

# Homogenization approach to the Taylor dispersion for reactive transport through porous media

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**Abstract for the International Workshop Mathematics in Chemical Kinetics and Engineering MACKiE-2009, Ghent, Belgium, February 8-11, 2009:**

We consider a saturated flow through a porous medium. The hydrodynamic dispersion is the averaged macroscopic picture of the motion of the tracer particles through the pore structure and of the chemical reactions of the solute with the solid walls and with other particles. It is caused by two basic transport phenomena involved: convection and molecular diffusion. Their simultaneous presence in the pore structure leads to a complex spreading of the tracer. The interaction between the solid pore interfaces and the fluid is related to the adsorption or deposition of tracer particles on the solid surface. Eventually, radioactive decay and chemical reactions within the fluid may also cause concentration changes.

Actually the hydrodynamic dispersion could be studied in three distinct regimes: a) *diffusion-dominated mixing*, b) *Taylor dispersion-mediated mixing* and c) *chaotic advection*.

In this work we study the second regime and in addition to dominant Peclet's number we also consider dominant non-dimensional numbers linked to the chemistry, like Damkohler's number.

We consider a periodic porous medium and in its fluid part the reactive diffusive transport by an incompressible flow of a single solute. Characteristic

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size of our porous medium is  $\varepsilon$ .

The unknowns are the concentrations  $c$  in the fluid and  $c_s$  on the solid pores boundaries. The equations for  $u_\varepsilon = c$  and  $v_\varepsilon = c_s$  in their non-dimensional form, with the characteristic time being of the characteristic global diffusion time scale, read (with the velocity  $\mathbf{v}_\varepsilon = \mathbf{v}$ )

$$\frac{\partial u_\varepsilon}{\partial t} + \mathbf{P}\mathbf{e} \mathbf{v}_\varepsilon(x, t) \cdot \nabla_x u_\varepsilon = D \Delta_x u_\varepsilon \quad \text{in } \Omega_\varepsilon \times (0, T) \quad (1)$$

$$-D \nabla_x u_\varepsilon \cdot \mathbf{n} = \frac{T_A}{T_{react}} \frac{\partial v_\varepsilon}{\partial t} = \frac{T_D}{T_{react}} k(u_\varepsilon - \frac{T_A}{T_{DE}} \frac{v_\varepsilon}{K}) \quad \text{on } \partial\Omega_\varepsilon \times (0, T), \quad (2)$$

$$u_\varepsilon(x, 0) = u^0(x), \quad x \in \Omega_\varepsilon, \quad v_\varepsilon(x, 0) = v^0(x), \quad x \in \partial\Omega_\varepsilon. \quad (3)$$

In the system (1)-(3)  $\mathbf{P}\mathbf{e}$  is Peclet's number,  $T_{DE}$  is the characteristic desorption time,  $T_A$  is the characteristic adsorption time and  $T_{react}$  is the superficial chemical reaction time scale. In the present work we make the following hypothesis.

$$\mathbf{P}\mathbf{e} \sim \frac{1}{\varepsilon}, \quad \mathbf{D}\mathbf{a} = \frac{T_D}{T_{react}} \sim \frac{1}{\varepsilon}, \quad \frac{T_A}{T_{react}} \sim \varepsilon, \quad \frac{T_A}{T_{DE}} \sim 1, \quad \mathbf{v}_\varepsilon(x, t) = \mathbf{b}\left(\frac{x}{\varepsilon}\right), \quad (4)$$

where  $\mathbf{b}$  is an 1-periodic divergence free vector field. Its normal component is zero on solid boundaries. Our goal is to find **the effective diffusion tensor** (= dispersion tensor), in the homogenization limit  $\varepsilon \rightarrow 0$ . We note that the problem differs from the Taylor dispersion in tubes by the choice of the characteristic time and the geometry is much more complicated. Therefore we can't apply the central manifold approach (see [3] and references therein) or anisotropic singular perturbation (see [6]).

For the derivation of Taylor's dispersion in porous media, in the case without chemical reactions and using formal two-scale expansions, we refer to [2] and the references therein. Here presence of the reaction complicates the situation and other approaches were tried (see e.g. [5]). Our approach uses the newly introduced **two-scale convergence with drift** in the recent papers [4] and [1].

Formally, this means that we search our concentrations using the following two-scale ansatz with drift:

$$u_\varepsilon = \sum_{i=1}^{+\infty} \varepsilon^i u_i(t, x - \frac{\mathbf{b}^* t}{\varepsilon}, \frac{x}{\varepsilon}); \quad v_\varepsilon = \sum_{i=1}^{+\infty} \varepsilon^i v_i(t, x - \frac{\mathbf{b}^* t}{\varepsilon}, \frac{x}{\varepsilon}), \quad (5)$$

where the drift  $\mathbf{b}^*$  is to be found. After inserting the expansions (5) into the system (1)-(3) we obtain a cascade of convection-diffusion problem in the periodicity pore. Applying Fredholm's alternative for their solvability, we obtain through the compatibility conditions that the drift is given by

$$\mathbf{b}^* = (|Y^0| + |\partial\Sigma^0|_{n-1} K)^{-1} \int_{Y^0} \mathbf{b}(y) dy, \quad (6)$$

where  $|Y^0|$  is the porosity,  $|\partial\Sigma^0|_{n-1}$  is the tortuosity and  $Y^0$  is the pore space in the unit cell. Next we find that  $u_0(x, t) = K v_0(x, t)$ .

The homogenized problem for  $u = u_0$  reads as follows:

$$(|Y^0| + K|\partial\Sigma^0|_{n-1})\partial_t u = \operatorname{div}_x(A^*\nabla_x u) \quad \text{in } \mathbb{R}^n \times (0, T), \quad (7)$$

$$u(x, 0) = \frac{|Y^0|u^0(x) + |\partial\Sigma^0|_{n-1}v^0(x)}{|Y^0| + K|\partial\Sigma^0|_{n-1}} \quad \text{in } \mathbb{R}^n. \quad (8)$$

Let auxiliary periodic functions  $\chi_i(y) \in H^1(Y^0)$  be given by

$$\begin{aligned} \mathbf{b}(y) \cdot \nabla \chi_i(y) - D \operatorname{div}(\nabla(\chi(y) + y)) &= b_i^* - b_i(y) \quad \text{in } Y^0, \\ D\nabla(\chi_i(y) + y_i) \cdot n &= Kb_i^* \quad \text{on } \partial\Sigma^0, \end{aligned} \quad (9)$$

Then the dispersion tensor  $A^*$  is positive definite and written as

$$A^* = \bar{A}_1 + D \int_{Y^0} (\mathbf{I} + \nabla_y \chi(y))(\mathbf{I} + \nabla_y \chi(y))^T dy. \quad (10)$$

The matrix  $\bar{A}_1$  is linked exclusively to the adsorption/desorption reactions, transported by the drift velocity, and given by

$$\bar{A}_1 = \frac{K^2}{k} |\partial\Sigma^0|_{n-1} \mathbf{b}^* \otimes \mathbf{b}^* = \left[ \frac{K^2}{k} |\partial\Sigma^0|_{n-1} b_i^* b_j^* \right]. \quad (11)$$

## References

- [1] G. Allaire, A.L. Raphael, *Homogenization of a convection-diffusion model with reaction in a porous medium*. C. R. Math. Acad. Sci. Paris 344 (2007), no. 8, p. 523–528.
- [2] J.L. Auriault, P.M. Adler, *Taylor dispersion in porous media : Analysis by multiple scale expansions*, Advances in Water Resources, Vol. 18 (1995), p. 217-226.
- [3] V. Balakotaiah, H.-C. Chang, *Dispersion of Chemical Solutes in Chromatographs and Reactors*, Philosophical Transactions: Physical Sciences and Engineering, Vol. 351 (1995), p. 39-75.
- [4] E. Marušić-Paloka, A. Piatnitskii, *Homogenization of a nonlinear convection-diffusion equation with rapidly oscillating coefficients and strong convection*, Journal of London Math. Soc., Vol. 72 (2005), No. 2, p. 391-409.
- [5] R. Mauri, *Dispersion, convection and reaction in porous media*, Phys. Fluids A (1991), p. 743-755.
- [6] A. Mikelić, V. Devigne, C.J. van Duijn : *Rigorous upscaling of the reactive flow through a pore, under dominant Peclet and Damkohler numbers*, SIAM J. Math. Anal., Vol. 38, Issue 4 (2006), p. 1262-1287.