



Mathematical Problems in Mechanics

Homogenization of a convection–diffusion model with reaction in a porous medium

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Abstract

We study the homogenization of a convection–diffusion equation with reaction in a porous medium when both the Péclet and Damkohler numbers are large. We prove that, up to a large drift, the homogenized equation is a diffusion equation. Our method is based on a factorization principle and two-scale convergence. The main consequence is that we obtain rigorous definitions of homogenized coefficients which justify heuristic arguments in the method of volume averaging. We perform 2-d numerical computations of the diffusion–dispersion homogenized coefficient which are in very good agreement with previous results obtained by the method of volume averaging. *To cite this article:* G. Allaire, A.-L. Raphael, *C. R. Acad. Sci. Paris, Ser. I 344 (2007)*.

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Résumé

Homogénéisation d'un modèle de convection–diffusion avec réaction en milieu poreux. On étudie l'homogénéisation d'un problème de convection–diffusion avec réaction en milieu poreux lorsque les nombres de Péclet et de Damkohler sont grands. Nous démontrons que, dans un repère dérivant à grande vitesse, l'équation homogénéisée est une équation de diffusion. Notre méthode est basée sur un principe de factorisation et sur la convergence à deux échelles. La conséquence pratique la plus importante est que nous obtenons ainsi une définition rigoureuse des coefficients homogénéisés qui justifie des arguments heuristiques utilisés dans la méthode de la prise de moyenne. Nous avons effectué des calculs numériques en 2-d du coefficient homogénéisé de diffusion–dispersion qui donnent des valeurs très semblables à celles obtenues par prise de moyenne. *Pour citer cet article :* G. Allaire, A.-L. Raphael, *C. R. Acad. Sci. Paris, Ser. I 344 (2007)*.

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On étudie l'homogénéisation du problème (1) de convection–diffusion avec réaction en milieu poreux. On note ϵ le rapport entre la taille de la cellule de périodicité et une dimension caractéristique macroscopique. La vitesse est alors de l'ordre de ϵ^{-1} , tandis que les réactions chimiques ou d'absorption sont de l'ordre de ϵ^{-2} dans le volume et de l'ordre de ϵ^{-1} sur les surfaces des pores. Cette mise à l'échelle de (1) correspond au cas de grands nombres de Péclet et de Damkohler, comme proposé dans [14]. Dans le cas sans réaction, $c(y) \equiv 0$ et $k = 0$, pour un champ de

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vitesse incompressible, $\operatorname{div}_y b = 0$, à moyenne nulle et non pénétrant, $b \cdot n = 0$ sur le bord des pores $\partial\mathbb{S}$, le résultat est bien connu [11,12]. De même, dans un domaine non perforé et sans réaction on peut citer le chapitre 2 de [10] et [13], ou bien plus généralement [15] pour le cas 1-d. Le cas général a été étudié dans la littérature physique [5,14] par des méthodes heuristiques de type développements asymptotiques. Le but de cette note est de justifier rigoureusement ces approches et de donner des formules pour calculer les coefficients homogénéisés de (1) qui justifient la méthode heuristique de prise de moyenne, traditionnellement utilisée [17,4]. Pour cela nous utilisons un principe de factorisation et une généralisation de la convergence à deux échelles (voir la Proposition 4.1).

Dans la Section 2 nous introduisons le problème spectral de cellule (2) ainsi que son adjoint (3). Grâce au théorème de Krein–Rutman, il existe une première valeur propre simple λ_1 commune pour (2) et (3), et les fonctions propres correspondantes sont strictement positives. La première fonction propre $\Psi_1(y)$ de (2) s'interprète comme le profil asymptotique microscopique d'équilibre entre convection–diffusion d'une part et réactions d'autre part. On peut ainsi introduire une nouvelle inconnue par la factorisation (4) et obtenir une forme simplifiée (5) du problème à homogénéiser. Dans cette nouvelle formulation il n'y a plus de termes de réaction et le champ de vitesse microscopique \tilde{b} est automatiquement à divergence nulle. Par contre, sa moyenne U^* n'est pas nécessairement nulle, ce qui nécessite une modification dans la méthode des développements asymptotiques à deux échelles comme expliqué dans la Section 3 : chaque terme de l'ansatz (7) est du type $v_i(t, x - U^*t/\epsilon, x/\epsilon)$ où la variable macroscopique x est transportée à la vitesse U^*/ϵ mais pas la variable microscopique $y = x/\epsilon$. Un autre problème de cellule pour le correcteur, (8), permet de définir un tenseur macroscopique de diffusion–dispersion A^* , voir (10). Les formules ainsi obtenues pour U^* et A^* sont très importantes pour les simulations numériques (voir [3] et la Section 5). Le résultat principal de cette Note est (voir le Théorème 4.1 pour un énoncé précis) :

Théorème 1. *Sous des hypothèses adéquates, la solution de (1) vérifie*

$$u_\epsilon(t, x) \approx e^{-(\lambda_1/\epsilon^2)t} \Psi_1\left(\frac{x}{\epsilon}\right) v\left(t, x - \frac{U^*}{\epsilon}t\right)$$

où $v(t, x)$ est la solution du problème homogénéisé

$$\frac{\partial v}{\partial t} - \operatorname{div}(A^* \nabla v) = 0 \quad \text{dans } \mathbb{R}^N \times (0, T), \quad v(x, t = 0) = v^0(x).$$

Remarquons que formellement on peut ré-écrire la solution de (1) sous la forme $u_\epsilon(t, x) \approx \Psi_1(\frac{x}{\epsilon}) w_\epsilon(t, x)$ où w_ϵ est solution de

$$\frac{\partial w_\epsilon}{\partial t} + \frac{U^*}{\epsilon} \cdot \nabla w_\epsilon - \operatorname{div}(A^* \nabla w_\epsilon) + \frac{\lambda_1}{\epsilon^2} w_\epsilon = 0 \quad \text{dans } \mathbb{R}^N \times (0, T), \quad w_\epsilon(x, t = 0) = v^0(x).$$

Autrement dit, $\epsilon^{-1}U^*$ apparaît bien comme une vitesse de convection macroscopique et $\epsilon^{-2}\lambda_1$ comme un coefficient de réaction effectif. Remarquons que la vitesse de dérive U^* n'est pas la moyenne du champ de vitesse original b . En particulier, il est tout à fait possible qu'un champ de vitesse microscopique à moyenne nulle, en présence de réactions, conduise à une convection macroscopique non nulle. Dans la Section 5 (voir aussi [3]) nous étudions l'influence couplée des nombres de Péclet et de Damkohler sur le tenseur de diffusion–dispersion homogénéisé A^* .

1. Introduction

We consider the homogenization of the following model of convection–diffusion with reaction

$$\begin{cases} \frac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(\frac{x}{\epsilon}\right) \nabla u_\epsilon\right) + \epsilon^{-1}b\left(\frac{x}{\epsilon}\right) \cdot \nabla u_\epsilon + \epsilon^{-2}c\left(\frac{x}{\epsilon}\right)u_\epsilon = 0 & \text{in } \Omega_\epsilon \times (0, T), \\ A\left(\frac{x}{\epsilon}\right) \nabla u_\epsilon \cdot n + \frac{k}{\epsilon}u_\epsilon = 0 & \text{on } \partial\Omega_\epsilon \times (0, T), \end{cases} \quad (1)$$

where Ω_ϵ is a porous medium defined by $\Omega_\epsilon = \mathbb{R}^N \setminus \bigcup_{i \in \mathbb{Z}^N} \mathbb{S}_i^\epsilon$ with identical solid obstacles $\mathbb{S}_i^\epsilon = \epsilon i + \epsilon\mathbb{S}$, obtained by translation and rescaling of a unit obstacle \mathbb{S} in the unit cell $(0, 1)^N$ (which we identify with the unit torus \mathbb{T}^N when it is supplemented by periodic boundary conditions). In (1), $b(y)$ is the periodic microscopic velocity field which is neither assumed to be incompressible nor of zero average, $A(y)$ is the molecular diffusion tensor which is bounded

and uniformly coercive, i.e., there exists $\nu > 0$ such that, $\forall y \in \mathbb{T}^N$ and $\forall \xi \in \mathbb{R}^N$, $A(y)\xi \cdot \xi \geq \nu |\xi|^2$, $c(y)$ and k are coefficients modelling chemical reaction or adsorption (they have no specified sign). All coefficients are periodic and bounded, namely they belong to $L^\infty(\mathbb{T}^N)$. Of course an initial data must be supplied to (1).

The scaling of (1) corresponds to large Péclet and Damkohler numbers as proposed in [14]. Computing the effective macroscopic coefficients for (1) is a generalization of the well-known Taylor dispersion problem. Although this model looks familiar its rigorous homogenization has not been obtained yet. Let us simply mention that, in the simpler case when $c(y) \equiv 0$, $k = 0$, $\operatorname{div}_y b(y) \equiv 0$, $b \cdot n = 0$ on $\partial\mathbb{S}$, and $\int_{\mathbb{T}^N} b(y) \, dy = 0$, the homogenization of (1) is well known [11,12]. The general case is still open although some contributions appeared as [15] for the 1-d case, [13] for the case without reactions and in non-perforated domain. Let us mention however some contributions in the mechanical literature as [5,14]. The goal of this note is to provide a rigorous version of these works and to justify definitions of homogenized coefficients which are used in the more heuristic method of volume averaging [17,4].

2. Spectral cell problems and factorization

We introduce two spectral cell problems which will allow us to simplify the original model (1). We first define the direct cell problem

$$\begin{cases} -\operatorname{div}_y(A(y)\nabla_y \Psi_1) + b(y) \cdot \nabla_y \Psi_1 + c(y)\Psi_1 = \lambda_1 \Psi_1 & \text{in } \mathbb{T}^N \setminus \mathbb{S}, \\ A(y)\nabla_y \Psi_1 \cdot n + k\Psi_1 = 0 & \text{on } \partial\mathbb{S}, \end{cases} \tag{2}$$

where \mathbb{S} is the solid obstacle and $\mathbb{T}^N \setminus \mathbb{S}$ the fluid pore, and then the adjoint cell problem

$$\begin{cases} -\operatorname{div}_y(A^T(y)\nabla_y \Psi_1^*) - \operatorname{div}_y(b(y)\Psi_1^*) + c(y)\Psi_1^* = \lambda_1 \Psi_1^* & \text{in } \mathbb{T}^N \setminus \mathbb{S} \\ A^T(y)\nabla_y \Psi_1^* \cdot n + b(y) \cdot n \Psi_1^* + k\Psi_1^* = 0 & \text{on } \partial\mathbb{S}, \end{cases} \tag{3}$$

where A^T is the adjoint matrix of A . Recall that \mathbb{T}^N is the unit torus so it automatically includes periodic boundary conditions. Both (2) and (3) are spectral problems. The corresponding operators are compact but not self-adjoint, so it is not clear whether they admit a full set of eigenvalues and orthonormal eigenvectors. However, they satisfy a maximum principle and, thanks to the Krein–Rutman theorem, they admit a common first eigenvalue which is real and simple, the corresponding eigenvectors being chosen positive. We normalize them such that $\|\Psi_1\|_{L^2(\mathbb{T}^N \setminus \mathbb{S})} = 1$ and $\int_{\mathbb{T}^N \setminus \mathbb{S}} \Psi_1 \overline{\Psi_1^*} \, dy = 1$. The eigenvalue λ_1 can be interpreted as a measure of the balance between reaction and convection–diffusion.

Remark 1. When there is no reactions, i.e., $c(y) \equiv 0$ and $k = 0$, and when the velocity is incompressible, $\operatorname{div}_y b = 0$, and does not penetrate the solid part, $b \cdot n = 0$ on $\partial\mathbb{S}$, we obtain that $\lambda_1 = 0$, $\Psi_1(y) \equiv 1$, and $\Psi_1^*(y) \equiv 1$.

We now simplify (1) by using a factorization principle as was already done in [2,6–8]. We introduce a new unknown

$$v_\epsilon(t, x) = e^{\lambda_1 t / \epsilon^2} \frac{u_\epsilon(t, x)}{\Psi_1(x/\epsilon)}, \tag{4}$$

and we multiply (1) by $\Psi_1^*(\frac{x}{\epsilon})$. Remark that (4) makes sense because $\Psi_1(y) > 0$ by the Krein–Rutman theorem. After some algebra we obtain that v_ϵ satisfies

$$\begin{cases} (\Psi_1 \Psi_1^*) \left(\frac{x}{\epsilon}\right) \frac{\partial v_\epsilon}{\partial t} - \operatorname{div} \left(\tilde{A} \left(\frac{x}{\epsilon}\right) \nabla v_\epsilon \right) + \epsilon^{-1} \tilde{b} \left(\frac{x}{\epsilon}\right) \cdot \nabla v_\epsilon = 0 & \text{in } \Omega_\epsilon \times (0, T), \\ \tilde{A} \left(\frac{x}{\epsilon}\right) \nabla v_\epsilon \cdot n = 0 & \text{on } \partial\Omega_\epsilon \times (0, T), \end{cases} \tag{5}$$

with $\tilde{A}(y) = \Psi_1(y)\Psi_1^*(y)A(y)$ and $\tilde{b}(y) = [\Psi_1 \Psi_1^* b + \Psi_1 A^T \nabla \Psi_1^* - \Psi_1^* A \nabla \Psi_1](y)$. One can easily check that the new velocity \tilde{b} is divergence free, $\operatorname{div}_y \tilde{b}(y) = 0$, and satisfies $\tilde{b} \cdot n = 0$ on $\partial\mathbb{S}$. By averaging \tilde{b} we define a constant drift velocity denoted by

$$U^* = \int_{\mathbb{T}^N \setminus \mathbb{S}} \tilde{b}(y) \, dy. \tag{6}$$

If it happens that the macroscopic convection vanishes, i.e., $U^* = 0$, then the homogenization of (5) is easy and well known [11,12]. On the other hand, if $U^* \neq 0$, then the homogenization of (5) is more subtle. In the absence of an obstacle one can refer to Chapter 2 of [10] and [13].

3. Two-scale asymptotic expansions with drift

Because of the large expected drift $\epsilon^{-1}U^*$, the usual method of two-scale asymptotic expansions needs to be slightly modified. We postulate the following ansatz for the solution of (5)

$$v_\epsilon(t, x) = \sum_{i=0}^{+\infty} \epsilon^i v_i \left(t, x - \frac{U^* t}{\epsilon}, \frac{x}{\epsilon} \right), \quad (7)$$

where each term $v_i(t, x, y)$ is periodic in y with period $(0, 1)^N$. The large drift is put only in the macroscopic variable. Therefore the ansatz (7) is not equivalent to the usual one upon the change of variable $x \rightarrow x - \frac{U^* t}{\epsilon}$. This large drift yields new terms in the usual cascade of equations. Plugging (7) into (5) and identifying powers of ϵ we first obtain that v_0 does not depend on y , i.e., $v_0(t, x, y) \equiv v(t, x)$, and then that v_1 can be written

$$v_1(t, x, y) = \sum_{k=1}^N w_k(y) \frac{\partial v}{\partial x_k}(t, x) + \tilde{v}_1(t, x),$$

where \tilde{v}_1 is an arbitrary function, which does not depend on y , and $w_k(y)$ is the solution of the corrector cell problem

$$-\operatorname{div}_y(\tilde{A}(e_k + \nabla_y w_k)) + \tilde{b} \cdot (e_k + \nabla_y w_k) = \Psi_1 \Psi_1^* U^* \cdot e_k \quad \text{in } \mathbb{T}^N \setminus \mathbb{S}, \quad \tilde{A}(e_k + \nabla_y w_k) \cdot n = 0 \quad \text{on } \partial \mathbb{S}. \quad (8)$$

It is easily seen that (8) is well-posed thanks to the definition (6) of U^* , i.e., it admits a unique solution up to an additive constant. Eventually, the compatibility condition for v_2 (the right hand side must have zero average) leads to the homogenized equation

$$\begin{cases} \frac{\partial v}{\partial t} - \operatorname{div}(A^* \nabla v) = 0 & \text{in } \mathbb{R}^N \times (0, T), \\ v(x, t = 0) = v^0(x), \end{cases} \quad (9)$$

where A^* is a positive definite symmetric tensor defined by

$$A_{ij}^* = \int_{\mathbb{T}^N \setminus \mathbb{S}} \tilde{A}(e_i + \nabla_y w_i) \cdot (e_j + \nabla_y w_j) dy, \quad 1 \leq i, j \leq N. \quad (10)$$

Remark 2. It is possible to perform a two-scale asymptotic expansion with drift, similar to (7), directly in the original formulation (1). However, the computation is more tedious although it yields the same results. In such a case, the corrector cell problem is posed, not for w_k as in (8), but for $\Psi_1 w_k$.

4. Convergence of the homogenization process

We use the method of two-scale convergence [1], [16] to rigorously prove that (5) is the correct homogenized problem. Because of the large drift we need to replace the standard two-scale convergence by the following generalization which was introduced in [13]. As usual T denotes some final time, $0 \leq T \leq +\infty$.

Proposition 4.1. ([13]) *Let $U^* \in \mathbb{R}^N$ be a given drift velocity. Let $(u_\epsilon)_{\epsilon>0}$ be a uniformly bounded sequence in $L^2((0, T) \times \mathbb{R}^N)$. There exists a subsequence, still denoted by ϵ , and a limit function $u_0(t, x, y) \in L^2((0, T) \times \mathbb{R}^N \times \mathbb{T}^N)$ such that u_ϵ two-scale converges with drift weakly to u_0 in the sense that*

$$\lim_{\epsilon \rightarrow 0} \int_0^T \int_{\mathbb{R}^N} u_\epsilon(t, x) \phi \left(t, x - \frac{U^* t}{\epsilon}, \frac{x}{\epsilon} \right) dt dx = \int_0^T \int_{\mathbb{R}^N} \int_{\mathbb{T}^N} u_0(t, x, y) \phi(t, x, y) dt dx dy \quad (11)$$

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

Thanks to the fact that the velocity \tilde{b} is divergence free, $\operatorname{div}_y \tilde{b}(y) = 0$, and satisfies $\tilde{b} \cdot n = 0$ on $\partial\mathbb{S}$, we easily obtain the following a priori estimate for the solution of (5), for any time $T > 0$,

$$\int_{\Omega_\epsilon} |v_\epsilon(T, x)|^2 dx + \int_0^T \int_{\Omega_\epsilon} |\nabla v_\epsilon(t, x)|^2 dt dx \leq C \int_{\Omega_\epsilon} |v_\epsilon(0, x)|^2 dx. \tag{12}$$

Theorem 4.1. Assume that the initial data for (5) is $v_\epsilon(0, x) = v^0(x) \in L^2(\mathbb{R}^N)$. Then, the solution of (5) two-scale converges with drift to $v(t, x)$ which is the unique solution of the homogenized equation (9).

Proof. Because of the uniform bound (12) we can use the two-scale convergence with drift of Proposition 4.1. In the variational formulation of (5) we use a test function

$$\phi_\epsilon(t, x) = \phi\left(t, x - \frac{U^*t}{\epsilon}\right) + \epsilon\phi_1\left(t, x - \frac{U^*t}{\epsilon}, \frac{x}{\epsilon}\right)$$

and we pass to the limit to obtain a combination of (8) and (9). \square

Remark 3. The initial data needs not to be well-prepared in Theorem 4.1 which holds up to extracting a subsequence. However, if $v_\epsilon(0, x) = v^0(x)$, then a stronger convergence can be achieved for v_ϵ and corrector results can also be derived. A weaker version of Theorem 4.1 can be obtained by a method of Bloch wave decomposition [3].

5. Numerical results

We performed some 2-d numerical computations of the homogenized coefficients using the FreeFem++ software [9]. For details on the computations we refer to [3]. Computing U^* and A^* amounts to solve two real non self-adjoint eigenvalue problems, (2) and (3), which yields $\lambda_1, \Psi_1(y)$ and $\Psi_1^*(y)$, and further to solve (8) for obtaining $w_k(y), 1 \leq k \leq N$.

In all our computations we take $A \equiv \text{Id}, c \equiv 0$ and b parallel to e_1 with a non-zero average (the obstacle \mathbb{S} is a disk). In a first test we assume there is no reaction, i.e., $k = 0$, in order to make a comparison with the usual volume averaging method for purely advective problems [17]. We vary the Péclet number Pe between 10^{-1} and $10^{3.5}$: the homogenized longitudinal diffusion–dispersion coefficient A_{11}^* is shown on Fig. 1 (left). We clearly see a transition around $Pe = 100$: for larger values of Pe the diffusion–dispersion coefficient varies like $Pe^{1.6}$ (the slope coefficient is indeed approximately equal to 1.6 as it should be).

In a second test we fix the Péclet number $Pe = 500$ and we vary the reaction coefficient k . As expected the homogenized longitudinal diffusion–dispersion coefficient A_{11}^* decreases when k increases and has a finite limit when $k \rightarrow +\infty$ (which corresponds to Dirichlet boundary conditions on $\partial\mathbb{S}$).

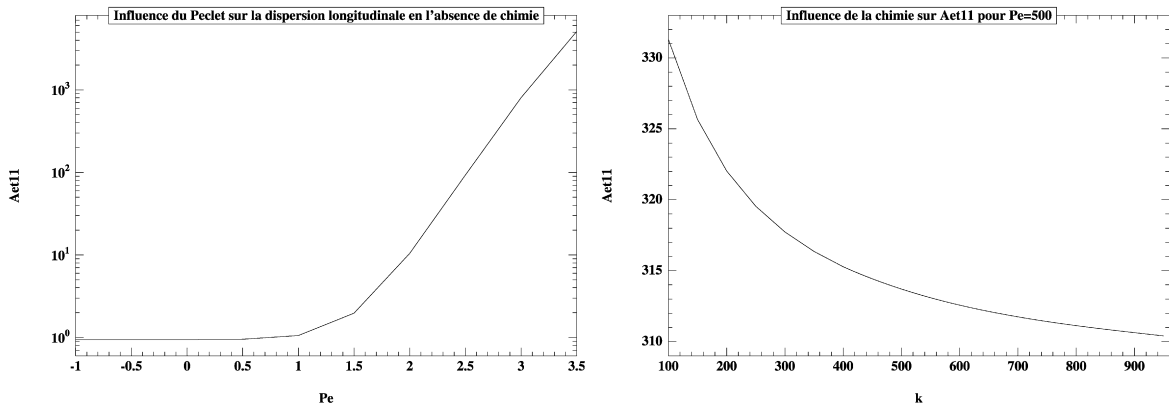


Fig. 1. Log–log plot of A_{11}^* in terms of the Péclet number with $k = 0$ (left). Variation of A_{11}^* in terms of the Damkohler number k with a fixed Péclet number (right).

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