)) \cdot e_i \text{ in } Y^* \\ D(y)\left(\nabla_y w_i + e_i\right) \cdot n = K b^* \cdot e_i \text{ on } \partial\mathcal{O} \\ y \to w_i(y) \ Y\text{-periodic} \end{cases}$$

Remark that the value of b^* is exactly the compatibility condition for the existence of w_i.

Equivalent homogenized equation

Define $\tilde{u}_\epsilon(t,x) = u_0\left(t, x - \frac{b^*}{\epsilon}t\right)$. Then, it is solution of

$$\begin{cases} \dfrac{\partial \tilde{u}_\epsilon}{\partial t} + \dfrac{1}{\epsilon} b^* \cdot \nabla \tilde{u}_\epsilon - \operatorname{div}\left(A^* \nabla \tilde{u}_\epsilon\right) = 0 & \text{in } \mathbb{R}^n \times (0,T) \\ \tilde{u}_\epsilon(t=0,x) = \dfrac{|Y^*| u^0(x) + |\partial \mathcal{O}|_{n-1} v^0(x)}{|Y^*| + K |\partial \mathcal{O}|_{n-1}} & \text{in } \mathbb{R}^n \end{cases}$$

-III- TWO-SCALE ANSATZ WITH DRIFT

To motivate our result, let us start with a formal process.

Standard two-scale asymptotic expansions should be modified to introduce an **unknown large drift** $b^* \in \mathbb{R}^n$

$$u_\epsilon(t,x) = \sum_{i=0}^{+\infty} \epsilon^i u_i \left(t, x - \frac{b^* t}{\epsilon}, \frac{x}{\epsilon} \right),$$

with $u_i(t,x,y)$ a function of the macroscopic variable x and of the periodic microscopic variable $y \in Y = (0,1)^n$.

Similarly

$$v_\epsilon(t,x) = \sum_{i=0}^{+\infty} \epsilon^i v_i \left(t, x - \frac{b^* t}{\epsilon}, \frac{x}{\epsilon} \right)$$

We plug these ansatz in the system of equations and use the usual chain rule derivation

$$\nabla\left(u_i\left(t, x-\frac{b^* t}{\epsilon}, \frac{x}{\epsilon}\right)\right) = \left(\epsilon^{-1}\nabla_y u_i + \nabla_x u_i\right)\left(t, x-\frac{b^* t}{\epsilon}, \frac{x}{\epsilon}\right),$$

plus a **new** contribution

$$\frac{\partial}{\partial t}\left(u_i\left(t, x-\frac{b^* t}{\epsilon}, \frac{x}{\epsilon}\right)\right) = \left(\frac{\partial u_i}{\partial t} - \underbrace{\epsilon^{-1} b^* \cdot \nabla_x u_i}_{new\, term}\right)\left(t, x, \frac{x}{\epsilon}\right)$$

$$
\begin{cases}
\dfrac{\partial u_\epsilon}{\partial t} + \dfrac{1}{\epsilon} b_\epsilon \cdot \nabla_x u_\epsilon - \operatorname{div}_x (D_\epsilon \nabla_x u_\epsilon) = 0 \quad \text{in} \ \ \Omega_\epsilon \times (0,T) \\
u_\epsilon(x,0) = u^0(x), \quad x \in \Omega_\epsilon, \\
-\dfrac{1}{\epsilon} D_\epsilon \nabla_x u_\epsilon \cdot n = \dfrac{\partial v_\epsilon}{\partial t} = \dfrac{k}{\epsilon^2}(u_\epsilon - \dfrac{v_\epsilon}{K}) \quad \text{on} \ \ \partial\Omega_\epsilon \times (0,T) \\
v_\epsilon(x,0) = v^0(x), \quad x \in \partial\Omega_\epsilon
\end{cases}
$$

Fredholm alternative in the unit cell

Lemma. The boundary value problem

$$\begin{cases} b(y)\cdot\nabla_y v(y) - \operatorname{div}_{\mathrm{y}}\left(D(y)\nabla_y v(y)\right) = g(y) \text{ in } Y^* \\ D(y)\nabla_y v(y)\cdot n = h(y) \text{ on } \partial\mathcal{O} \\ y \to v(y)\ Y\text{-periodic} \end{cases}$$

admits a unique solution in $H^1(Y^*)$, up to an additive constant, **if and only if**

$$\int_{Y^*} g(y)\,dy + \int_{\partial\mathcal{O}} h(y)\,ds = 0.$$

Recall that $Y = Y^* \cup \mathcal{O}$ with Y^* = fluid part and $\mathcal{O}$ = solid obstacle.

Cascade of equations

Equation of order ϵ^{-2}:

$$\left\{\begin{array}{l} b(y)\cdot\nabla_y u_0 - \operatorname{div}_y\left(D(y)\nabla_y u_0\right) = 0 \text{ in } Y^* \\ D(y)\nabla_y u_0\cdot n = 0 = k\Big(u_0 - \frac{v_0}{K}\Big) \text{ on } \partial\mathcal{O} \\ y \to u_0, v_0(t,x,y)\ Y\text{-périodique} \end{array}\right.$$

We deduce

$$\boxed{u_0(t,x,y) \equiv u_0(t,x) \text{ and } v_0(t,x,y) \equiv K u_0(t,x)}$$

Equation of order ϵ^{-1}:

$$\begin{cases} -b^* \cdot \nabla_x u_0 + b(y) \cdot (\nabla_x u_0 + \nabla_y u_1) - \operatorname{div_y}(D(y)(\nabla_x u_0 + \nabla_y u_1)) = 0 \text{ in } Y^* \\ -D(y)(\nabla_x u_0 + \nabla_y u_1) \cdot n = -b^* \cdot \nabla_x v_0 \cdot n = k\Big(u_1 - \frac{v_1}{K}\Big) \text{ on } \partial\mathcal{O} \\ y \to u_1, v_1(t,x,y) \; Y\text{-periodic} \end{cases}$$

We deduce

$$\boxed{u_1(t,x,y) = \sum_{i=1}^{n} \frac{\partial u_0}{\partial x_i}(t,x) w_i(y) \quad \text{and} \quad v_1 = K u_1 + \frac{K^2}{k} b^* \cdot \nabla_x u_0}$$

Cell problem

$$\begin{cases} b(y) \cdot \nabla_y w_i - \operatorname{div_y}\left(D(y)\left(\nabla_y w_i + e_i\right)\right) = \left(b^* - b(y)\right) \cdot e_i \text{ in } Y^* \\ D(y)\left(\nabla_y w_i + e_i\right) \cdot n = K b^* \cdot e_i \text{ on } \partial\mathcal{O} \\ y \to w_i(y) \; Y\text{-periodic} \end{cases}$$

The compatibility condition (Fredholm alternative) for the existence of w_i is

$$b^* = \left(|Y^*| + |\partial\mathcal{O}|_{n-1} K\right)^{-1} \int_{Y^*} b(y) dy.$$

Equation of order ϵ^0:

$$\begin{cases} b \cdot \nabla_y u_2 - \operatorname{div}_y \left(D \nabla_y u_2 \right) = b^* \cdot \nabla_x u_1 - b \cdot \nabla_x u_1 \\ + \operatorname{div}_y \left(D \nabla_x u_1 \right) + \operatorname{div}_x \left(D (\nabla_y u_1 + \nabla_x u_0) \right) - \frac{\partial u_0}{\partial t} \quad \text{in } Y^* \\ -D(y) \left(\nabla_y u_2 + \nabla_x u_1 \right) \cdot n = \frac{\partial v_0}{\partial t} - b^* \cdot \nabla_x v_1 = k \Big(u_2 - \frac{v_2}{K} \Big) \text{ on } \partial \mathcal{O} \\ y \to u_2, v_2(t,x,y) \ Y\text{-periodic} \end{cases}$$

Compatibility condition for the existence of u_2:

$$\int_{Y^*} \Big(b^* \cdot \nabla_x u_1 - b \cdot \nabla_x u_1 + \operatorname{div}_y \big(D \nabla_x u_1 \big) + \operatorname{div}_x \big(D (\nabla_y u_1 + \nabla_x u_0) \big) \\ - \frac{\partial u_0}{\partial t} \Big) dy - \int_{\partial \mathcal{O}} \Big(D \nabla_x u_1 \cdot n + \frac{\partial v_0}{\partial t} - b^* \cdot \nabla_x v_1 \Big) ds = 0$$

Replacing u_1 by its previous value in terms of $\nabla_x u_0$ we obtain the **homogenized problem**.

Homogenized equation

$$
\begin{cases}
\dfrac{\partial u_0}{\partial t} - \operatorname{div}\left(A^*\nabla u_0\right) = 0 & \text{in } \mathbb{R}^n \times (0,T) \\
u_0(t=0,x) = \dfrac{|Y^*|u^0(x) + |\partial\mathcal{O}|_{n-1}v^0(x)}{|Y^*| + K|\partial\mathcal{O}|_{n-1}} & \text{in } \mathbb{R}^n,
\end{cases}
$$

The initial condition is an average of

$$u_0(t=0,x) \approx u_\epsilon(t=0,x) = u^0(x) \text{ in } Y^*$$

and

$$v_0(t=0,x) = K u_0(t=0,x) \approx v_\epsilon(t=0,x) = v^0(x) \text{ on } \partial\mathcal{O}$$

-IV- RIGOROUS PROOF

The proof is made of 3 steps

1. A priori estimates.
2. Passing to the limit by two-scale convergence with drift.
3. Strong convergence.

A priori estimates

For any final time $T > 0$, there exists a constant $C > 0$ that does not depend on ϵ such that

$$\|u_\epsilon\|_{L^\infty(0,T;L^2(\Omega_\epsilon))} + \sqrt{\epsilon}\|v_\epsilon\|_{L^\infty(0,T;L^2(\partial\Omega_\epsilon))} + \|\nabla u_\epsilon\|_{L^2((0,T)\times\Omega_\epsilon)}$$

$$\leq C\left(\|u^0\|_{L^2(\mathbb{R}^n)} + \|v^0\|_{H^1(\mathbb{R}^n)}\right).$$

$$\|v_\epsilon\|_{L^2(0,T;H^1(\Omega_\epsilon))} \leq C(\|u_\epsilon\|_{L^2(0,T;H^1(\Omega_\epsilon))} + \epsilon\|v^0\|_{H^1(\mathbb{R}^n)}).$$

$$\|\frac{1}{K}v_\epsilon - u_\epsilon\|_{L^2((0,T)\times\Omega_\epsilon)} \leq C\epsilon$$

Proof. Multiply the fluid equation by u_ϵ and the solid boundary equation by $\epsilon v_\epsilon/K$, integrate by parts to get the usual parabolic estimates. (v_ϵ is extended to the whole Ω_ϵ.)

Two-scale convergence

Proposition. (Nguetseng, A.)

Let w_ϵ be a bounded sequence in $L^2(\mathbb{R}^n)$. Up to a subsequence, there exist a limit $w(x,y) \in L^2(\mathbb{R}^n \times \mathbb{T}^n)$ such that w_ϵ two-scale converges to w in the sense that

$$\lim_{\epsilon \to 0} \int_{\mathbb{R}^n} w_\epsilon(x) \phi\left(x, \frac{x}{\epsilon}\right) dx = \int_{\mathbb{R}^n} \int_{\mathbb{T}^n} w(x,y) \phi(x,y) \, dx \, dy$$

for all functions $\phi(x,y) \in L^2\left(\mathbb{R}^n; C(\mathbb{T}^n)\right)$.

Two-scale convergence with drift

Proposition (Marusic-Paloka, Piatnitski). Let $\mathcal{V} \in \mathbb{R}^N$ be a given drift velocity. Let w_ϵ be a bounded sequence in $L^2((0,T) \times \mathbb{R}^n)$. Up to a subsequence, there exist a limit $w_0(t,x,y) \in L^2((0,T) \times \mathbb{R}^n \times \mathbb{T}^n)$ such that w_ϵ two-scale converges with drift weakly to w_0 in the sense that

$$\lim_{\epsilon \to 0} \int_0^T \int_{\mathbb{R}^n} w_\epsilon(t,x) \phi\left(t, x + \frac{\mathcal{V}}{\epsilon} t, \frac{x}{\epsilon}\right) dt\, dx = \int_0^T \int_{\mathbb{R}^n} \int_{\mathbb{T}^n} w_0(t,x,y) \phi(t,x,y)\, dt\, dx\, dy$$

for all functions $\phi(t,x,y) \in L^2\left((0,T) \times \mathbb{R}^n; C(\mathbb{T}^n)\right)$.

Passing to the limit

We multiply the equation by an oscillating test function with drift $\mathcal{V} = -b^*$

$$\Psi_\epsilon = \phi\left(t, x + \frac{\mathcal{V}}{\epsilon}t\right) + \epsilon\, \phi_1\left(t, x + \frac{\mathcal{V}}{\epsilon}t, \frac{x}{\epsilon}\right)$$

and we use the two-scale convergence with drift to get the homogenized equation.

STRONG CONVERGENCE

If the initial data are well prepared, i.e., $v^0(x) = Ku^0(x)$, then we use the notion of strong two-scale convergence with drift.

Proposition. If $w_\epsilon(t,x)$ two-scale converges with drift weakly to $w_0(t,x,y)$ (assumed to be smooth enough) and

$$\lim_{\epsilon\to 0} \|w_\epsilon\|_{L^2((0,T)\times\mathbb{R}^n)} = \|w_0\|_{L^2((0,T)\times\mathbb{R}^n\times\mathbb{T}^n)},$$

then it converges strongly in the sense that

$$\lim_{\epsilon\to 0} \left\| w_\epsilon(t,x) - w_0\left(t, x - \frac{b^*}{\epsilon}t, \frac{x}{\epsilon}\right)\right\|_{L^2((0,T)\times\mathbb{R}^n)} = 0$$

If $v^0(x) \neq Ku^0(x)$, then we need to take into account a time initial layer.

Bon anniversaire Alain !