DISPERSION AND CONVECTION IN PERIODIC MEDIA

BY

JACOB RUBINSTEIN

AND

ROBERTO MAURI

IMA Preprint Series # 188

October 1985

INSTITUTE FOR MATHEMATICS AND ITS APPLICATIONS

UNIVERSITY OF MINNESOTA

514 Vincent Hall

206 Church Street S.E.

Minneapolis, Minnesota 55455

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DISPERSION AND CONVECTION IN PERIODIC POROUS MEDIA

Jacob Rubinstein(1) and Roberto Mauri(2)

(1) Institute for Mathematics and its Applications, University of Minnesota, Minneapolis, MN 55455

(2) Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139

Abstract

The problem of transport of a passive solute in a porous medium by convection and dispersion is analysed by the method of homogenization. Assuming that the geometry is periodic, the expressions for the macroscopic dispersion coefficients are derived. A few possible scalings are compared and we find that the most interesting one provides a local balance between drift and diffusion.

1. Introduction

The problem of solute transport in a porous material by convection and dispersion is a long-standing question [2], [5]. In general it is not possible to solve the full microscopic equations, so one would like to evaluate the effective (macroscopic) values of the dispersion coefficients and the convective velocity. While the study of the effective convection goes back to Darcy in the 19th century, the derivation of the macroscopic dispersion coefficients started only about 25 years ago. Saffman [7] tried to apply the successful theory of Taylor dispersion (which was formulated originally for the flow in a tube) to a flow in porous media which were modeled as a network of capillaries. However, his approach and several others which followed along the same lines were based on many ad hoc assumptions and their validity is doubtful (see the discussion in [5]). A different approach was suggested by Brenner [5]. Here the discussion was restricted to periodic structures applying the method of moments ([1], [4]) to derive a sequence of equations for the moments of the (normalized) concentration.

An asymptotic expression for the first and second moments was derived for long time and the effective dispersion parameters are evaluated herewith. We analyze here a similar problem. Our techniques, however, are completely different; namely the homogenization method which is studied extensively in [3]. The advantages of this approach are twofold:

(i) We use directly the fact that the structure is spatially periodic.

(ii) Several scalings can be analyzed within the same framework.

In the next section we formulate the problem under the appropriate scaling, and then derive the effective equation. In Section 3 we compare these results with Brenner's, examine other possible scalings, and show how the current theory reduces to the familiar Taylor dispersion phenomena ([8], [4]) in the special case of porous media composed of parallel straight tubes.

2. Derivation of the effective equations

In a spatially periodic porous material consider the two length scales ℓ and L corresponding to the cell size (i.e., the period of the structure) and the size of the region in question, respectively. Assume:

$$\varepsilon = \ell/L \ll 1 \tag{2.1}$$

We want to perform an asymptotic analysis to pass from the microscopic description to the effective (macroscopic) mass transfer equation.

Each quantity will be assumed to depend both on the macroscopic position vector $\underline{x}$ and on its microscopic counterpart $\underline{y} = \underline{x}/\varepsilon$. (The dependence on $\underline{y}$ will be assumed to be periodic.)

Consider a domain $S \in R^3$. Then the microscopic convective-diffusive equation for the solute concentration $P(\underline{x},\underline{y},t)$ reads:

$$\frac{\partial P}{\partial t} + \underline{v} \cdot \nabla P = D \Delta P \qquad \text{in} \quad S' \tag{2.2}$$

here $\underline{v}(y)$ is the fluid velocity (which is taken as periodic), D is the diffusion coefficient, while S' is the fluid region within S.

Eq. (2.2) is supplemented by

$$P(\underline{x},\underline{y},0) = f(\underline{x}) \tag{2.3}$$

where f is a smooth function with a compact support in S, and by

$$\underline{n} \cdot \nabla P = 0 \quad \text{on} \quad \partial_p \tag{2.4}$$

where ∂p denotes the boundaries of the solid particle in a cell and $\underline{n}$ indicates a unit vector normal to ∂p.

The effects of the outer boundaries are not considered here. One can assume, for example, that S is much larger than the support of $f(\underline{x})$.

The most natural way to analyze this problem is to define the following hierarchy of time scales [6]:

$$\tau_1 = \ell/V_0 \qquad \tau_2 = \ell^2/D \tag{2.5}$$

$$\tau_3 = L/V_0 \qquad \tau_4 = L^2/D$$

where V_0 is the characteristic value of the velocity field. There are two related nondimensional numbers which appear here -- the local and global Peclet numbers:

$$Pe_\ell = \frac{\tau_2}{\tau_1}$$

$$Pe_g = \frac{\tau_4}{\tau_3} \ , \tag{2.6}$$

representing the ratio between convection and diffusion locally and globally, respectively.

The most interesting case to analyze is when

$$Pe_\ell = O(1) \ (\rightarrow Pe_g = O(\frac{1}{\varepsilon})) \ . \tag{2.7}$$

Now, scaling (2.2) according to τ_4 (which is the longest time) and defining $\underline{u} = \underline{v}/V_0$, we obtain:

$$\frac{\partial P}{\partial t} + \frac{1}{\varepsilon} \underline{u} \cdot \nabla P = \Delta P \ . \tag{2.8}$$

Our homogenization technique proceeds as follows. Expand

$$P = P_0(\underline{x},\underline{y},t) + \varepsilon P_1(\underline{x},\underline{y},t) + \varepsilon^2 P_2(\underline{x},\underline{y},t) + \ldots$$

$$\nabla = \frac{1}{\varepsilon} \nabla_y + \nabla_x \ . \tag{2.9}$$

Eq. (2.8) can be rewritten as

$$\frac{\partial P}{\partial t} + \frac{1}{\varepsilon}[\underline{u} \cdot \nabla P - \langle \underline{u} \rangle \cdot \nabla_x P_0] = \Delta P - \frac{1}{\varepsilon} \langle u \rangle \cdot \nabla_x P_0 \qquad (2.10)$$

where for every integrable function $g(\underline{x},\underline{y},t)$ we define its cell average as

$$\langle g \rangle(\underline{x},t) = \frac{1}{|\Omega|} \int_\Omega g(\underline{x},\underline{y},t)d\underline{y} \; . \qquad (2.11)$$

where Ω is the cell region.

We shall treat $\underline{x},\underline{y}$ as independent variables and, furthermore, the second term on the right hand side of (2.10) will be taken as of $O(1)$. (A justification for such an asymptotic expansion is given in the Appendix).

Substituting (2.9) into (2.10) and collecting equal powers of ε one gets:

$$O(\varepsilon^{-2}) \qquad \Delta_y P_0 - \underline{u} \cdot \nabla_y P_0 = 0$$

$$\underline{n} \cdot \nabla_y P_0 = 0 \quad \text{on} \quad \partial_p \; .$$

hence $P_0 = P_0(\underline{x},t)$.

$$O(\varepsilon^{-1}) \qquad \Delta_y P_1 - \underline{u} \cdot \nabla_y P_1 = (\underline{u} - \langle \underline{u} \rangle) \cdot \nabla_x P_0 \; ,$$

$$\underline{n} \cdot \nabla_y P_1 = -\underline{n} \cdot \nabla_x P_0 \quad \text{on} \quad \partial p$$

Setting

$$P_1(\underline{x},\underline{y},t) = \underline{\chi}(\underline{y}) \cdot \nabla_x P_0(\underline{x},t),$$

we find $\Delta_y \underline{\chi} - \underline{u} \cdot \nabla_y \underline{\chi} = \underline{u} - \langle \underline{u} \rangle$ in Ω ,

$$\underline{n} \cdot \nabla_y \underline{\chi} = -\underline{n} \quad \text{on} \quad \partial_p \; , \qquad (2.12)$$

$\underline{\chi}(y)$ is periodic and $\langle \underline{\chi} \rangle = 0$.

It is easy to verify that (2.12) is solvable since:

$$\underline{\nabla} \cdot \underline{u} = 0 \; , \quad \underline{u} = 0 \quad \text{on} \quad \partial_p \; , \quad \text{and} \quad \int_{\partial_p} \underline{n} \, ds = 0 \; .$$

O(1):

$$\Delta_y P_2 - \underline{u} \cdot \nabla_y P_2 = \frac{\partial P_0}{\partial t} + \underline{u} \cdot \nabla_x P_1 - \Delta_x P_0 - 2\nabla_x \nabla_y P_1 + \frac{1}{\varepsilon} \langle \underline{u} \rangle \cdot \nabla_x P_0 \,, \qquad (2.13)$$

$$n \cdot \nabla_y P_2 = -\underline{n} \cdot \nabla_x P_1 \quad \text{on} \quad \partial_p \,.$$

The solvability condition for (2.13) gives

$$\frac{\partial P_0}{\partial t} + \frac{1}{\varepsilon} \langle \underline{u} \rangle \cdot \nabla_x P_0 = \underline{g} : \nabla_x \nabla_x P_0 \,, \qquad (2.14)$$

where

$$\underline{\underline{g}} = \underline{\underline{I}} + 2\langle \nabla \chi \rangle - \langle \underline{u}\ \underline{\chi} \rangle - \frac{1}{|\Omega|} \int_{\partial_p} \underline{n}\ \underline{\chi}\ ds \,. \qquad (2.15)$$

Rescaling (2.14) according to τ_3 we finally obtain:

$$\frac{\partial P_0}{\partial t} + \langle \underline{u} \rangle \cdot \nabla_x P_0 = \varepsilon \underline{\underline{D}}^* \nabla_x \nabla_x P_0 \,, \qquad (2.16)$$

where:

$$\frac{\underline{\underline{D}}^*}{D} = I + \mathrm{sym}[\langle 2\nabla \underline{\chi} - \underline{u}\ \underline{\chi} \rangle - \frac{1}{|\Omega|} \int_{\partial_p} \underline{n}\ \underline{\chi}\ ds]. \qquad (2.17)$$

3. Discussion

1) The macroscopic diffusion tensor (2.15) can be expressed in an alternative form as follows. Multiplying (2.10) by $\underline{\chi}$ and averaging over Ω, we find:

$$\underline{\underline{g}} = I + 2\langle\nabla\underline{\chi}\rangle + \langle\nabla\underline{\chi}^+\nabla\underline{\chi}\rangle$$

where we have considered that $\langle\underline{\chi}\ \underline{u}\ \nabla\underline{\chi}\rangle$ is antisymmetric, while:

$$\underline{\underline{g}} = \underline{\underline{I}} + 2\ \langle\underline{\chi}\Delta\underline{\chi}\rangle = -\frac{1}{|\Omega|}\int_{\partial_p}\underline{n}\ \underline{\chi}\ ds - \langle\nabla\underline{\chi}^+\cdot\nabla\underline{\chi}\rangle\ ,$$

Set now

$$\underline{B}(\underline{y}) = -(\underline{\chi}(\underline{y}) + \underline{y})\ ,$$

then $\underline{B}$ solves the following cell problem:

$$\begin{aligned}\Delta_y\underline{B} - \underline{u}\cdot\nabla_y\underline{B} &= \langle\underline{u}\rangle\ ,\\ \underline{n}\cdot\nabla_y\underline{B} &= 0 \quad \text{on } \partial_p\ ,\\ \langle B\rangle &= -\langle\underline{y}\rangle\ .\end{aligned} \tag{3.1}$$

while $\underline{\underline{g}}$ is given by:

$$\underline{\underline{g}} = \langle\nabla\underline{B}^+\cdot\nabla B\rangle\ . \tag{3.2}$$

(3.1) and (3.2) agree with Brenner's results [5]. For the case of free diffusion (i.e. for $\underline{u} = 0$), it is easily found that (3.2) can be simplified, yielding:

$$\underline{\underline{g}} = \text{sym}(\nabla\underline{B}).$$

2) Notice that (2.16) implies that in the global scale, convection prevails over diffusion, while as can be seen from (2.7) or (2.12), they are balanced

locally. Of course, we can also analyze by the same method the case $Pe_g = O(1)$, which means $Pe_\ell = O(\varepsilon)$, i.e. diffusion is dominant in the local process.

3) For the case where f is a rapidly changing function, our treatment cannot be applied and a different analysis is called for (see Ref. [3]).

4) As a by-product of our analysis, let us see how it collapses into the familiar Taylor dispersion theory when the porous medium is composed of straight parallel tubes in the x-direction. The only relevant diffusion coefficient is q_{11} .

$$q_{11} = 1 + \langle 2\frac{\partial \chi_1}{\partial y_1} - u_1 \underline{\chi_1} \rangle - \frac{1}{|\Omega|} \int_{\partial p} n_1 \chi_1 ,$$

while the cell problem for χ_1 reads:

$$\Delta_y \chi_1 - u_1(y_2,y_3) \frac{\partial \chi_1}{\partial y_1} = u_1 - \langle u_1 \rangle .$$

Since by obvious symmetry $\chi_1 = \chi_1(y_2,y_3)$, we are left with

$$\Delta_y \chi_1 = u_1 - \langle u_1 \rangle . \tag{3.3}$$

Thus, since $n_1 = 0$, we get

$$q_{11} = 1 - \langle u_1 \chi_1 \rangle . \tag{3.4}$$

(3.3) and (3.4) indeed give the well-known Taylor dispersion coefficient in a tube ([1]).

Acknowledgement

We would like to thank Professors George Papanicolaou and Howard Brenner for valuable discussions concerning this problem. The research of J.R. was supported in part by the Sloan Foundation.

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Appendix

We justify here the asymptotic procedure we used in Section 2 for a somewhat simpler problem, namely

$$\Delta P - \frac{1}{\varepsilon}\ \underline{u}\left(\frac{\chi}{\varepsilon}\right) \cdot \nabla P - \lambda P = f \quad \text{in} \quad S \tag{A.1}$$

$$P = 0 \quad \text{on} \quad \partial S \ .$$

(this is the Laplace transform of (2.2) - (2.3)). Motivated by the expansion in Section 2 we set

$$P = P_0(\underline{\chi}) + \varepsilon \chi_i\left(\frac{\chi}{\varepsilon}\right) \frac{\partial P_0(\chi)}{\partial x_i} + \varepsilon^2\ \psi_{ij}\left(\frac{\chi}{\varepsilon}\right) \frac{\partial^2 P_0}{\partial x_i \partial x_j} + P_r \tag{A.2}$$

where P_0, χ_i and ψ_{ij} are given by:

$$(\delta_{ij} + q_{ij}) \frac{\partial^2 P_0}{\partial x_i \partial x_j} - \frac{1}{\varepsilon} < \underline{u} > \nabla P_0 - \lambda P_0 = f \quad \text{in} \quad S \tag{A.3}$$

$$P_0 = 0 \quad \text{on} \quad \partial S,$$

$$(\Delta - u_j \frac{\partial}{\partial x_j}) \chi_i = u_i - <u_i> \quad \text{in } \Omega \tag{A.4}$$

χ_i periodic ,

$$(\Delta - u_i \frac{\partial}{\partial x_i})\ \psi_{\kappa\ell} = q_{k\ell} - 2 \frac{\partial \chi_\kappa}{\partial x_\ell} - u_\kappa \chi_\ell \quad \text{in } \Omega \tag{A.5}$$

$$\psi_{\kappa\ell} \ \text{periodic} ,$$

while

$$q_{\kappa\ell} = < 2 \frac{\partial \chi_\ell}{\partial x_\ell} - u_\kappa \chi_\ell > . \tag{A.6}$$

Let L be the differential operator defined in (A.1). Then

$$L[P_r] = L[P] - L[P_0 + \varepsilon \chi_i \frac{\partial P_0}{\partial x_i} + \varepsilon^2 \psi_{\kappa\ell} \frac{\partial^2 P_0}{\partial x_\kappa \partial x_\ell}] =$$

$$= \varepsilon\,(\chi_i \frac{\partial^3 P_0}{\partial x_j^2 \partial x_i} - \lambda \chi_i \frac{\partial P_0}{\partial x_i} + 2 \frac{\partial \psi_{\kappa\ell}}{\partial x_j} \frac{\partial^3 P_0}{\partial x_j \partial x_\kappa \partial x_\ell} -$$

$$- u_i \psi_{\kappa\ell} \frac{\partial^3 P_0}{\partial x_i \partial x_\kappa \partial x_\ell}) + \varepsilon^2(\lambda \psi_{\kappa\ell} \frac{\partial^2 P_0}{\partial x_\kappa \partial x_\ell} +$$

$$+ \psi_{\kappa\ell} \frac{\partial^4 P_0}{\partial x_j^2 \partial x_\kappa \partial x_\ell}) .$$

Hence, for $\underline{u} \in C^1(S)$ and smooth f

$$L[P_r] = \varepsilon h \quad , \quad \sup_{x \in S} |h| \leq c .$$

Also

$$P_r = - \varepsilon \chi_i \frac{\partial P_0}{\partial x_i} - \varepsilon\, \psi_{\kappa\ell} \frac{\partial^2 P_0}{\partial x_\kappa \partial x_\ell} \qquad \text{on} \quad \partial S ,$$

and so we get

$$\sup_{x \in S} |p - P_0| \leq C\, \varepsilon .$$

Notice that due to the singular nature of (A.3) we need $f \in C^4(S)$ to guarantee that the derivatives of P_0 are bounded up to fourth order uniformly in ε .