

TAYLOR DISPERSION FOR REACTIVE TRANSPORT THROUGH PERIODIC POROUS MEDIA

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Work supported by the GNR MOMAS

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MOMAS, 23-25 November 2009

-I- INTRODUCTION

We consider an infinite 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:

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

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 $\ell \ll L_R$: 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:

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

Scaling (continued)

New unknowns:

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

and dimensionless equations

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

and

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

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 time-scale, 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

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

We assume

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

Scaling (continued)

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

Assumptions:

- ✗ Unit cell $Y = (0, 1)^n = Y^* \cup \mathcal{O}$ with fluid part Y^*
- ✗ Stationary incompressible periodic flow $b_\epsilon(x) = b\left(\frac{x}{\epsilon}\right)$ 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 $D_\epsilon(x) = D\left(\frac{x}{\epsilon}\right)$

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

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

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

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

Homogenized coefficients

The homogenized diffusion tensor is

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

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

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

$$\left\{ \begin{array}{l} b(y) \cdot \nabla_y w_i - \operatorname{div}_y (D(y) (\nabla_y w_i + e_i)) = (b^* - b(y)) \cdot e_i \text{ in } Y^* \\ D(y) (\nabla_y w_i + e_i) \cdot n = K b^* \cdot e_i \text{ on } \partial\mathcal{O} \\ y \rightarrow w_i(y) \text{ } Y\text{-periodic} \end{array} \right.$$

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

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

Remark. The case without adsorption on the pore boundaries is recovered for $K = 0$ (and $v^0 \equiv 0$).

-III- TWO-SCALE ANSATZ WITH DRIFT

A formal proof of our result is obtained as follows.

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

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

We recall the equations

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

Fredholm alternative in the unit cell

Lemma. The boundary value problem

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

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} :

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

We deduce

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

Equation of order ϵ^{-1} :

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

We deduce

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

Cell problem

$$\left\{ \begin{array}{l} b(y) \cdot \nabla_y w_i - \operatorname{div}_y (D(y) (\nabla_y w_i + e_i)) = (b^* - b(y)) \cdot e_i \text{ in } Y^* \\ D(y) (\nabla_y w_i + e_i) \cdot n = Kb^* \cdot e_i \text{ on } \partial\mathcal{O} \\ y \rightarrow w_i(y) \text{ } Y\text{-periodic} \end{array} \right.$$

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

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

Equation of order ϵ^0 :

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

Compatibility condition for the existence of u_2 :

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

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

Homogenized equation

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

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

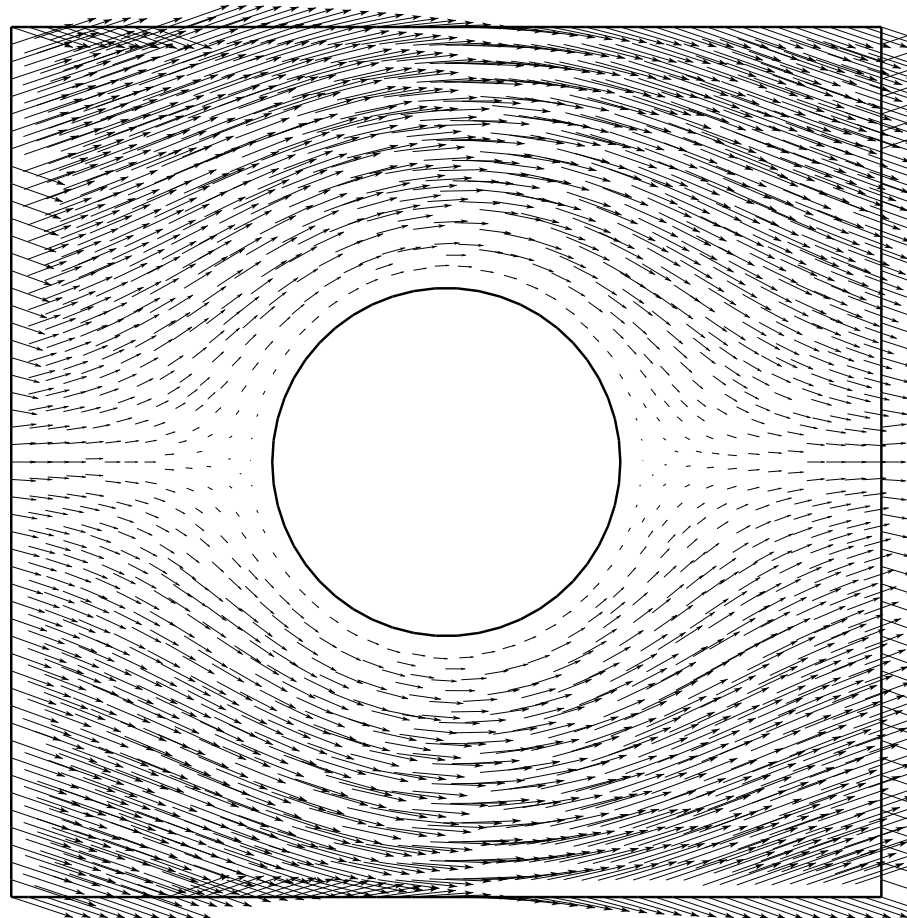
$$v_0(t = 0, x) = K u_0(t = 0, x) \approx v_\epsilon(t = 0, x) = v^0(x) \text{ on } \partial \mathcal{O}$$

-IV- NUMERICAL RESULTS

Numerical computations done with FreeFem++ in 2-d for circular obstacles.

The velocity $\mathbf{b}(y)$ is generated by solving the following filtration problem in the fluid part Y^* of the unit cell Y

$$\left\{ \begin{array}{ll} \nabla_y p - \Delta_y \mathbf{b} = \mathbf{e}_i & \text{in } Y^*; \\ \operatorname{div}_y \mathbf{b} = 0 & \text{in } Y^*; \\ \mathbf{b} = 0 & \text{on } \partial\mathcal{O}; \\ p, \mathbf{b} & \text{are } Y\text{-periodic.} \end{array} \right.$$

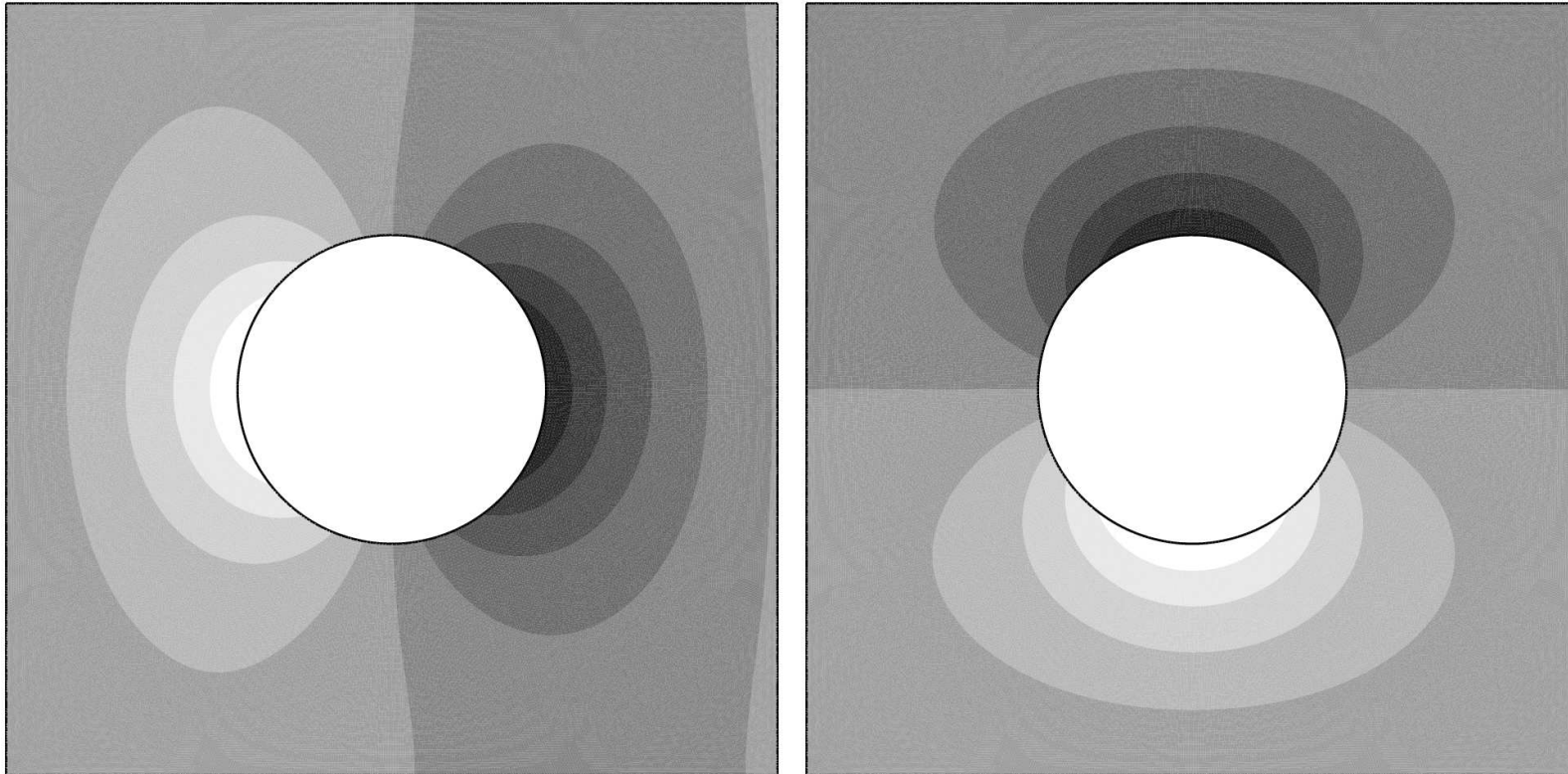


<i>PARAMETERS</i>	<i>VALUES</i>
Observation length : L_R	10 m,
Pore length : ℓ	10^{-5} m
$\epsilon = \ell/L_R$	10^{-6}
Characteristic velocity: V_R :	10^{-3} m/sec
Diffusion coefficient: D^* :	10^{-8} m ² /sec,
Péclet's number: Pe :	10^6
Adsorption rate \hat{k}^* :	10^{-3} m/sec
Adsorption equilibrium constant K^*	10^{-5} m
Damköhler's number: Da	10^6
Local Péclet's number: Pe _{loc}	1
Local Damköhler's number: Da _{loc}	1

Cell problem

$$\left\{ \begin{array}{l} b(y) \cdot \nabla_y w_i - D \Delta_y w_i = (b^* - b(y)) \cdot e_i \text{ in } Y^* \\ D (\nabla_y w_i + e_i) \cdot n = K b^* \cdot e_i \text{ on } \partial \mathcal{O} \\ y \rightarrow w_i(y) \text{ } Y\text{-periodic} \end{array} \right.$$

w_1, w_2



The homogenized velocity is

$$\mathbf{b}^* = \begin{pmatrix} 0.01808 \\ -6.759 \cdot 10^{-6} \end{pmatrix}$$

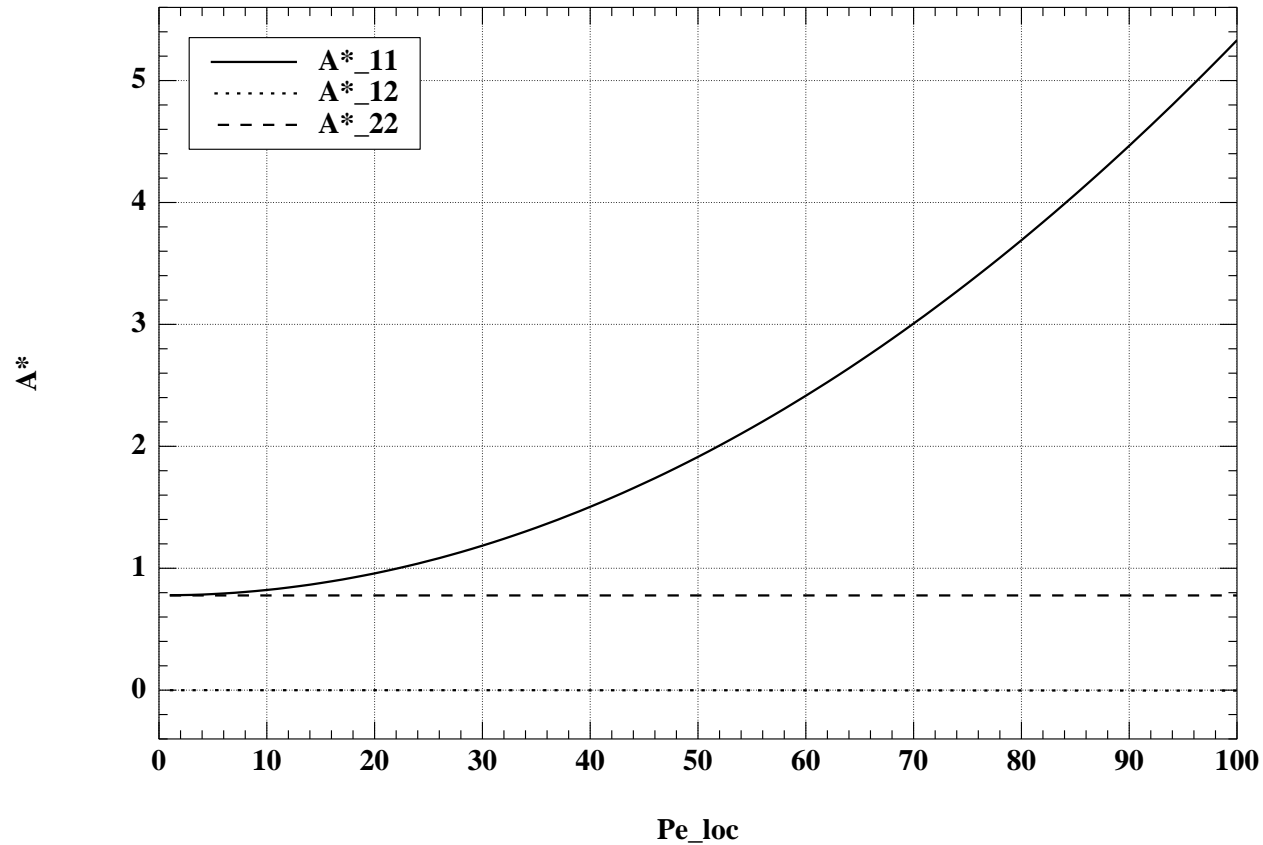
The homogenized tensor is

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

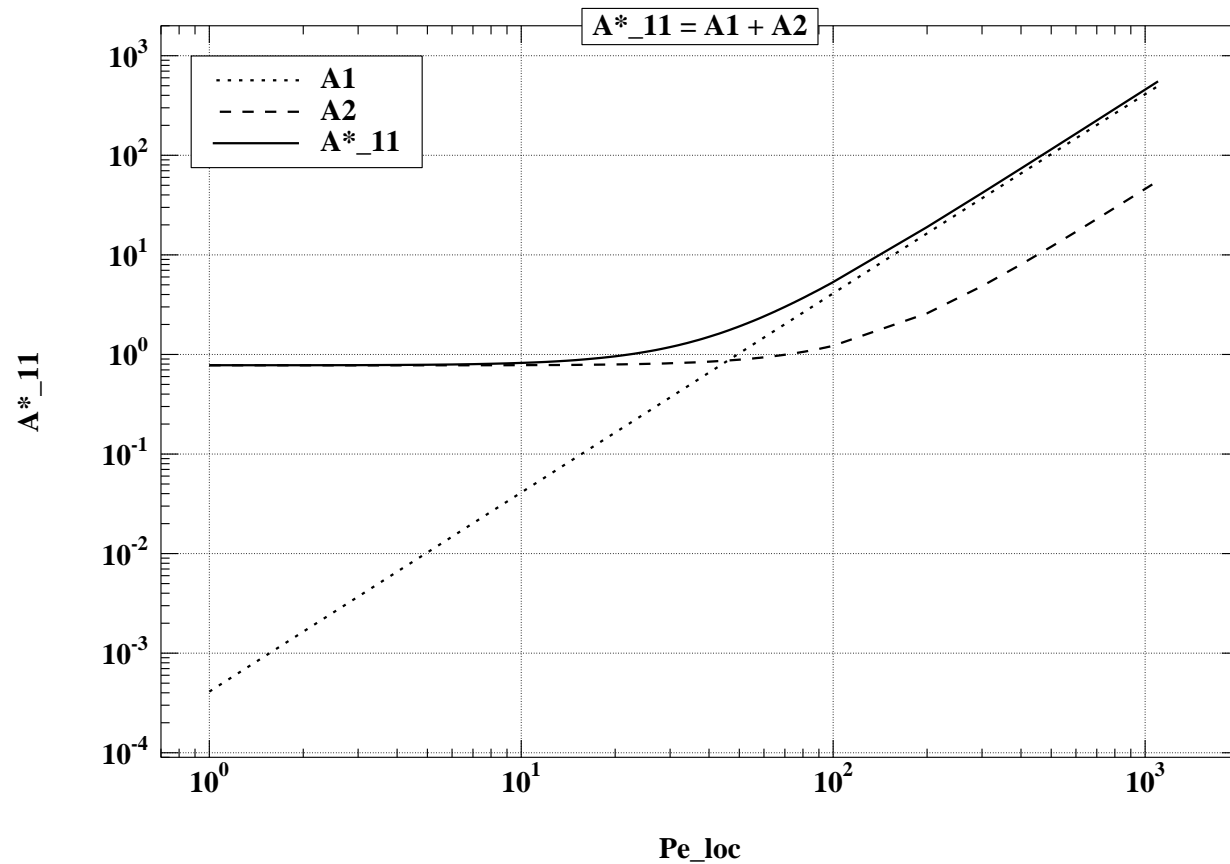
$$\text{with } A_1^* = \frac{K^2}{k} |\partial\mathcal{O}|_{n-1} b^* \otimes b^* \quad \text{and} \quad A_2^* = \int_{Y^*} D(\mathbf{I} + \nabla_y w(y)) (\mathbf{I} + \nabla_y w(y))^T dy$$

For $\mathbf{Pe}_{loc} = 1$ and $\mathbf{Da}_{loc} = 1$, we get $(|Y^*| + K|\partial\mathcal{O}|_{n-1}) = 2.13097$ and

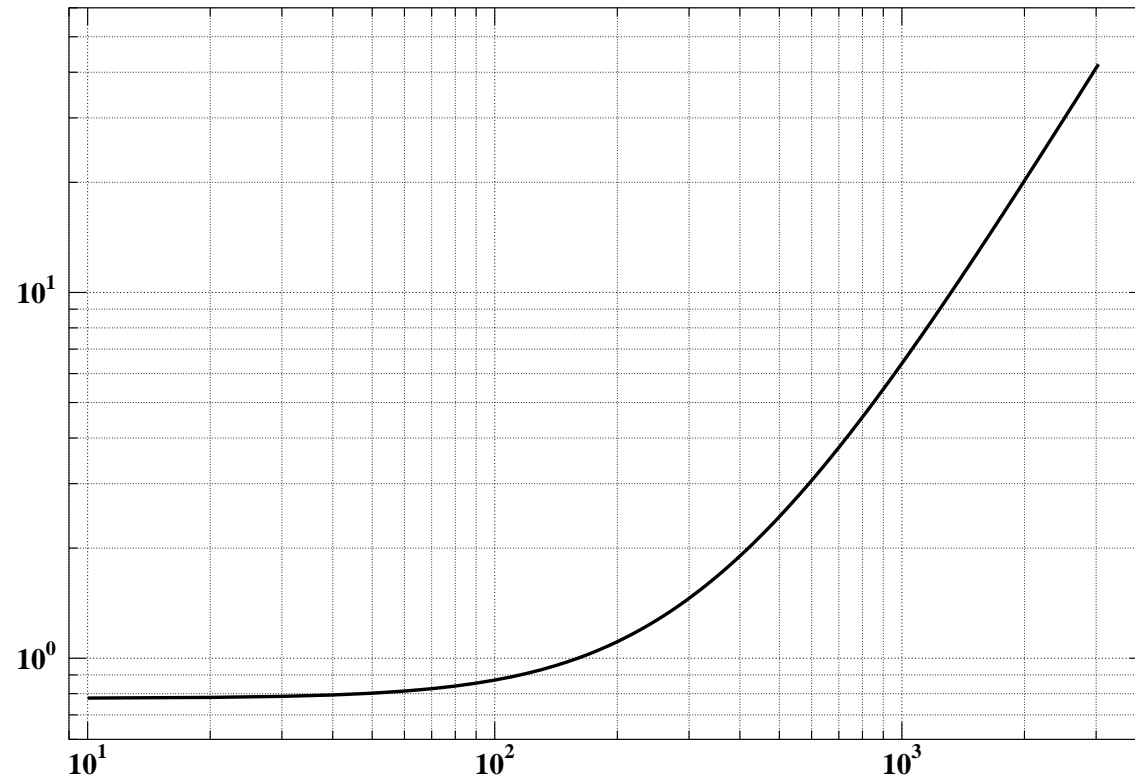
$$A_1^* = \begin{pmatrix} 4.10 \cdot 10^{-4} & -3.43 \cdot 10^{-7} \\ -3.43 \cdot 10^{-7} & 2.87 \cdot 10^{-11} \end{pmatrix}, \quad A_2^* = \begin{pmatrix} 0.778 & -1.49 \cdot 10^{-4} \\ -1.49 \cdot 10^{-4} & 0.776 \end{pmatrix}.$$



Entries A^*_{11} , A^*_{12} and A^*_{22} of the dispersion matrix A^* as a function of the local Péclet's number, for $Da_{loc} = 1$.



Log-log plot of the (1,1) entry of the dispersion matrix $A^* = A_1 + A_2$, together with its 2 components A_1 and A_2 , as a function of the local Péclet's number, for $Da_{loc} = 1$ (asymptotic slope ≈ 2).



Log-log plot of the longitudinal dispersion A_{11}^* as a function of the local Péclet's number, in the absence of chemical reactions, $K^* = 0$ (asymptotic slope ≈ 1.7).