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## HOMOGENIZATION

AN INTRODUCTION BASED ON REACTIVE POROUS MEDIA  
FLOW MODELS

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# Chapter 1

## Introduction

This is an introduction to homogenization based on reactive porous media flows. The aim is to bridge the gap between the pore scale and the laboratory scale and beyond. In other words, the focus is on the upscaling of models (differential equations) posed in complex domains or involving strongly oscillatory characteristics.

Motivation:

- The main interest is in the averaged/effective behavior of the system and not in the detailed description within each pore (the micro scale).
- The full model involving all features from the pore (micro-) scale to the scale of interest (the core/macro-scale) is generally too complex for being solved in full details.

Typical example: water flow in the soil. Within each pore, the flow is governed by the (Navier-)Stokes system. When averaged to the core scale, the fluid velocity is given by the Darcy law.

Material is inspired from Chapters 1 and 6 of the book *U. Hornung (ed.), Homogenization and porous media, Interdisciplinary Applied Mathematics, 6. Springer-Verlag, New York, 1997*. It is under development, therefore no further particular references are given.

## 1.1 The basic idea

Let  $u$  be a quantity involving rapidly oscillating characteristics. It can be smoothed by *averaging* over a representative elementary volume (*REV*). Its choice is ruled by the following principle: the *REV* is sufficiently large to include all oscillations and to allow for a correct averaging, but at the same time sufficiently small s.t. small spatial translations of the *REV* do not affect the averaged quantity significantly. Given a point  $x$  in the space,  $V(x)$  - the *REV* around it - leads to the averaged quantity

$$\langle u \rangle (x) = \frac{1}{|V(x)|} = \int_{V(x)} u(y)dy, \text{ with } |V(x)| = \int_{V(x)} dy.$$

The first step in the homogenization is to identify and separate the different scales. As an example, in a porous media one can consider  $\ell$  and  $L$  as length scales for the pore, resp the domain of interest. Then introducing

$$\varepsilon = \frac{\ell}{L},$$

the solution including all oscillatory features will depend on the (dimensionless) parameter  $\varepsilon$ :  $u = u^\varepsilon$ . In homogenization one assumes that  $\varepsilon$  is small, and investigates the limit behavior of  $u^\varepsilon$  as  $\varepsilon \searrow 0$ :

$$\bar{u} = \lim_{\varepsilon \searrow 0} u^\varepsilon.$$

Without being specific on the meaning of the limit and on its eventual existence,  $\bar{u}$  is then a good expression of the (averaged) quantity describing the behavior of the process at the macro scale.

**Remark 1.1.1** *In general,  $u^\varepsilon$  and its limit cannot be determined explicitly. Therefore the main focus in the homogenization is to identify the averaged/effective/upscaled equation satisfied by the macro-scale  $\bar{u}$ .*

## 1.2 A one-dimensional example

To illustrate some of the features in the homogenization procedure we consider a simple model problem in one spatial dimension (an elliptic equation). Let  $m, M > 0$  be two

positive numbers and  $a : [0, 1] \rightarrow \mathbb{R}$  be a given function satisfying  $m \leq a(x) \leq M$  for all  $x \in [0, 1]$ . Consider the problem

$$(P) \quad \begin{cases} -\frac{d}{dx} \left( a(x) \frac{d}{dx} u(x) \right) = 0, & \text{for } x \in (0, 1), \\ u(0) = 0, \quad u(1) = 1. \end{cases} \quad (1.1)$$

This equation is a simplified diffusion model. Here  $u$  stands for the concentration of a substance in a medium, and  $a$  for the diffusion. To describe a heterogeneous context, where the diffusion coefficient depends on the location, we assume  $a$  non-constant.

Clearly, one can integrate (1.1)<sub>1</sub> twice and use the boundary condition to determine the explicit solution

$$u(x) = \frac{\int_0^x \frac{1}{a(z)} dz}{\int_0^1 \frac{1}{a(z)} dz}. \quad (1.2)$$

We seek an approximation of the solution of problem (1.1), solving an averaged problem involving no variable quantities. In doing so we adopt an ad-hoc approach having physical motivation. Specifically, we define the *flux*

$$q(x) = -a(x) \frac{d}{dx} u(x), \quad (1.3)$$

and observe that this quantity remains constant over  $(0, 1)$ , as resulting from (1.1)<sub>1</sub>:

$$q(x) = q^*, \quad \text{for all } x \in (0, 1). \quad (1.4)$$

From (1.2) and (1.4) one obtains

$$\frac{d}{dx} u(x) = -\frac{q^*}{a(x)},$$

and, since  $u(0) = 0$ ,

$$u(x) = -q^* \int_0^x \frac{1}{a(z)} dz.$$

To identify the constant flux  $q^*$  one can now use the second boundary condition  $u(1) = 1$  and obtain

$$q^* = -1 \Big/ \int_0^1 \frac{1}{a(z)} dz .$$

From the last two equations we obtain

$$u(x) = \int_0^x \frac{1}{a(z)} dz \Big/ \int_0^1 \frac{1}{a(z)} dz . \quad (1.5)$$

Note that (1.1) involves a variable diffusion coefficient. Although at this point it might seem nothing particular in having variable coefficients, but have in mind that later these variations will be very rapid. Therefore we seek for an approximation  $u^*$  of  $u$ , which solves a simplified, constant coefficient model:

$$(P^*) \quad \begin{cases} -\frac{d}{dx} (a^* \frac{d}{dx} u^*(x)) = 0, & \text{for } x \in (0, 1), \\ u^*(0) = 0, \quad u^*(1) = 1. \end{cases} \quad (1.6)$$

The question here is to find a proper value for the diffusion coefficient  $a^*$ . Once this is obtained,  $u^*$  can be found explicitly by solving (1.6). The "averaged" coefficient  $a^*$  and the corresponding solution  $u^*$  will be named *effective* or *upscaled*. Before doing this we observe that since  $a^*$  is constant, it can be immediately divided out in (1.6)<sub>1</sub>, and the solution is obtained straightforwardly:

$$u^*(x) = x. \quad (1.7)$$

Therefore it might seem unclear why this coefficient plays such an important role. Recall that (1.6) is just a toy model taken to illustrate the idea, and for any extension of the model (i. e. by simply taking a non-zero right hand side) one cannot eliminate the coefficient  $a^*$ .

To find  $a^*$ , a physical concept can be used: since by (1.4) the flux  $q$  in (1.1) is constant, the corresponding quantity in the *averaged* model should have the same value,  $q^*$ . Analogous to (1.3), the flux becomes

$$q^* = -a^* \frac{d}{dx} u^*(x), \quad \text{for all } x \in (0, 1). \quad (1.8)$$

By (1.7), we obtain the effective diffusion

$$a^* = \frac{1}{\int_0^1 \frac{1}{a(z)} dz}. \quad (1.9)$$

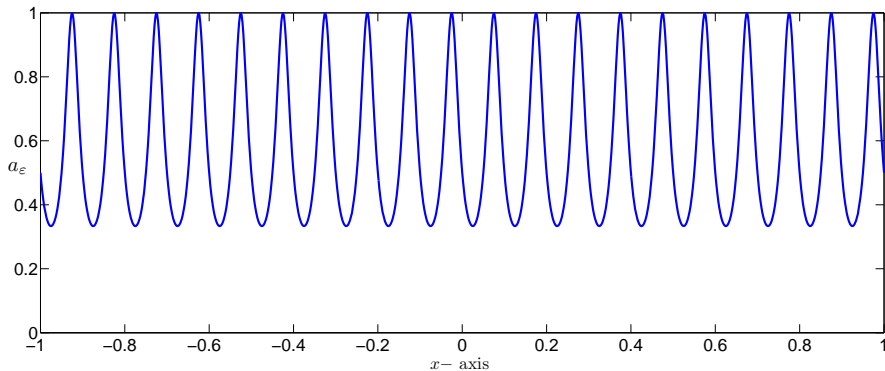


Figure 1.1: A periodic function  $a$

Note that  $a^*$  is the *harmonic mean* over  $(0, 1)$  of the function  $a$ .

The problem (1.1) involves a non-constant coefficient. At the first glance nothing seems to be difficult here: the exact solution can be computed, and a numerical solution can be also easily compute. However, the situation may change when assuming that the diffusion coefficient is rapidly oscillating. Then having a simpler model with constant coefficients makes sense. The natural question appearing here is in how far the simplified model ( $P^*$ ) approximates the original one, ( $P$ ). We will give the answer below, for a situation involving rapid oscillations. In this sense, let  $n \in \mathbb{N}$  be given and define  $\varepsilon = \frac{1}{n}$ . Assume that the function  $a$  introduced above is *1-periodic* (i.e. periodic with period 1):

$$a(y) = a(y + 1) \quad \text{for all } y \in [0, 1).$$

Clearly, by this  $a$  is defined over the entire real axis  $\mathbb{R}$ . Consider now the coefficient function  $a^\varepsilon : \mathbb{R} \rightarrow \mathbb{R}$  defined as

$$a^\varepsilon(x) = a\left(\frac{x}{\varepsilon}\right), \quad \text{for all } x \in \mathbb{R}.$$

Clearly, we have  $a^\varepsilon(x) = a^\varepsilon(x + \varepsilon) = a^\varepsilon(x + 2\varepsilon) = \dots a^\varepsilon(x + k\varepsilon)$  for all  $k \in \mathbb{Z}$ . An example in this sense is presented in Figure 1.2.



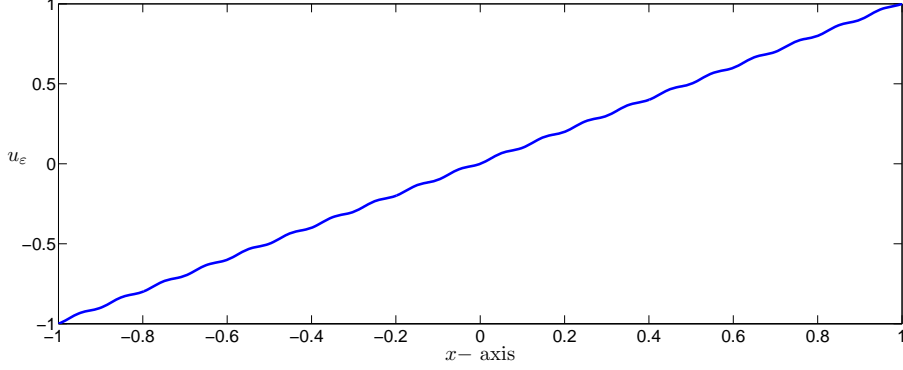


Figure 1.2: The oscillatory solution  $u$

We define the  $\varepsilon$ -dependent problem

$$(P^\varepsilon) \quad \begin{cases} -\frac{d}{dx} \left( a^\varepsilon(x) \frac{d}{dx} u^\varepsilon(x) \right) = 0, & \text{for } x \in (0, 1), \\ u^\varepsilon(0) = 0, \quad u^\varepsilon(1) = 1, \end{cases} \quad (1.10)$$

having  $u^\varepsilon$  as solution. As before, this can be found explicitly:

$$u^\varepsilon(x) = \frac{\int_0^x \frac{1}{a^\varepsilon(z)} dz}{\int_0^1 \frac{1}{a^\varepsilon(z)} dz}. \quad (1.11)$$

Its graph is presented in Figure 1.2

Letting  $k = \left[ \frac{x}{\varepsilon} \right]$  (where  $[\alpha]$  stands for the integer part of the real number  $\alpha$ ), note that a change of variable  $y = \frac{z}{\varepsilon}$ , the definition of  $a^\varepsilon$  and the periodicity of  $a$  give

$$\int_0^x \frac{1}{a^\varepsilon(z)} dz = \int_0^{\frac{x}{\varepsilon}} \frac{\varepsilon}{a(y)} dy = k\varepsilon \int_0^1 \frac{1}{a(y)} dy + \varepsilon \int_k^{\frac{x}{\varepsilon}} \frac{1}{a(y)} dy. \quad (1.12)$$

By this we obtain

$$u^\varepsilon(x) = \frac{\int_0^{\frac{x}{\varepsilon}} \frac{1}{a(y)} dy}{\int_0^1 \frac{1}{a(y)} dy},$$

and for the corresponding effective coefficient

$$a^* = \frac{1}{\int_0^1 \frac{1}{a^\varepsilon(z)} dz} = \frac{1}{\int_0^1 \frac{1}{a(y)} dy}. \quad (1.13)$$

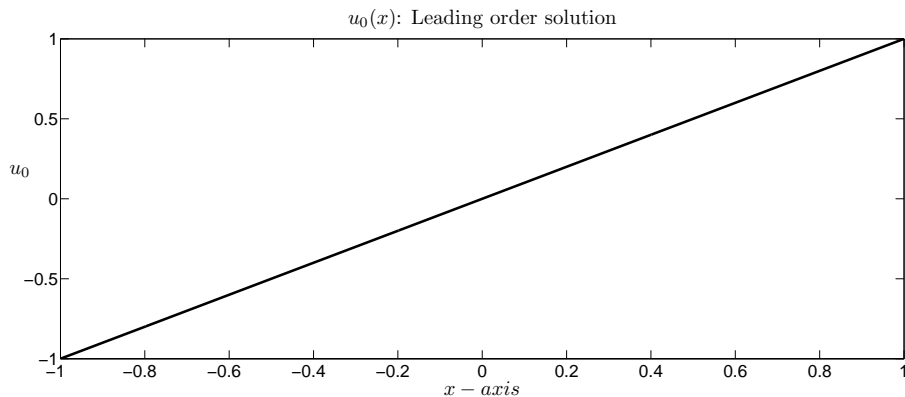


Figure 1.3: The non-oscillatory component  $u$

With this one gets

$$u^\varepsilon(x) = \varepsilon a^* \int_0^{\frac{x}{\varepsilon}} \frac{1}{a(y)} dy = x + \varepsilon \int_0^{\frac{x}{\varepsilon}} \left( \frac{a^*}{a(y)} - 1 \right) dy. \quad (1.14)$$

Recalling the definition of  $u^*$  in (1.7), with

$$u_1(s) = \int_0^s \left( \frac{a^*}{a(y)} - 1 \right) dy,$$

the solution  $u^\varepsilon$  satisfies

$$u^\varepsilon(x) = u^*(x) + \varepsilon u_1\left(\frac{x}{\varepsilon}\right). \quad (1.15)$$

In the above we have identified two parts: the *non-oscillatory* component  $u^*$  and a *first order corrector*  $u_1$  that includes oscillations. Following from the exercises below,  $u_1$  remains bounded (in the order of 1) and hence the total oscillations are of order  $\varepsilon$ . Figures 1.2 and 1.2 display the two solutions  $u^*$  and  $u_1$ . Figure 1.2 gives an idea about how well  $u_0$  approximates the original solution  $u^\varepsilon$ .

**Remark 1.2.1** *In what follows, by  $O(\varepsilon^k)$  we mean the order of  $\varepsilon^k$ , i.e. a quantity behaving like the  $k$ -th power of  $\varepsilon$ . For  $k = 0$  we get terms of order 1.*

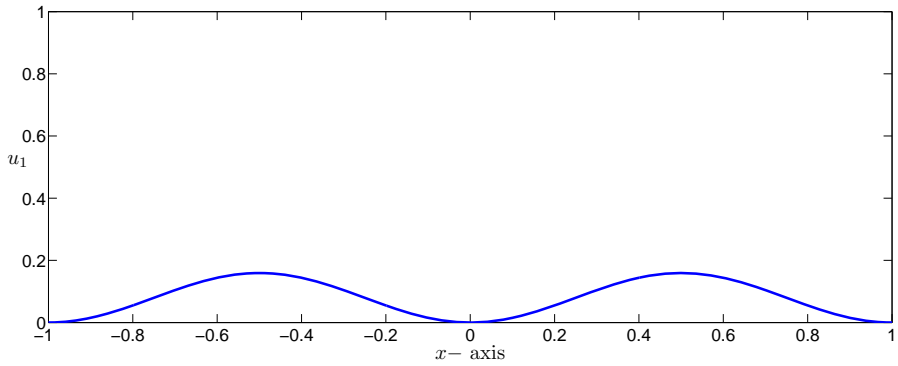


Figure 1.4: The first order corrector  $u_1$

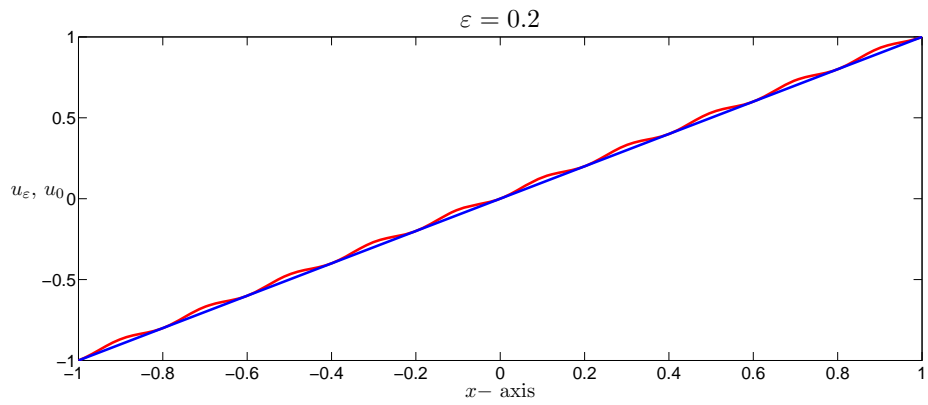


Figure 1.5: The solution  $u^\varepsilon$  and the non-oscillatory approximation  $u_0$

### 1.3 Exercises

1 Derive the calculations for (1.5), (1.12), (1.11). Show that the function  $u_1$  is *uniformly bounded*, i.e. there exist a constant  $C > 0$  such that, for all  $s \in \mathbb{R}$ ,  $|u_1(s)| \leq C$ . Find a uniform estimate for the difference  $|u^\varepsilon - u^*|$ .

2 Let  $n \in \mathbb{N}$  and  $\varepsilon = \frac{1}{n}$ . Let  $F \in \mathbb{R}$  be given and consider the problem

$$\begin{cases} -\frac{d}{dx} \left( a^\varepsilon(x) \frac{d}{dx} u^\varepsilon(x) \right) = 0, & \text{for } x \in (0, 1), \\ u^\varepsilon(0) = 0, \quad -\frac{1}{2} \frac{d}{dx} u^\varepsilon(1) = F, \end{cases}$$

where  $a^\varepsilon(x) = \frac{1}{2 + \sin \frac{2\pi x}{\varepsilon}}$ . Determine the solution  $u^\varepsilon$ , the corresponding effective model, effective solution  $u^*$  and estimate the error of approximating  $u^\varepsilon$  by  $u^*$ .

3 As before let  $\varepsilon = \frac{1}{n}$  and consider the boundary value problem (BVP)

$$(P^\varepsilon) \begin{cases} -u_{xx}^\varepsilon + \frac{1}{\varepsilon} b_\varepsilon(x) u_x^\varepsilon = 0, & x \in (0, 1), \\ u^\varepsilon(0) = 0, & u^\varepsilon(1) = 1, \end{cases}$$

where  $b_\varepsilon(x) = b(x/\varepsilon)$  with  $b - 1$  periodic and  $\int_0^1 b(y) dy = 0$ . Show that, as  $\varepsilon \searrow 0$ ,  $u^\varepsilon$  converges to  $\bar{u}$  solving

$$(P^*) \begin{cases} -a^* u_{xx}^*(x) = 0, & x \in (0, 1), \\ u^*(0) = 0, & u^*(1) = 1. \end{cases}$$

*Note:* The effective equation does not contain first order terms!

# Chapter 2

## The asymptotic expansion method

The example considered in the previous chapter gives an idea about the objectives of the upscaling and homogenization: approximating models involving highly oscillating characteristics by averaged, effective ones. The approach in Chapter 1 method is rather ad-hoc, based on explicit calculations that are tailored to the given example. This chapter presents the basics of a systematic approach, the *asymptotic expansion method*. The method involves formal calculus (derivation) and Taylor expansion, and is presented in connection with the assumption on the periodicity of the oscillating features. Further, it implies the existence of a two scales: a *fast scale* used for the rapidly oscillating characteristics and a *slow scale*, related to the averaged behavior of the system. The details will be given below.

### 2.1 Background

To introduce the method we disregard the modelling details and consider the problem strictly from mathematical point of view, written in dimensionless form. As in Chapter 1 we deal with a diffusion problem, but now posed in a bounded (multi-dimensional) domain  $\Omega \subset \mathbb{R}^d$ , ( $d \geq 1$ ) (the region of interest). Its boundary is denoted by  $\partial\Omega$ . We

consider the problem

$$(P^\varepsilon) \quad \begin{cases} -\nabla \cdot (a^\varepsilon \nabla u^\varepsilon) = f, & \text{for all } x \in \Omega, \\ u^\varepsilon = 0, & \text{on } \partial\Omega. \end{cases} \quad (2.1)$$

As before,  $\varepsilon > 0$  is a small *scale parameter*,  $u^\varepsilon$  can be interpreted as the concentration of a chemical substance,  $f$  a (bulk) reaction term and  $a^\varepsilon$  the diffusion coefficient. Motivated by the heterogeneity of the medium, this coefficient is assumed strongly oscillatory. To become more precise, we introduce the following. With  $Y = [0, 1]^d$  denoting the (closed) *unit cube* and given the constants  $m, M > 0$ , we consider the function  $a : \mathbb{R}^d \rightarrow \mathbb{R}$  satisfying

$$\begin{aligned} 0 < m \leq a(y_1, \dots, y_d) \leq M < \infty, \\ a(y_1, y_2, \dots, y_d) &= a(y_1 + 1, y_2, \dots, y_d) = a(y_1, y_2 + 1, \dots, y_d) \\ &= \dots = a(y_1, y_2, \dots, y_d + 1), \end{aligned} \quad (2.2)$$

for all points  $y = (y_1, \dots, y_d)$  in  $Y$ . Note that the first equation is nothing but the (uniform) boundedness of  $a$ , while the second one is expressing the  $Y$ -*periodicity* of the function  $a$ . Clearly, having defined  $a$  on  $Y$ , by periodicity one automatically extends this function on the entire  $\mathbb{R}^d$ . Having this in mind, we define  $a^\varepsilon$  as

$$a^\varepsilon(x) = a\left(\frac{x}{\varepsilon}\right), \quad \text{for all } x = (x_1, \dots, x_d) \in \Omega, \quad (2.3)$$

(the fraction should be understood componentwise).

Assuming  $\varepsilon$  small, we are interested again in identifying an effective model (and the corresponding equation) which approximates the original problem  $(P^\varepsilon)$  without containing the oscillations. to this end we make use of the *homogenization ansatz*, meaning that  $u^\varepsilon$  can be (formally) written as

$$u^\varepsilon(x) = u_0(x, y) + \varepsilon u_1(x, y) + \varepsilon^2 u_2(x, y) + \dots, \quad (2.4)$$

where the vector  $y$  is defined as  $y = \frac{x}{\varepsilon}$ , while the functions  $u_k$  are  $Y$ -periodic w.r.t. the second argument  $y$  (see also (2.2)). Further, all functions  $u_k$  are assumed to have an order of magnitude that does not depend on  $\varepsilon$ .

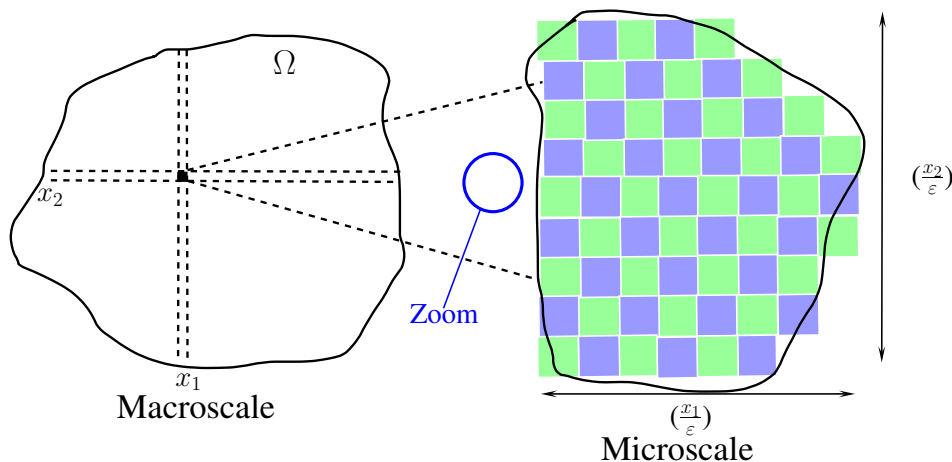


Figure 2.1: A medium involving two scales

Such an assumption deserves some explanations. First, we have separated  $u_0$ , the *macroscopic* part of  $u^\varepsilon$ , which has the order of magnitude 1. Without making this statement rigorous, in a limit process one can view  $u_0$  as

$$u_0 = \lim_{\varepsilon \searrow 0} u^\varepsilon.$$

Having identified  $u_0$ , the remainder  $u^\varepsilon - u_0$  is of order  $\varepsilon$ . In analogy to  $u_0$ ,  $u_1$  can be seen as

$$u_1 = \lim_{\varepsilon \searrow 0} \frac{1}{\varepsilon} (u^\varepsilon - u_0),$$

and the procedure can continue further with  $u_2$ , etc.

Second, note that each of the  $u_k$ 's depend on two variables:  $x$ -the *slow* one, and  $y$ -the *fast* one. However, as  $y = \frac{x}{\varepsilon}$ , all functions depend in fact on one variable. To explain this we refer to Figure 2.1 and imagine that behind each "macroscopic" point located at  $x$ , a whole "microscopic" world can be found, including the oscillatory characteristics. This micro-structure cannot be seen from the macro scale, it requires a zoomed out view. Then the oscillations inside the micro structure are described by the fast variable  $y$ , while the location of the microstructure inside the macro system is at  $x$ . For the slow variable one has  $x \in \Omega$ , so it remains bounded. At the first instance, this also means that as  $\varepsilon$

approaches 0, the fast variable  $y$  blows up. However, one should consider the situation differently: the rapidly oscillating characteristics are encountered at the micro-scale (thus within an  $O(\varepsilon)$  range). To capture this at the macro-scale ( $O(1)$ ) one uses a zoomed-out (fast) variable  $y = x/\varepsilon$ , which transfers the rapid oscillations at the ( $O(1)$ ) scale, whereas the slow variations are still described by the slow variable  $x$ . Therefore  $y$  remains within a bounded domain, which is here denoted by  $Y$ . By rescaling (an example in this sense being given in Chapter 6),  $Y$  becomes the unit cube  $(0, 1)^d$ .

Periodicity (in the sense of (2.2)) is assumed only with respect to  $y$ , so it appears only at the micro-scale level and does not lead to periodic macro-structures. Moreover, the assumption on periodicity is made only for the ease of presentation. Similar results can be obtained, for example, in the case of randomness.

**Remark 2.1.1** *In (1.15) we have separated the scales explicitly; compared to the asymptotic expansion ansatz (2.4) we get  $u_0(x, y) = x$  and  $u_1(x, y) = \int_0^y \left( \frac{a^*}{a(z)} - 1 \right) dz$ . Note that  $u_0$  does not depend on the fast variable  $y$ , while  $u_1$  only depend on  $y$ . What are the other functions  $u_k$  in this case?*

## 2.2 The Diffusion problem

In this part we study the model problem  $(P^\varepsilon)$  introduced in the previous paragraph,

$$(P^\varepsilon) \quad \begin{cases} -\nabla \cdot (a^\varepsilon \nabla u^\varepsilon) = f, & \text{for all } x \in \Omega, \\ u^\varepsilon = 0, & \text{on } \partial\Omega, \end{cases} \quad (2.5)$$

with  $\Omega \subset \mathbb{R}^d, (d \geq 1)$  being a  $d$ -dimensional domain. As before, we assume that the diffusion coefficient is a strongly oscillatory function (compare to (2.2) and (2.3)). To determine an effective model approximating  $(P^\varepsilon)$  we make use of the asymptotic expansion method. Specifically, we expand  $u^\varepsilon$  as in (2.4) and equate in the resulting the terms of the same order. But before doing so we recall the assumption relating the fast and the slow variable. In this case, for any function  $u = u(x, y)$ , if  $y = \frac{x}{\varepsilon}$ , then in fact



we deal with a different function  $\tilde{u}(x) = u(x, \frac{x}{\varepsilon})$  and the partial derivatives have to be changed accordingly. With  $x = (x_1, \dots, x_d)$ , and  $y = (y_1, \dots, y_d)$  satisfying  $y_i = \frac{x_i}{\varepsilon}$  for all  $i = 1, \dots, d$ , by the chain rule we have

$$\frac{\partial \tilde{u}}{\partial x_i}(x) = \frac{du}{dx_i}\left(x, \frac{x}{\varepsilon}\right) = \frac{\partial u}{\partial x_i}(x, y) + \frac{\partial y_i}{\partial x_i} \frac{\partial u}{\partial y_i}(x, y) = \frac{\partial u}{\partial x_i}(x, y) + \frac{1}{\varepsilon} \frac{\partial u}{\partial y_i}(x, y). \quad (2.6)$$

By this we have separated the derivatives w.r.t. the slow, respectively fast variables. In this way one can formally replace the gradient by the linear combination of two gradients, one in  $x$  and the other in  $y$ ,

$$\nabla = \nabla_x + \frac{1}{\varepsilon} \nabla_y, \quad (2.7)$$

where the indices denote the the variable w.r.t. which the partial derivatives are computed. Clearly, the divergence behaves similarly.

Using (2.4) and the above into the first equation of (2.5), since  $a^\varepsilon(x) = a(\frac{x}{\varepsilon}) = a(y)$  for a  $Y$ -periodic function  $a$  we obtain

$$\begin{aligned} -(\nabla_x + \frac{1}{\varepsilon} \nabla_y) \cdot [a(y) (\nabla_x + \frac{1}{\varepsilon} \nabla_y) (u_0(x, y) \\ + \varepsilon u_1(x, y) + \varepsilon^2 u_2(x, y) + \dots)] = f. \end{aligned} \quad (2.8)$$

We can now group the terms having the same order of magnitude:

$$\begin{aligned} & -\frac{1}{\varepsilon^2} \nabla_y \cdot (a(y) \nabla_y u_0(x, y)) \\ & -\frac{1}{\varepsilon} \{ \nabla_x \cdot [a(y) \nabla_y u_0(x, y)] + \nabla_y \cdot [a(y) (\nabla_x u_0(x, y) + \nabla_y u_1(x, y))] \} \\ & - \{ \nabla_x \cdot [a(y) (\nabla_x u_0(x, y) + \nabla_y u_1(x, y))] \\ & \quad + \nabla_y \cdot [a(y) (\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] \} \\ & -O(\varepsilon) = f. \end{aligned} \quad (2.9)$$

### 2.2.1 The $\varepsilon^{-2}$ problem

Having assumed the smallness of  $\varepsilon$ , i.e.  $1 \gg \varepsilon \gg \varepsilon^2 \gg \dots$  (which means essentially that the scales are well separated), we can equate the terms w.r.t.  $\varepsilon$  and obtain the

problems corresponding to each of the orders of magnitude. The idea behind this is justified by the following argument. Multiplying (2.9) by  $\varepsilon^2$  we get

$$-\nabla_y \cdot (a(y)\nabla_y u_0(x, y)) + O(\varepsilon) = O(\varepsilon^2).$$

This equality holds for all  $y \in Y$ . For small values of  $\varepsilon$  (or as  $\varepsilon \searrow 0$ ) we have obtained in fact the  $\varepsilon^{-2}$  problem

$$(P^{-2})(x) \quad \begin{cases} -\nabla_y \cdot (a(y)\nabla_y u_0(x, y)) = 0, & \text{for all } y \in Y, \\ u_0(x, y) \text{ is } Y\text{-periodic.} \end{cases} \quad (2.10)$$

Problem  $P^{-2}(x)$  is defined in the microscopic domain  $Y$ , but for each macroscopic point  $x \in \Omega$ . Moreover, if the diffusion coefficient (function)  $a^\varepsilon$  would have been taken in such a way that  $a^\varepsilon(x) = a(x, \frac{x}{\varepsilon})$ , where  $a : \mathbb{R}^d \times Y \rightarrow \mathbb{R}$  is  $Y$ -periodic for any fixed  $x$ , then for each  $x \in \Omega$  the problem  $P^{-2}(x)$  would involve the function  $a(x, y)$  and it would therefore depend explicitly on  $x$ . To emphasize this we include an  $x$ -dependency in the label  $P^{-2}$ . Obviously, a function  $u_0 = u_0(x)$  (thus constant w.r.t.  $y$ ) is a solution to this problem. Mathematical arguments show that no other kind of solutions is possible (see also the exercises below). We therefore get

$$u_0(x, y) = u_0(x) \quad \text{and} \quad \nabla_y u_0(x, y) = 0 \quad \text{for all } y \in Y. \quad (2.11)$$

This gives precious information over  $u_0$  appearing in the homgenization ansatz (2.4). As  $u_0$  is  $O(1)$ , it can be interpreted as the macro-scale component of  $u^\varepsilon$ , since one has

$$u^\varepsilon(x) = u_0(x) + O(\varepsilon).$$

However, this is not enough to determine  $u_0$ , or an equation that is solved by this function. Therefore we proceed by analyzing the remaining terms in (2.9).

### 2.2.2 The $\varepsilon^{-1}$ problem

Knowing the above, the first line in (2.9) vanishes (as it is equally 0). Multiplying the remaining by  $\varepsilon$  and reasoning as above, for small values of  $\varepsilon$  we obtain the  $\varepsilon^{-1}$  problem

in the unknown  $u_1$

$$(P^{-1})(x) \begin{cases} -\nabla_y \cdot (a(y)\nabla_y u_1(x, y)) = \nabla_y \cdot (a(y)\nabla_x u_0(x)), \\ \text{for all } y \in Y, \\ u_1(x, y) \text{ is } Y\text{-periodic.} \end{cases} \quad (2.12)$$

The dependence of this problem on the macro-scale variable  $x$  is now implicit, through  $u_0$ . Further, we observe that if  $u_0$  would be a known function, the solution  $u_1$  could be obtained by solving Problem  $P^{-1}(x)$ . In fact we can determine  $u_1$  as a function of  $u_0$  itself, eliminating it in this way  $u_1$  from the system. Specifically, with  $\vec{e}_j = (0, \dots, 0, 1, 0, \dots, 0)$  being the unit vector in the  $j^{\text{th}}$  direction ( $j = 1, \dots, d$ ) we start by observing that

$$\nabla_x u_0(x) = \sum_{j=1}^d \vec{e}_j \partial_{x_j} u_0(x). \quad (2.13)$$

Since Problem  $P^{-1}(x)$  is linear, one can find the solution  $u_1$  as a linear combination involving the solutions of some *cell problems* similar to (2.12), but where  $\vec{e}_j$  replaces  $\nabla_x u_0$ . To be exact, for all  $j = 1, \dots, d$  we consider

$$(P_j^{-1})(x) \begin{cases} -\nabla_y \cdot (a(y)\nabla_y w^j(x, y)) = \nabla_y \cdot (a(y) \vec{e}_j), \\ \text{for all } y \in Y, \\ w^j(x, y) \text{ is } Y\text{-periodic.} \end{cases} \quad (2.14)$$

**Remark 2.2.1** Clearly, having found a solution  $w^j$ , then for all constant  $C \in \mathbb{R}$  (in fact  $C$  might even change from one  $x$  to another, thus can be seen as a function of  $x$ ) the function  $\tilde{w}^j(x, y) = w^j(x, y) + h(x)$  is still a solution of (2.14). So as for  $P^{-2}$ , each of the cell problems  $P_j^{-1}(x)$  have a solution  $w^j$  that is unique up to addition of a function depending only on  $x$  (thus constant w.r.t.  $y$ ). To identify the solution  $w^j$  uniquely we assume also that  $w^j$  has the average 0 over  $Y$ ,

$$\int_Y w^j(x, y) dy = 0, \quad \text{for all } x \in \Omega.$$

From now on by the solution of the cell problems we will understand the function  $w^j$  solving (2.14) and having the average 0.

Having found the functions  $w^j$  for all  $j = 1, \dots, d$ , the solution  $u_1$  of Problem  $P^{-1}(x)$  can be expressed as

$$u_1(x, y) = \tilde{u}_1(x) + \sum_{j=1}^d w^j(x, y) \partial_{x_j} u_0(x), \quad (2.15)$$

with  $\tilde{u}_1(x)$  being an arbitrary function of  $x$  (thus constant in  $y$ ) that can be chosen for convenience. In fact, as we will see below, in this case  $\tilde{u}_1$  plays no role. It is easy to check that  $u_1$  defined above solves Problem  $P^{-1}(x)$  for any  $x \in \Omega$ .

Note that by this one can get a better estimate of the original unknown  $u^\varepsilon$ , since

$$u^\varepsilon(x) = u_0(x) + \varepsilon u_1(x, y) + O(\varepsilon^2).$$

However, one still has to find  $u_0$ , which immediately provides  $u_1$  by (2.15). This is the step in the next.

### 2.2.3 The $\varepsilon^0$ problem

As before, we can now eliminate the second line in (2.9) (as it is equally 0) and equate the  $O(1)$  terms to obtain the  $\varepsilon^{-2}$  problem in the unknown  $u_2$

$$(P^0)(x) \begin{cases} -\nabla_x \cdot [a(y)(\nabla_x u_0(x) + \nabla_y u_1(x, y))] \\ \quad -\nabla_y \cdot [a(y)(\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] = f, \\ \text{for all } y \in Y, \\ u_2(x, y) \text{ is } Y\text{-periodic.} \end{cases} \quad (2.16)$$

Since now we have expressed  $u_1$  in terms of  $u_0$  explicitly, it is possible to proceed as before and determine the solution  $u_2$ , depending on  $u_0$ . Carrying out such a step would improve the accuracy of the upscaling procedure we consider here (and is indeed performed for problems where the scales cannot be properly separated, i.e.  $\varepsilon$  is not sufficiently small). Again, by (2.4),

$$u^\varepsilon(x) = u_0(x) + \varepsilon u_1(x, y) + \varepsilon^2 u_2(x, y) + O(\varepsilon^3),$$

which means we have a very good approximation of  $u_0$ . However, this does not provide any further information on the quantity of primary interest, the function  $u_0$ , which is still unknown. Instead, we proceed by eliminating  $u_2$  out of (2.16) and seek for an equation for  $u_0$ . If this is found, one immediately obtains  $u_1$  and proceed by finding  $u_2$  if needed.

To determine the equation for  $u_0$  we average (integrate) (2.16) over  $Y$  and obtain

$$\begin{aligned} & -\nabla_x \cdot \left[ \int_Y a(y) (\nabla_x u_0(x) + \nabla_y u_1(x, y)) dy \right] \\ & - \int_Y \nabla_y \cdot [a(y) (\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] dy = f(x), \end{aligned} \quad (2.17)$$

for all  $x \in \Omega$ . Here we have used the fact that  $Y$  has volume 1, i.e.  $\int_Y dy = 1$ . By Gauß theorem, the last integral on the left of (2.17) becomes

$$\begin{aligned} & \int_Y \nabla_y \cdot [a(y) (\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] dy \\ & = \int_{\partial Y} \vec{\nu} \cdot [a(y) (\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] d\sigma_y, \end{aligned} \quad (2.18)$$

where  $d\sigma_y$  is the area element over  $\partial Y$ , the boundary of the unit cell  $Y$ , and  $\vec{\nu}$  the unit normal to  $\partial Y$  pointing outwards to  $Y$ .

We proceed now by analyzing the boundary integral in the above. Restricting to the case  $d = 2$  (the argument being absolutely the same for other spatial dimensions), then any point  $y \in Y$  has two components  $y = (y_1, y_2)$  and we see that  $\partial Y$  is the unit square and contains four segments:  $\partial Y_1 = \{(y_1, 0), y_1 \in (0, 1)\}$ ,  $\partial Y_2 = \{(0, y_2), y_2 \in (0, 1)\}$ ,  $\partial Y_3 = \{(y_1, 1), y_1 \in (0, 1)\}$ , and  $\partial Y_4 = \{(1, y_2), y_2 \in (0, 1)\}$ . The corresponding unit normals are  $\vec{\nu}_1 = (0, -1)$ ,  $\vec{\nu}_2 = (-1, 0)$ ,  $\vec{\nu}_3 = (0, 1)$ , and  $\vec{\nu}_4 = (1, 0)$ , thus  $\vec{\nu}_1 = -\vec{\nu}_3$  and  $\vec{\nu}_2 = -\vec{\nu}_4$ . We refer to Figure 2.2.3 for the situation described here.

The term on the right in (2.18) is decomposed into

$$\begin{aligned} & \int_{\partial Y} \vec{\nu} \cdot [a(y) (\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] d\sigma_y \\ & = \sum_{k=1}^4 \int_{\partial Y_k} \vec{\nu}_k \cdot [a(y) (\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] d\sigma_y. \end{aligned}$$

Recalling that  $u_1$  and  $u_2$  are assumed periodic in  $Y$ , so the same holds for their gradients  $\nabla_x u_1$  and  $\nabla_y u_2$ . Together with the  $Y$ -periodicity of  $a$ , for all  $y_1 \in (0, 1)$  we have

$$\begin{aligned} & \vec{\nu}_1 \cdot [a(y_1, 0) (\nabla_x u_1(x, (y_1, 0)) + \nabla_y u_2(x, (y_1, 0)))] \\ & = -\vec{\nu}_3 \cdot [a(y_1, 1) (\nabla_x u_1(x, (y_1, 1)) + \nabla_y u_2(x, (y_1, 1)))] \end{aligned}$$

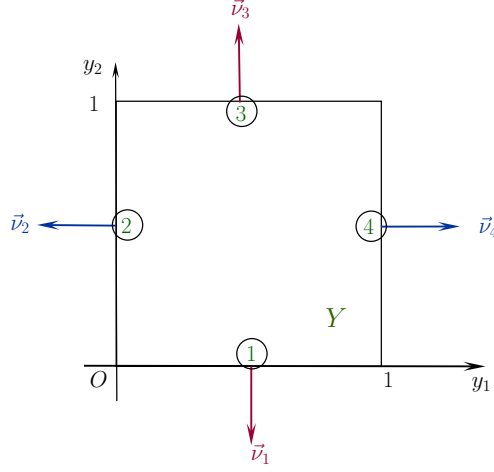


Figure 2.2: The boundaries of the unit square and the corresponding unit normals

where instead of the vector argument  $y$  along  $\partial Y_1$  or  $\partial Y_3$  we use either  $(y_1, 0)$  or  $(y_1, 1)$ . Therefore the arguments in the boundary integrals over  $\partial Y_1$  and  $\partial Y_3$  are equal in absolute value, but of opposite signs. This immediately implies that

$$\begin{aligned} & \int_{\partial Y_1} \vec{v}_1 \cdot [a(y)(\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] d\sigma_y \\ & + \int_{\partial Y_3} \vec{v}_3 \cdot [a(y)(\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] d\sigma_y = 0. \end{aligned}$$

In a similar manner one can show that the integrals along  $\partial Y_2$  and  $\partial Y_4$  add up to 0, implying that

$$\int_Y \nabla_y \cdot [a(y)(\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] dy = 0,$$

so the last integral on the left in (2.17) vanishes.

To deal with the first integral in (2.17) we make use of (2.15) and obtain

$$\nabla_y u_1(x, y) = \sum_{j=1}^d \partial_{x_j} u_0(x) \nabla_y w^j(x, y),$$

leading to

$$-\nabla_x \cdot \left[ \int_Y a(y) \left( \nabla_x u_0(x) + \sum_{j=1}^d \partial_{x_j} u_0(x) \nabla_y w^j(x, y) \right) dy \right] = f(x).$$

This can be rewritten as

$$-\sum_{i=1}^d \left[ \partial_{x_i} \sum_{j=1}^d \left( \int_Y a(y) (\delta_{ij} + \partial_{y_i} w^j(x, y)) dy \right) \partial_{x_j} u_0(x) \right] = f(x),$$

where  $\delta_{ij} = 1$  if  $i = j$  and  $\delta_{ij} = 0$  if  $i \neq j$ . Recalling the boundary conditions in (2.5), we rewrite the above in a compact form to conclude that the effective (upscaled) approximation of  $u^\varepsilon$  is  $U(x) = u_0(x)$  is solving

$$(P) \quad \begin{cases} -\nabla \cdot (A^* \nabla U) = f, & \text{for all } x \in \Omega, \\ U = 0, & \text{on } \partial\Omega, \end{cases} \quad (2.19)$$

where the matrix-valued function  $A^* : \Omega \rightarrow \mathbb{R}^{d \times d}$  has the elements

$$\begin{aligned} a_{ij}^* : \Omega &\rightarrow \mathbb{R}, \quad (i, j = 1, \dots, d) \\ a_{ij}^*(x) &= \int_Y a(y) (\delta_{ij} + \partial_{y_i} w^j(x, y)) dy. \end{aligned} \quad (2.20)$$

**Remark 2.2.2** *The  $x$ -dependency in the coefficients  $a_{ij}$  appear only through the solutions  $w^j$  of the cell problems  $P_j^{-1}$ . However, since the function  $a$  defining  $a^\varepsilon$  depends only on the fast scale variable  $y$ , the same holds for  $w^j$  and therefore the coefficients  $a_{ij}^*$  in (2.20) are constant. The situation would change if, for example, one has  $a^\varepsilon(x) = a(x, \frac{x}{\varepsilon})$ , thus when  $a$  depends on both  $x$  and  $y$  (remaining  $Y$ -periodic in  $y$  for every  $x$ ).*

We started with the problem  $P^\varepsilon$ , involving a highly oscillatory but scalar diffusion coefficient. The homogenization procedure explained above leads to the upscaled problem  $P$ , with a diffusion tensor  $A^*$  that may be non-isotropic. The matrix  $A^*$  contains no oscillations (in fact it is even constant here), giving an effective model that is much easier to solve. The micro-scale oscillations in the original model are reflected at the macro-scale through the fact that the effective diffusion is not simply the average of the original ones,  $\int_Y a(y) dy$ , but includes the additional (non-diagonal) terms  $\int_Y \partial_{y_i} w^j(x, y) dy$ . For the effective diffusion matrix one has the following

**Lemma 2.2.1** *Let  $a$  fulfill the conditions in (2.2) and  $A^*$  be the effective diffusion tensor in (2.20). It holds*

- a)  $A^*$  is symmetric, i.e.  $a_{ij}^* = a_{ji}^*$  for all  $i, j = 1, \dots, d$ .
- b)  $A^*$  is positive definite, i.e. there exist a constant  $C > 0$  s.t. for all (column vectors)  $z \in \mathbb{R}^d$ ,  $z^T(A^*z) \geq C(z^Tz)$ .

## 2.3 Exercises

- 1 Apply the asymptotic expansion method to derive the upscaled equation corresponding to the one dimensional situation given in (1.10).
- 2 With  $a$  introduced in (2.2), but for the two-dimensional case ( $d = 2$ ) consider a *layered medium*, where the function  $a$  depends only on (say) the second component of  $y = (y_1, y_2)$ :  $a(y) = a(y_2)$ . Show that the effective matrix is diagonal (i.e.  $a_{ij}^* = 0$  whenever  $i \neq j$ ), and determine (explicitly, depending on  $a$ ) the elements of  $A$  on the main diagonal.
- 3 Redo the calculations in Section 2.2, but considering now a more general situation where (compare with (2.2)) the function  $a : \Omega \times \mathbb{R}^d \rightarrow \mathbb{R}$  depends on two vector variables,  $x$  and  $y$ , and for all  $x = (x_1, \dots, x_d) \in \Omega$  and  $y = (y_1, \dots, y_d) \in Y$  it satisfies

$$\begin{aligned}
 0 < m &\leq a(x_1, \dots, x_d, y_1, \dots, y_d) \leq M < \infty, \\
 a(x_1, \dots, x_d, y_1, \dots, y_d) &= a(x_1, \dots, x_d, y_1 + 1, \dots, y_d) \\
 &= \dots = a(x_1, \dots, x_d, y_1, \dots, y_d + 1),
 \end{aligned}$$

and  $a^\varepsilon$  is defined as  $a^\varepsilon(x) = a(x, \frac{x}{\varepsilon})$  for all  $x = (x_1, \dots, x_d) \in \Omega$ .

- 4 Prove Lemma 2.2.1.
- 5 Show that the only possible solutions to Problem (2.10) are functions not depending on  $y$ .



# Chapter 3

## Diffusion in perforated domains

In Chapter 2 we considered the case when the diffusion was strongly oscillatory. The domain instead was fairly standard. In this chapter we consider a problem where the highly oscillatory characteristics are due to the domain, which is assumed complex. Specifically, we consider a domain including periodic perforations. These are small (of order  $\varepsilon$ ), but located within "elementary cells" that are of the same order. Therefore we deal with a domain including small, but many perforations. A typical example in this sense is the reactive fluid transport through porous media (such as soils). At the pore scale, such a medium consists of solid grains surrounded by void spaces (the pores). We assume that all pores are filled by a fluid (water) containing dissolved components (solute). The solute may be redistributed within water by diffusion. For the ease of presentation we only focus on the stationary diffusion process, but later we extend the approach to more realistic situations.

In the specific situation mentioned above, the pores are at the micro scale. The flow domain is strictly the union of all pores (the void space). No flow is encountered inside grains, thus these can be viewed as perforations of the domain. We apply the techniques in Chapter 2 to derive an effective, homogenized model that is valid at the laboratory scale, and defined on the entire domain, including the locations where originally perforations (solid grains) were encountered.

### 3.1 The complex domain

We consider a bounded (multi-dimensional) domain  $\Omega \subset \mathbb{R}^d$ , ( $d \geq 1$ ) (the total region of interest). This includes the perforations as well. Its (outer) boundary is denoted by  $\partial\Omega$ . As mentioned before, this domain includes perforations. We assume that the domain is a finite union of  $\varepsilon$ -sized cubes ( $\varepsilon$  being again a small positive parameter). To be specific, with  $Y = (0, 1)^d$  we let  $\vec{k} = (k_1, \dots, k_d) \in \mathbb{Z}^d$  be a vector of integers. For a given set  $Z \subset \mathbb{R}^d$ , consider

$$Z_{\vec{k}} = \left\{ x + \vec{k}/x \in Z \right\}, \quad \text{and} \quad \varepsilon Z = \{ \varepsilon x / x \in Z \}. \quad (3.1)$$

Given the parameter  $\varepsilon$ , we assume that

$$\bar{\Omega} = \cup \left\{ \varepsilon(\vec{k} + \bar{Y})/\vec{k} \in \mathcal{K}_\varepsilon \right\} \quad (3.2)$$

for some set of vector indices  $\mathcal{K}_\varepsilon$ . For an open set  $Z$ , by  $\bar{Z}$  we mean here the union of  $Z$  and its boundary  $\partial Z$ .

To describe the complex geometry we first consider the unit cube  $Y$  and assume it is separated into two sub-domains: the "inner" grain  $\mathcal{G}$  surrounded by the pore  $\mathcal{P}$ . With  $\Gamma$  being the boundary of  $\mathcal{G}$ , we have

$$Y = \mathcal{P} \cup \mathcal{G} \cup \Gamma.$$

This defines a typical elementary cell at the micro scale, in a zoomed view. In view of (3.2), this allows defining

$$\Omega^\varepsilon = \cup \left\{ \varepsilon(\vec{k} + \mathcal{P})/\vec{k} \in \mathcal{K}_\varepsilon \right\}, \quad (3.3)$$

which can be seen as the total pore space in the porous medium  $\Omega$ . As announced before, we consider the diffusion problem in the complex/perforated domain  $\Omega^\varepsilon$ . For this domain we identify two kinds of boundaries: the *outer* boundary  $\partial\Omega$ , coinciding with the boundary of the entire medium, and the *inner* boundary

$$\Gamma^\varepsilon = \cup \left\{ \varepsilon(\vec{k} + \Gamma)/\vec{k} \in \mathcal{K}_\varepsilon \right\}, \quad (3.4)$$

which is nothing but the total grain surface (the pore walls). The situation is sketched in Figure 3.1.

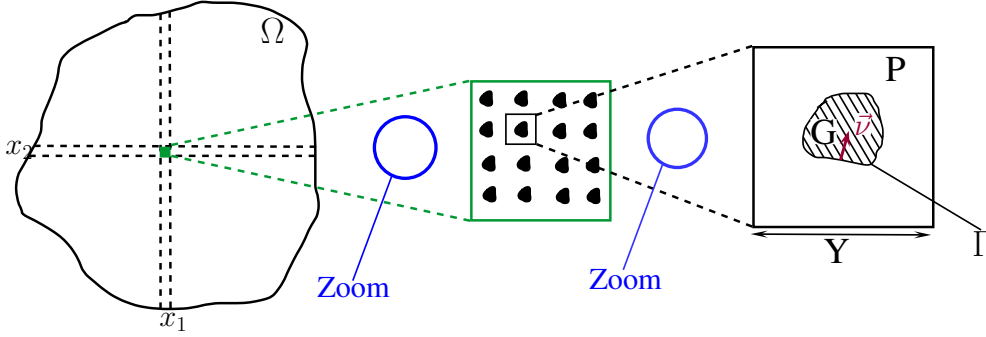


Figure 3.1: Different scales in a perforated medium

## 3.2 The diffusion problem

Assuming that the grains are impervious to the fluid and no adsorption or desorption processes are encountered at the grain surfaces, we consider the following problem

$$(P^\varepsilon) \begin{cases} -\nabla \cdot (A^\varepsilon \nabla u^\varepsilon) = f, & \text{in } \Omega^\varepsilon, \\ -\vec{\nu} \cdot (A^\varepsilon(x) \nabla u^\varepsilon) = 0, & \text{on } \Gamma^\varepsilon, \\ u^\varepsilon = 0, & \text{on } \partial\Omega. \end{cases} \quad (3.5)$$

Note that, since  $\Omega^\varepsilon$  is perforated and thus has inner boundaries, one has to impose boundary conditions there as well. With  $\vec{\nu}$  being the unit normal to  $\Gamma^\varepsilon$  pointing *into* the grains, the condition at the inner boundary means that there is no (normal) flow into the grains.

As before, we let  $\varepsilon > 0$  be a small parameter and  $A^\varepsilon$  be the diffusion matrix, which is assumed strongly oscillatory. More precisely, we consider a *matrix-valued* function  $A : \Omega \times \mathbb{R}^d \rightarrow \mathbb{R}^{d \times d}$  depending on the vector variables  $x$  and  $y$ , and for all  $x = (x_1, \dots, x_d) \in \Omega$  and  $y = (y_1, \dots, y_d) \in Y$  it satisfies

$$\begin{aligned} 0 < m \leq A(x_1, \dots, x_d, y_1, \dots, y_d) \leq M < \infty, \\ A(x_1, \dots, x_d, y_1, \dots, y_d) &= A(x_1, \dots, x_d, y_1 + 1, \dots, y_d) \\ &= \dots = A(x_1, \dots, x_d, y_1, \dots, y_d + 1). \end{aligned} \quad (3.6)$$

Again,  $A^\varepsilon$  is defined by  $A^\varepsilon(x) = A(x, \frac{x}{\varepsilon})$  for all  $x = (x_1, \dots, x_d) \in \Omega$ . For simplicity we define  $A$  over the entire unit cell  $Y$ , whereas our interest is in the void space  $\mathcal{P}$ . Note

that now the diffusion tensor has variations in both micro- and macro scales, expressed through the explicit dependence on  $y = \frac{x}{\varepsilon}$  and on  $x$ .

When compared to the situation in Chapter 2, note that the domain includes now small but many perforations. Due to this, an internal boundary has to be taken into account:  $\Gamma^\varepsilon$  - the boundary of the perforations. Furthermore, since  $A$  includes both macro- and micro-scale variations, the resulting cell problems (see (2.14)) are  $x$ -dependent. For finding an upscaled model we proceed as in Chapter 2, and recall that  $x$  and  $y = \frac{x}{\varepsilon}$  provide the separation of the original  $x$  into slow and fast variables, implying that any partial derivative is rewritten as

$$\frac{\partial}{\partial x_i} = \frac{\partial}{\partial x_i} + \frac{1}{\varepsilon} \frac{\partial}{\partial y_i}, \quad \text{for all } i = 1, \dots, d, \quad (3.7)$$

as well as the homogenization ansatz

$$u^\varepsilon(x) = u_0(x, y) + \varepsilon u_1(x, y) + \varepsilon^2 u_2(x, y) + \dots, \quad (3.8)$$

where the functions  $u_k$  are  $Y$ -periodic w.r.t. the second argument  $y$ .

As in Section 2.2, we use (3.7) and (3.8) into (3.5) and group together the terms having the same order of magnitude. For the first equation, we obtain

$$\begin{aligned} & -\frac{1}{\varepsilon^2} \nabla_y \cdot (A(x, y) \nabla_y u_0(x, y)) \\ & -\frac{1}{\varepsilon} \{ \nabla_x \cdot [A(x, y) \nabla_y u_0(x, y)] \\ & \quad + \nabla_y \cdot [A(x, y) (\nabla_x u_0(x, y) + \nabla_y u_1(x, y))] \} \\ & - \{ \nabla_x \cdot [A(x, y) (\nabla_x u_0(x, y) + \nabla_y u_1(x, y))] \\ & \quad + \nabla_y \cdot [A(x, y) (\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] \} \\ & -O(\varepsilon) = f. \end{aligned} \quad (3.9)$$

Due to the presence of perforations, the problem under consideration involves an *internal* boundary condition. In a similar fashion on  $\Gamma^\varepsilon$  one has

$$-\vec{\nu} \cdot \left( A(x, y) \left( \nabla_x + \frac{1}{\varepsilon} \nabla_y \right) (u_0(x, y) + \varepsilon u_1(x, y) + \varepsilon^2 u_2(x, y) + \dots) \right) = 0,$$

implying

$$\begin{aligned}
& -\frac{1}{\varepsilon} \left\{ \vec{\nu} \cdot (A(x, y) \nabla_y u_0(x, y)) \right\} - \left\{ \vec{\nu} \cdot (A(x, y) (\nabla_x u_0(x, y) + \nabla_y u_1(x, y))) \right\} \\
& -\varepsilon \left\{ \vec{\nu} \cdot (A(x, y) (\nabla_x u_1(x, y) + \nabla_y u_2(x, y))) \right\} + O(\varepsilon^2) = 0.
\end{aligned} \tag{3.10}$$

As before, we equate terms of similar orders of magnitude in both the equation (3.9) and the boundary condition (3.10) to find more information about  $u_0$ ,  $u_1$ , etc.

### 3.2.1 The $\varepsilon^{-2}$ problem and the $\varepsilon^{-1}$ boundary condition

For small values of  $\varepsilon$  (or as  $\varepsilon \searrow 0$ ),  $O(\varepsilon^{-2})$  terms in (3.9) and the  $O(\varepsilon^{-1})$  terms in (3.10) give

$$(P^{-2})(x) \begin{cases} -\nabla_y \cdot (A(x, y) \nabla_y u_0(x, y)) = 0, & \text{for all } y \in \mathcal{P}, \\ -\vec{\nu} \cdot (A(x, y) \nabla_y u_0(x, y)) = 0, & \text{for all } y \in \Gamma, \\ u_0(x, y) \text{ is } Y\text{-periodic.} \end{cases} \tag{3.11}$$

Note that, due to the perforations  $\mathcal{G}$  in  $Y$ , the equation (3.11)<sub>1</sub> is defined in the domain  $\mathcal{P}$  and not in the entire  $Y$ . Further, by the rescaling  $y = x/\varepsilon$ , taking  $x \in \Gamma^\varepsilon$  implies  $y \in \Gamma$ . Due to the explicit dependence of  $A$  on the slow variable  $x$ , Problem  $P^{-2}(x)$  also depends on the "macro-scale" location  $x \in \Omega$ . As in Section 2.2, a function  $u_0 = u_0(x)$  (thus constant w.r.t.  $y$ ) is a solution to this problem, and this is the only possible type of solution. Therefore

$$u_0(x, y) = u_0(x) \quad \text{and} \quad \nabla_y u_0(x, y) = 0 \quad \text{for all } y \in \mathcal{P}, \tag{3.12}$$

so  $u_0$  is in fact the upscaled approximation of  $u^\varepsilon$ . Again, we will further use the remaining terms in (3.9) and (3.10) to determine  $u_0$ .

### 3.2.2 The $\varepsilon^{-1}$ problem and the $\varepsilon^0$ boundary condition

Considering now  $O(\varepsilon^{-1})$  terms in (3.9) and the  $O(1)$  terms in (3.10) gives a problem in the unknown  $u_1$ , depending on  $u_0$

$$(P^{-1})(x) \left\{ \begin{array}{l} -\nabla_y \cdot (A(x, y) \nabla_y u_1(x, y)) = \nabla_y \cdot (A(x, y) \nabla_x u_0(x)), \\ \qquad \qquad \qquad \text{for all } y \in \mathcal{P}, \\ -\vec{\nu} \cdot (A(x, y) \nabla_y u_1(x, y)) = \vec{\nu} \cdot (A(x, y) \nabla_x u_0(x, y)), \\ \qquad \qquad \qquad \text{for all } y \in \Gamma, \\ u_1(x, y) \text{ is } Y\text{-periodic.} \end{array} \right. \quad (3.13)$$

To determine  $u_1$  as a function of  $u_0$  itself, we can proceed as in Section 2.2 and rewrite

$$\nabla_x u_0(x) = \sum_{j=1}^d \vec{e}_j \partial_{x_j} u_0(x), \quad (3.14)$$

where  $\vec{e}_j = (0, \dots, 0, 1, 0, \dots, 0)$  is the unit vector in the  $j^{\text{th}}$  direction ( $j = 1, \dots, d$ ). Using the linearity of Problem  $P^{-1}(x)$ ,  $u_1$  can be expressed in terms of the partial  $x$ -derivatives of  $u_0$  and of the solutions  $w^j$  of the cell problems ( $j = 1, \dots, d$ )

$$(P_j^{-1})(x) \left\{ \begin{array}{l} -\nabla_y \cdot (A(x, y) \nabla_y w^j(x, y)) = \nabla_y \cdot (A(x, y) \vec{e}_j), \\ \qquad \qquad \qquad \text{for all } y \in \mathcal{P}, \\ -\vec{\nu} \cdot (A(x, y) \nabla_y w^j(x, y)) = \vec{\nu} \cdot (A(x, y) \vec{e}_j), \\ \qquad \qquad \qquad \text{for all } y \in \Gamma, \\ w^j(x, y) \text{ is } Y\text{-periodic.} \end{array} \right. \quad (3.15)$$

For uniqueness, we further require that  $w^j$  has the average 0 over  $\mathcal{P}$  (see also Remark 2.2.1). This yields

$$u_1(x, y) = \tilde{u}_1(x) + \sum_{j=1}^d w^j(x, y) \partial_{x_j} u_0(x), \quad (3.16)$$

with  $\tilde{u}_1(x)$  being an arbitrary function of  $x$ , but playing no role in the final form of the upscaled model.

### 3.2.3 The $\varepsilon^0$ problem and the $\varepsilon^1$ boundary condition

Finally, taking the  $O(1)$  terms in (3.9) and the  $O(\varepsilon)$  terms in (3.10) gives

$$(P^0)(x) \left\{ \begin{array}{l} -\nabla_x \cdot [A(x, y)(\nabla_x u_0(x) + \nabla_y u_1(x, y))] \\ \quad -\nabla_y \cdot [A(x, y)(\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] = f, \\ \qquad \qquad \qquad \text{for all } y \in \mathcal{P}, \\ -\vec{\nu} \cdot (A(x, y)\nabla_y u_2(x, y)) = \vec{\nu} \cdot (A(x, y)\nabla_x u_1(x, y)), \\ \qquad \qquad \qquad \text{for all } y \in \Gamma, \\ u_2(x, y) \text{ is } Y\text{-periodic.} \end{array} \right. \quad (3.17)$$

Again, instead of trying to find  $u_2$ , we eliminate it by integrating over the entire domain  $\mathcal{P}$ , which gives an equation for  $u_0$

$$\begin{aligned} -\nabla_x \cdot \left[ \int_{\mathcal{P}} A(x, y)(\nabla_x u_0(x) + \nabla_y u_1(x, y)) dy \right] \\ - \int_{\mathcal{P}} \nabla_y \cdot [A(x, y)(\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] dy = |\mathcal{P}|f(x), \end{aligned} \quad (3.18)$$

for all  $x \in \Omega$ , where  $|\mathcal{P}| = \int_{\mathcal{P}} dy$  is the ( $d$ -dimensional) volume of the set  $\mathcal{P}$ .

For the last integral on the left in (3.18) we use the Gauß theorem, to obtain

$$\begin{aligned} \int_{\mathcal{P}} \nabla_y \cdot [A(x, y)(\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] dy \\ = \int_{\partial\mathcal{P}} \vec{\nu} \cdot [A(x, y)(\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] d\sigma_y, \end{aligned} \quad (3.19)$$

where  $d\sigma_y$  is the area element over  $\partial\mathcal{P}$ , the boundary of the void space  $\mathcal{P}$ , and  $\vec{\nu}$  the unit normal to  $\partial\mathcal{P}$  pointing outwards to  $\mathcal{P}$ . Compared to the situation in Chapter 2, the boundary of  $\mathcal{P}$  contains now two parts:  $\partial Y$ , the boundary of the unit cube  $Y$ , and  $\Gamma$ , the grain boundary, see also Figure 3.2.3. Thus

$$\begin{aligned} \int_{\mathcal{P}} \nabla_y \cdot [A(x, y)(\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] dy \\ = \int_{\partial Y \cup \Gamma} \vec{\nu} \cdot [A(x, y)(\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] d\sigma_y, \end{aligned} \quad (3.20)$$

As in Section 2.2, the integral over  $\partial Y$  is 0 due to the  $Y$ -periodicity of  $A$ ,  $u_1$  and  $u_2$  and the fact that on  $\partial Y$  the unit normals can be grouped into pairs having opposite senses.

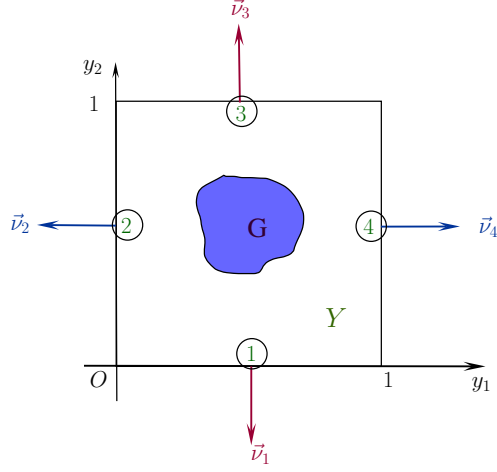


Figure 3.2: The boundaries of a reference pore  $\mathcal{P}$

Further, using the boundary condition (3.17)<sub>2</sub> shows that the boundary integral on  $\Gamma$  vanishes as well, giving

$$\int_{\mathcal{P}} \nabla_y \cdot [A(x, y)(\nabla_x u_1(x, y) + \nabla_y u_2(x, y))] dy = 0.$$

so the last integral on the left in (2.17) vanishes.

To deal with the first integral in (3.18) we use (3.16) to obtain

$$-\nabla_x \cdot \left[ \int_{\mathcal{P}} A(x, y) \left( \nabla_x u_0(x) + \sum_{j=1}^d \partial_{x_j} u_0(x) \nabla_y w^j(x, y) \right) dy \right] = |\mathcal{P}| f(x).$$

Using the outer boundary conditions in (3.5), we obtain that  $U(x) = u_0(x)$ , the upscaled approximation of  $u^\varepsilon$  solves the upscaled model

$$(P) \quad \begin{cases} -\nabla \cdot (A^*(x) \nabla U) = f, & \text{for all } x \in \Omega, \\ U = 0, & \text{on } \partial\Omega, \end{cases} \quad (3.21)$$

with the tensor  $A^* : \Omega \rightarrow \mathbb{R}^{d \times d}$  having the elements  $(V_1 \cdot V_2)$  standing for the inner product of the vectors  $V_1, V_2 \in \mathbb{R}^d$ :

$$\begin{aligned} a_{ij}^* : \Omega &\rightarrow \mathbb{R}, \quad (i, j = 1, \dots, d) \\ a_{ij}^*(x) &= \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} (A(x, y)(\vec{e}_j + \nabla_y w^j(x, y))) \cdot \vec{e}_i dy. \end{aligned} \quad (3.22)$$



**Remark 3.2.1** *Since now the solutions  $w^j$  of the cell problems  $P_j^{-1}$  depend on  $x$ , the cell problems (3.15) have to be solved for each  $x \in \Omega$ . However, this still simplifies the original problem  $P^\varepsilon$ , as it allows decoupling the perforated structure from the upscaled problem  $P$ . The difference is subtle. In the original problem, the variable characteristics are present at all scales and in the complex, perforated domain  $\Omega^\varepsilon$ , and in a strongly coupled manner. The upscaled model instead involves essentially variations at the macro scale and, of course, no perforations (so the domain is not complex). However, for every  $x \in \Omega$ , to determine the value of the diffusion tensor  $A^*(x)$  one has to solve the cell problems  $P_j^{-1}(x)$ . Note that these problems reflect the rapidly oscillating characteristics and are decoupled from the macro-scale variations. For computational point of view, the importance of this decoupling becomes obvious: instead of solving the full problem, requiring a sufficiently fine grid and thus highly complex calculations, in the upscaled case one solves much simpler problems, their number being essentially the number of nodes of a coarse grid. Moreover, as seen in Chapter 2, if no macro-scale variations are encountered (i.e.  $A = A(y)$ , thus  $x$ -independent), one only has to solve the cell problems once, as these become  $x$ -independent as well.*

As in the non-perforated case, one has the following

**Lemma 3.2.1** *Let  $A$  be a symmetric tensor function fulfilling the conditions in (3.6), and  $A^*$  be the effective diffusion matrix in (3.22). It holds*

- a)  $A^*$  is symmetric, i.e.  $a_{ij}^* = a_{ji}^*$  for all  $i, j = 1, \dots, d$ .
- b)  $A^*$  is positive definite, i.e. there exist a constant  $C > 0$  s.t. for all (column vectors)  $z \in \mathbb{R}^d$ ,  $z^T(A^*z) \geq C(z^Tz)$ .

### 3.3 Exercises

- 1 Prove Lemma 3.2.1.

# Chapter 4

## The formal derivation of the Darcy law

In this chapter we still work in a perforated medium, but consider another application: the flow of a fluid through the pores of the medium. Due to the complexity of the domain, it is impossible to carry out large scale simulations by starting at the pore scale. Instead, one should consider models for flow that are valid at the macro scale, a classical example in this sense being the Darcy law. Here apply the asymptotic expansion techniques described in Chapter 3 and derive this upscaled law by starting from a flow model valid at the micro scale, the Stokes model.

### 4.1 The micro scale flow problem

We work in the framework given in Chapter 3 and consider a perforated domain. Related to a porous medium, the perforations are the grains (the solid matrix) within the porous medium, while the flow domain is the union of all pores (the voids). We refer to Section 3.1 for the definition of the flow domain  $\Omega^\varepsilon$  and of the inner boundary  $\Gamma^\varepsilon$  (equations (3.2) and (3.3)). At the pore scale, the flow is described by the Stokes equations. Considering

a the Navier-Stokes model would make no difference. At the pore scale we have

$$\begin{cases} \varepsilon^2 \mu \Delta \vec{q}^\varepsilon = \nabla p^\varepsilon(x), & \text{in } \Omega^\varepsilon \\ \nabla \cdot \vec{q}^\varepsilon(x) = 0, & \text{in } \Omega^\varepsilon \\ \vec{q}^\varepsilon(x) = 0, & \text{on } \Gamma^\varepsilon, \end{cases} \quad (4.1)$$

completed by boundary conditions on the external boundary  $\partial\Omega$ . For simplicity, on the solid grain boundaries ( $\Gamma^\varepsilon$ ) we assume no-slip, and no internal forces acting on the fluid are considered.

Note the  $\varepsilon^2$  scaling in front of the viscosity  $\mu$ . Physically speaking, this means that the viscosity ( $\varepsilon^2 \mu$ ) is in balance with the friction of the fluid on the solid pore boundaries, appearing due to the no-slip conditions there. In other words, the pressure gradient is large enough for determining an effective displacement of the fluid within the pores. In this framework, this is also the only possible choice that leads to a non-trivial limit of the velocity field  $\vec{q}^\varepsilon$ . For example, if viscosity would be larger (say  $\varepsilon \mu$ , or  $\mu$ ), as  $\varepsilon \searrow 0$  this would simply lead to a “frozen” profile ( $\vec{q} = 0$ ), since viscous forces are dominating. As  $\varepsilon \searrow 0$ , the pores are very small, so the fluid will be simply blocked.

As before we start with assuming that  $\vec{q}^\varepsilon$  and  $p^\varepsilon$  can be expanded asymptotically as:

$$\begin{aligned} \vec{q}^\varepsilon &= \vec{q}_0(x, y) + \varepsilon \vec{q}_1(x, y) + \varepsilon^2 \vec{q}_2(x, y) + \dots \\ p^\varepsilon &= p_0(x, y) + \varepsilon p_1(x, y) + \varepsilon^2 p_2(x, y) + \dots \end{aligned} \quad (4.2)$$

all functions  $\vec{q}_k$  and  $p_k$  being  $Y$ -periodic w.r.t.  $y$  ( $k = 1, \dots, d$ ). Similar to the previous chapters, we rewrite the differential operators as

$$\nabla \rightarrow \nabla_x + \frac{1}{\varepsilon} \nabla_y, \quad \Delta \rightarrow \Delta_x + \frac{1}{\varepsilon} \nabla_x \cdot \nabla_y + \frac{1}{\varepsilon} \nabla_y \cdot \nabla_x + \frac{1}{\varepsilon^2} \Delta_y$$

and proceed by identifying the terms having the same order in  $\varepsilon$ . Using these relations into (4.1) we end up with

$$\left\{ \begin{aligned} & \mu \Delta_y \vec{q}_0(x, y) + \varepsilon \mu [(\nabla_x \cdot \nabla_y + \nabla_y \cdot \nabla_x) \vec{q}_0 + \Delta_y \vec{q}_1] + O(\varepsilon^2) \\ & = \frac{1}{\varepsilon} \nabla_y p_0 + (\nabla_x p_0 + \nabla_y p_1) + \varepsilon (\nabla_x p_1 + \nabla_y p_2) + O(\varepsilon^2), & \text{in } \Omega^\varepsilon \\ & \frac{1}{\varepsilon} \nabla_y \cdot \vec{q}_0 + (\nabla_x \cdot \vec{q}_0 + \nabla_y \cdot \vec{q}_1) + \varepsilon (\nabla_x \cdot \vec{q}_1 + \nabla_y \cdot \vec{q}_2) + O(\varepsilon^2) = 0, & \text{in } \Omega^\varepsilon \\ & \vec{q}_0 + \varepsilon \vec{q}_1 + \varepsilon^2 \vec{q}_2 + O(\varepsilon^2) = \vec{0}, & \text{on } \Gamma^\varepsilon. \end{aligned} \right. \quad (4.3)$$

The  $\varepsilon^{-1}$  term in the first equation gives

$$\nabla_y p_0(x, y) = 0, \quad (4.4)$$

thus  $p_0$  is  $y$ -independent.

The  $\varepsilon^0$  terms in the first and last equations in (4.3), and the  $\varepsilon^{-1}$  term in the middle one lead to

$$\left\{ \begin{array}{ll} \mu \Delta_y \vec{q}_0(x, y) = \nabla_x p_0(x) + \nabla_y p_1(x, y), & \text{in } \Omega^\varepsilon \\ \nabla_y \cdot \vec{q}_0(x, y) = 0, & \text{in } \Omega^\varepsilon \\ \vec{q}_0(x, y) = 0, & \text{on } \Gamma^\varepsilon \\ \vec{q}_0, p_1 - Y\text{-periodic.} \end{array} \right. \quad (4.5)$$

As before, we want to simplify the  $p_0$ -dependence of  $\vec{q}_0$  through ‘‘cell problems’’. With  $\nabla_x p_0(x) = \sum_{j=1}^d \vec{e}_j \partial_{x_j} p_0(x)$  we construct the cell problems ( $j = 1, \dots, d$ )

$$(P_j) \left\{ \begin{array}{ll} -\Delta_y \vec{\chi}^j(y) = \nabla_y \Pi^j(y) + \vec{e}_j, & \text{in } \mathcal{P} \\ \nabla_y \cdot \vec{\chi}^j(y) = 0, & \text{in } \mathcal{P} \\ \vec{\chi}^j(y) = 0, & \text{on } \Gamma \\ \vec{\chi}^j, \Pi^j - Y\text{-periodic.} \end{array} \right. \quad (4.6)$$

In this way we have identified both  $\vec{q}_0$  and  $p_1$  in terms of  $p_0$  and the solutions of the cell problems,

$$\vec{q}_0(x, y) = -\frac{1}{\mu} \sum_{j=1}^d \partial_{x_j} p_0(x) \cdot \vec{\chi}^j(y), \quad p_1(x, y) = \sum_{j=1}^d \partial_{x_j} p_0(x) \cdot \Pi^j(y). \quad (4.7)$$

Note that we have chosen not to include the viscosity  $\mu$  in the cell problems, and the presence of the  $-$  sign there. This choice is made purely for convenience: as follow from below, in this way the resulting upscaled equation can be written in the form that is more common for the Darcy law.

Defining the averaged velocity as

$$\vec{q}(x) = \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} \vec{q}_0(x, y) dy, \quad (4.8)$$

from (4.7) we obtain that  $\vec{q}$  satisfies the Darcy law

$$\vec{q}(x) = -\frac{1}{\mu} \mathbf{K} \nabla p_0(x) \quad (\text{for all } x \text{ in } \Omega), \quad (4.9)$$

where the permeability tensor  $\mathbf{K}$  has the components

$$k_{ij} = \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} \chi_i^j(y) dy,$$

for all  $i, j = 1, \dots, d$ . Here by  $\chi_i^j$  we mean the  $i$ -th component of  $\vec{\chi}^j = (\chi_1^j, \dots, \chi_d^j)$ .

To see that  $\vec{q}$  and  $p_0$  (the effective velocity and pressure) really satisfy a Darcy law, we also have to show that  $\vec{q}$  is divergence-free. This follows by integrating the  $\varepsilon^0$ -term in the second equation of (4.3) over  $\mathcal{P}$ ,

$$\begin{aligned} \nabla_x \cdot \vec{q}(x) &= \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} \nabla_x \cdot \vec{q}_0(x, y) dy \\ &= -\frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} \nabla_y \cdot \vec{q}_1(x, y) dy \\ &= -\frac{1}{|\mathcal{P}|} \int_{\partial\mathcal{P}} \vec{\nu} \cdot \vec{q}_1(x, y) dy \\ &= -\frac{1}{|\mathcal{P}|} \int_{\partial Y} \vec{\nu} \cdot \vec{q}_1(x, y) dy - \frac{1}{|\mathcal{P}|} \int_{\Gamma} \vec{\nu} \cdot \vec{q}_1(x, y) ds \end{aligned} \quad (4.10)$$

In the first step we have used the equality  $\nabla_x \vec{q}_0 + \nabla_y \vec{q}_1 = 0$ , resulting from the second equation of (4.3). Finally, the first boundary integral on the right vanishes due to  $Y$ -periodicity of  $\vec{q}_1$ , while for the second one we recall that  $\vec{q}_1 = \vec{0}$  on  $\Gamma$  (this being the boundary condition in (4.3)). This shows that at the macro-scale, the Darcy flow is divergence free.

As for the diffusion problems, we have the following

**Lemma 4.1.1** *The tensor  $\mathbf{K}$  is symmetric and positive definite.*

**Remark 4.1.1** *The microscopic model can be considered more complex, by adding forces acting on the fluid, or considering a Navier-Stokes model. The upscaled result will be fairly the same (a Darcy law).*

## 4.2 Exercises

- 1 Prove Lemma 4.1.1.

# Chapter 5

## Chemical processes in porous media

In the previous chapter we have provided the asymptotic expansion method, and applied it to different examples: diffusion problem in both continuum and perforated domains, and Stokes flow in porous media. The corresponding effective equations are derived. We are going now to use these results for homogenizing more complex models describing miscible displacement. Note that formally there are no particular difficulties to apply the techniques employed before to derive effective models, rigorous mathematical proofs for the convergence of the homogenization procedure are seldom available, mostly for simple cases. As in Chapters 3 and 4, here we consider a complex domain including small (of order  $\varepsilon$ ) perforations distributed periodically. This part is motivated by the reactive fluid transport through porous media (like soils), and elaborates on Chapter 3.

### 5.1 Bulk-reactive flow in porous media

We consider a porous medium filled by a fluid that flows through its void space (the pores). The geometry is given in Section 3.1, and the flow is governed by the Stokes

system

$$\begin{cases} \varepsilon^2 \mu \Delta \vec{q}^\varepsilon = \nabla p^\varepsilon, & \text{in } \Omega^\varepsilon, \\ \nabla \cdot \vec{q}^\varepsilon = 0, & \text{in } \Omega^\varepsilon, \\ \vec{q}^\varepsilon(x) = \vec{0}, & \text{on } \Gamma^\varepsilon, \end{cases} \quad (5.1)$$

complemented by boundary conditions on the outer boundary of the domain. Here  $\vec{q}^\varepsilon$  is the fluid velocity and  $p^\varepsilon$  the pressure inside the fluid.

Further, we assume that certain chemical species are dissolved into (and transported by) the fluid. For simplicity, we only consider one species, but the situation can be immediately extended to multiple species. Denoting by  $u^\varepsilon$  the concentration of the solute, allowing diffusion, convection, and reaction to take place, we end up with the following parabolic problem in  $u^\varepsilon$

$$\partial_t u^\varepsilon(t, x) + \nabla \cdot (\vec{q}^\varepsilon(x) u^\varepsilon(x)) = \nabla \cdot (a^\varepsilon(x) \nabla u^\varepsilon(x)) + R(u^\varepsilon(t, x)), \quad (5.2)$$

defined for all  $t > 0$  and  $x \in \Omega^\varepsilon$ . By  $a^\varepsilon$  we denote the diffusion coefficient of the species  $u^\varepsilon$ , while  $R$  models the reaction. Further, as in (2.3),

$$a^\varepsilon(x) = a\left(\frac{x}{\varepsilon}\right), \quad \text{with } a \text{ being } Y\text{-periodic.}$$

If only bulk reactions are encountered, thus excluding reactions at the grain surface or in its interior, on the grain surface we have

$$-a(y) \vec{\nu} \cdot \nabla u^\varepsilon(t, x) = 0, \quad \text{on } \Gamma^\varepsilon. \quad (5.3)$$

Note that we have also assumed no-slip boundary conditions for the fluid,  $\vec{q}^\varepsilon = \vec{0}$  on  $\Gamma^\varepsilon$ . Assuming that the fluid properties are not affected by the chemical processes, the flow problem (5.1) can be considered independently. As seen in Chapter 4, as  $\varepsilon \searrow 0$  we end up with a Darcy law for the averaged flow

$$\begin{aligned} \vec{q} &= -\frac{1}{\mu} \mathbf{K} \nabla p, & \text{in } \Omega \\ \nabla \cdot \vec{q} &= 0, & \text{in } \Omega. \end{aligned} \quad (5.4)$$

Now we turn our attention to the chemistry. Using the homogenization ansatz,

$$u^\varepsilon(t, x) = u_0(t, x, y) + \varepsilon u_1(t, x, y) + \varepsilon^2 u_2(t, x, y) + \dots$$

we have for the gradient and the diffusion term

$$\nabla \rightarrow \nabla_x + \frac{1}{\varepsilon} \nabla_y, \quad \Delta \rightarrow \Delta_x + \frac{1}{\varepsilon} \nabla_x \cdot \nabla_y + \frac{1}{\varepsilon} \nabla_y \cdot \nabla_x + \frac{1}{\varepsilon^2} \Delta_y.$$

Using the above, (5.2) yields

$$\begin{aligned} & \partial_t (u_0(t, x, y) + \varepsilon u_1(t, x, y) + \dots) + \frac{1}{\varepsilon} \nabla_y \cdot (\vec{q}_0(x, y) u_0(t, x, y)) \\ & + (\nabla_x \cdot \vec{q}_0(x, y) u_0(t, x, y)) + \nabla_y \cdot (\vec{q}_0(x, y) u_1(t, x, y) + \vec{q}_1(x, y) u_0(t, x, y)) \\ & + \varepsilon \{ \nabla_x \cdot (\vec{q}_0(x, y) u_1(t, x, y) + \vec{q}_1(x, y) u_0(t, x, y)) \\ & + \nabla_y \cdot (\vec{q}_0(x, y) u_2(t, x, y) + \vec{q}_1(x, y) u_1(t, x, y) + \vec{q}_2(x, y) u_0(t, x, y)) \} + O(\varepsilon^2) \\ & = \frac{1}{\varepsilon^2} \nabla_y \cdot (a(y) \nabla_y u_0(t, x, y)) \tag{5.5} \\ & + \frac{1}{\varepsilon} \{ \nabla_x \cdot (a(y) \nabla_y u_0) + \nabla_y \cdot (a(y) (\nabla_x u_0(t, x, y) + \nabla_y u_1(t, x, y))) \} \\ & + \{ \nabla_x \cdot (a(y) (\nabla_x u_0(t, x, y) + \nabla_y u_1(t, x, y))) \\ & + \nabla_y \cdot (a(y) (\nabla_x u_1(t, x, y) + \nabla_y u_2(t, x, y))) \} \\ & + R(u_0) + R'(u_0) \{ \varepsilon u_1(t, x, y) + \varepsilon^2 u_2(t, x, y) \} + O(\varepsilon). \end{aligned}$$

Here we have used the Taylor expansion for  $R$  around  $u_0$ . Analogously, the grain boundary condition (5.3) becomes

$$-\vec{\nu} \cdot a(y) \left( \frac{1}{\varepsilon} \nabla_y u_0(t, x, y) + (\nabla_x u_0(t, x, y) + \nabla_y u_1(t, x, y)) + O(\varepsilon) \right) = 0$$

Now we can identify the  $\varepsilon^k$ -problems, where  $k = -2, -1, \dots$

$$\begin{cases} \nabla_y \cdot (a(y) \nabla_y u_0(t, x, y)) = 0, & \text{in } \mathcal{P} \\ -\vec{\nu} \cdot (a(y) \nabla_y u_0(t, x, y)) = 0, & \text{on } \Gamma \\ u_0 \text{ is } Y\text{-periodic.} \end{cases} \tag{5.6}$$

As before, (5.6) implies that  $u_0(t, x, y) = u_0(t, x)$  (thus,  $u_0$  is  $y$ -independent). We go on



with

$$\left\{ \begin{array}{ll} \nabla_y \cdot (\vec{q}_0(x, y)u_0(t, x, y)) - \nabla_x(a(y)\nabla_y u_0) \\ -\nabla_y \cdot \{a(y)(\nabla_x u_0(t, x) + \nabla_y u_1(t, x, y))\} = 0 & \text{in } \mathcal{P}, \\ -\nu \cdot \{a(y)(\nabla_x u_0(t, x) + \nabla_y u_1(t, x, y))\} = 0, & \text{on } \Gamma, \\ u_1 \text{ is } Y\text{-periodic} \end{array} \right. \quad (5.7)$$

Since  $u_0$  does not depend on  $y$  and  $\nabla_y \cdot \vec{q}_0(x, y) = 0$  (see also (4.5)<sub>2</sub>) we obtain for  $u_1$ ,

$$\left\{ \begin{array}{ll} -\nabla_y \cdot (a(y)\nabla_y u_1(t, x, y)) = \nabla_y \cdot (a(y)\nabla_x u_0(t, x)), & \text{in } \mathcal{P} \\ -\vec{\nu} \cdot (a(y)\nabla_y u_1(t, x, y)) = \vec{\nu} \cdot (a(y)\nabla_x u_0(t, x)), & \text{on } \Gamma \\ u_1 \text{ is } Y\text{-periodic.} \end{array} \right. \quad (5.8)$$

As in Chapter 3 (note that now  $a$  does not depend on  $x$ ),  $u_1$  can be obtained by solving the cell problems

$$\left\{ \begin{array}{ll} -\nabla_y \cdot (a(y)\nabla_y w^j(y)) = \nabla_y \cdot (a(y)\vec{e}_j) & \text{in } \mathcal{P} \\ -\vec{\nu} \cdot (a(y)\nabla_y w^j(y)) = \vec{\nu} \cdot (a(y)\vec{e}_j) & \text{on } \Gamma \\ w^j \text{ is } Y\text{-periodic.} \end{array} \right. \quad (5.9)$$

This gives

$$u_1(t, x, y) = \tilde{u}_1(t, x) + \sum_{j=1}^d \partial_{x_j} u_0(t, x) w^j(y).$$

Finally, the  $O(1)$  terms in the expanded equation yields

$$\left\{ \begin{array}{l} \partial_t u_0(t, x) + \nabla_x \cdot (\vec{q}_0(x, y)u_0(t, x, y)) + \nabla_y \cdot (\vec{q}_0(x, y)u_1(t, x, y) + \vec{q}_1(x, y)u_0(t, x, y)) \\ = \{\nabla_x \cdot (a(y)(\nabla_x u_0(t, x, y) + \nabla_y u_1(t, x, y))) \\ + \nabla_y \cdot (a(y)(\nabla_x u_1(t, x, y) + \nabla_y u_2(t, x, y)))\} + R(u_0), \text{ in } \mathcal{P} \\ -\nu \cdot \{a(y)(\nabla_x u_1(t, x) + \nabla_y u_2(t, x, y))\} = 0, \text{ on } \Gamma \\ u_2 \text{ is } Y\text{-periodic} \end{array} \right. \quad (5.10)$$

With

$$\vec{q}(x) = \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} \vec{q}_0(x, y) dy,$$

we average the above equation over  $\mathcal{P}$  to obtain

$$\left\{ \begin{aligned} \partial_t u_0 + \nabla_x \cdot (\vec{q} u_0) + \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} \nabla_y \cdot (\vec{q}_0 u_1 + \vec{q}_1 u_0) dy \\ = \nabla_x \cdot \left\{ \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} a(y) dy \cdot \nabla_x u_0 \right\} + \frac{1}{|\mathcal{P}|} \nabla_x \cdot \left( \int_{\mathcal{P}} a(y) \nabla_y u_1 dy \right) \\ + \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} \nabla_y \cdot \{ a(y) (\nabla_x u_1 + \nabla_y u_2) \} dy + \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} R(u_0) dy. \end{aligned} \right. \quad (5.11)$$

The last integral on the left becomes

$$\int_{\mathcal{P}} \nabla_y \cdot (\vec{q}_0 u_1 + \vec{q}_1 u_0) dy = \int_{\partial Y} \vec{\nu} \cdot (\vec{q}_0 u_1 + \vec{q}_1 u_0) ds + \int_{\Gamma} \vec{\nu} \cdot (\vec{q}_0 u_1 + \vec{q}_1 u_0) ds = 0,$$

where we have used the periodicity (for the first boundary integral) and the boundary condition at  $\Gamma$ .

To deal with the terms on the right, which include derivatives, we proceed as in Section 3.2 and obtain the effective diffusion operator

$$\nabla \cdot (A^* \nabla u_0(t, x)) \quad \text{with } A^* = (A_{ij}^*)_{i,j=1,\dots,d}$$

and

$$A_{ij}^* = \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} a(y) (\vec{e}_j + \nabla_y w^j(y)) \vec{e}_i dy, \quad i, j = 1, \dots, d$$

Thus, we end up with the effective reaction-diffusion-convection equation for the effective concentration  $U = u_0$

$$\partial_t u_0(t, x) + \nabla_x \cdot (\vec{q}(x) u_0(t, x)) = \nabla_x \cdot (A^* \nabla u_0(t, x)) + R(u_0(t, x)) \quad (5.12)$$

with  $\vec{q}$  being the Darcy velocity. Hence, the homogenized system is

$$\left\{ \begin{aligned} \vec{q} &= -\frac{1}{\mu} \mathbf{K} \nabla P, & \text{in } \Omega \text{ (Darcy),} \\ \nabla \cdot \vec{q} &= 0, & \text{in } \Omega \text{ (incompressibility)} \\ \partial_t U + \nabla(\vec{q}U) &= \nabla \cdot (A^* \nabla U) + R(U) & \text{in } (0, T] \times \Omega \text{ (mass balance/solute)} \end{aligned} \right. \quad (5.13)$$

**Remark 5.1.1** *Further extensions can be considered by adding  $y$ -dependence of  $R$ , or  $x$ -dependence of  $A$ .*

## 5.2 Adsorption/desorption effects

Here we extend the bulk-reaction model discussed above by including processes like adsorption and desorption, which are encountered at the grain boundaries  $\Gamma^\varepsilon$ . Considering processes like precipitation, dissolution, or other kind of reactions can be done in the same fashion. When compared to Section 5.1, the homogeneous boundary condition (5.3) becomes more complicated. In particular, to model the adsorption/desorption effects one includes a new unknown  $v^\varepsilon$  that models the concentration of the adsorbed species. Note that compared to  $u^\varepsilon$ , which is a bulk (volumetric) concentration of the solute,  $v^\varepsilon$  is a surface concentration and is defined therefore only on the grain surface  $\Gamma^\varepsilon$  and not in the void space  $\Omega^\varepsilon$ .

Without giving its specific form, we assume that the adsorption and desorption are modeled by a rate  $b^\varepsilon$ , depending on the concentrations  $u^\varepsilon$  and  $v^\varepsilon$  and on the location  $x$ . This may include linear, Freundlich, Langmuir, or other isotherms proposed in the literature. In this case, the normal flux of the solute at the grain is proportional to the changes due to the chemical processes encountered there. This translates into the boundary condition

$$-a(y)\vec{\nu} \cdot \nabla u^\varepsilon(t, x) = \varepsilon b^\varepsilon(x, u^\varepsilon, v^\varepsilon), \quad \text{on } \Gamma^\varepsilon \text{ and for all } t > 0. \quad (5.14)$$

By letting the rate depend on  $x$  - the location on the grain boundary  $\Gamma^\varepsilon$ , we include the case of heterogeneous processes. As done previously, we separate the original variable  $x$  into its slow component (still denoted by  $x$ ) and the fast one  $y = \frac{x}{\varepsilon}$ , and assume that  $b^\varepsilon$  is periodic w.r.t. the fast variable. Specifically,  $b^\varepsilon$  satisfies

$$b^\varepsilon(x, u, v) = b\left(x, \frac{x}{\varepsilon}, u, v\right), \quad \text{for all } x \in \Gamma^\varepsilon \text{ and } u, v \in \mathbb{R}, \quad (5.15)$$

where  $b : \mathbb{R}^{2d+2} \rightarrow \mathbb{R}$  is  $Y$ -periodic (in the sense of (2.2)).

Note the factor  $\varepsilon$  on the right of (5.15). As explained in Chapter 6, such a factor appears naturally when bringing the model to a dimensionless form. Further, the need to include an  $\varepsilon$  factor is justified by the following observation. In the three dimensional case

and for spherical grains having a radius of order  $\varepsilon$ , the surface of a grain is proportional to  $\varepsilon^2$ . Assuming that the grains are uniformly distributed on an  $\varepsilon$ -sized grid, and that the medium occupies a region over a length scale of order 1 (this being thus also the order of the volume of the medium), the total number of grains is of order  $\varepsilon^{-3}$ . This means that the total grain surface  $\Gamma^\varepsilon$  in the medium is of order  $\varepsilon^{-1}$ , and thus it goes to infinity as  $\varepsilon$  approaches 0. Having adsorption/desorption rates of order 1 means that the total amount of adsorbed species behaves similarly,  $O(\varepsilon^{-1})$ , in finite times. However, such models are finite at both micro and macro scale, so an increase in the total grain surface is compensated by a factor  $\varepsilon$  multiplying the rate  $b^\varepsilon$ . Clearly, the same argumentation holds for other spatial dimensions, or for other grain shapes having a regular shape.

Since the model discussed here involves two species,  $u^\varepsilon$  and  $v^\varepsilon$ . To complete the model, at the grain boundary we add an equation describing the dynamics of the adsorbed species

$$\partial_t v^\varepsilon = b^\varepsilon(x, u^\varepsilon, v^\varepsilon) + R_\Gamma(v^\varepsilon), \quad \text{on } \Gamma^\varepsilon \text{ and for all } t > 0. \quad (5.16)$$

The term  $R_\Gamma$  models the eventual reactions concerning strictly the adsorbed species (thus not the interaction with the solute) encountered at the grain surface. One may further include surface diffusion effects.

Recalling the construction on Section 5.1, we end up with the following model at the micro scale.

*Flow:*

$$\begin{cases} \varepsilon^2 \mu \Delta \vec{q}^\varepsilon = \nabla p^\varepsilon, & \text{in } \Omega^\varepsilon, \\ \nabla \cdot \vec{q}^\varepsilon = 0, & \text{in } \Omega^\varepsilon, \\ \vec{q}^\varepsilon(x) = \vec{0}, & \text{on } \Gamma^\varepsilon, \end{cases} \quad (5.17)$$

*Chemistry:*

$$\begin{cases} \partial_t u^\varepsilon(t, x) = \nabla \cdot (a^\varepsilon(x) \nabla u^\varepsilon(x)) \\ \quad - \nabla \cdot (\vec{q}^\varepsilon(x) u^\varepsilon(x)) + R(u^\varepsilon(t, x)), & \text{in } (0, T] \times \Omega^\varepsilon, \\ -a(y) \vec{\nu} \cdot \nabla u^\varepsilon(t, x) = \varepsilon b^\varepsilon(x, u^\varepsilon, v^\varepsilon), & \text{on } (0, T] \times \Gamma^\varepsilon, \\ \partial_t v^\varepsilon = b^\varepsilon(x, u^\varepsilon, v^\varepsilon) + R_\Gamma(v^\varepsilon), & \text{on } (0, T] \times \Gamma^\varepsilon. \end{cases} \quad (5.18)$$

Note that the flow component is completely decoupled from the chemistry. As explained in Chapter 4, the upscaled velocity in (4.8) satisfies the Darcy law

$$\vec{q}(x) = -\frac{1}{\mu} \mathbf{K} \nabla p_0(x) \quad \text{and} \quad \nabla_x \cdot \vec{q}(x) = 0, \quad (\text{for all } x \text{ in } \Omega), \quad (5.19)$$

where the conductivity tensor  $\mathbf{K}$  is determined by the solutions of the *Stokes*-type cell problems (4.6). We focus now on the chemistry, in particular on the changes that are due to the processes on the grains. Expanding  $v^\varepsilon$  as

$$v^\varepsilon(t, x) = v_0(t, x, y) + \varepsilon v_1(t, x, y) + \varepsilon^2 v_2(t, x, y) + \dots$$

in terms of the  $Y$ -periodic functions  $v_k$ , and proceeding similarly for the rate  $b$  (recall the assumption (5.15))

$$\begin{aligned} b^\varepsilon(x, u^\varepsilon, v^\varepsilon) &= b(x, y, u_0, v_0) + \varepsilon \partial_u b(x, y, u_0, v_0)(u_1(t, x, y) + \varepsilon u_2(t, x, y) + \dots) \\ &+ \varepsilon \partial_v b(x, y, u_0, v_0)(v_1(t, x, y) + \varepsilon v_2(t, x, y) + \dots) + O(\varepsilon^2), \end{aligned}$$

the boundary condition (5.14) transforms into

$$\begin{aligned} -a(y) \vec{\nu} \cdot (\nabla_x + \frac{1}{\varepsilon} \nabla_y) (u_0(t, x, y) + \varepsilon u_1(t, x, y) + \varepsilon^2 u_2(t, x, y) + \dots) \\ = \varepsilon b(x, y, u_0, v_0) + \varepsilon^2 (\partial_u b(x, y, u_0, v_0) u_1(t, x, y) + \partial_v b(x, y, u_0, v_0) v_1(t, x, y)) + \dots, \end{aligned} \quad (5.20)$$

the dots standing for higher order terms. Similarly, (5.16) gives

$$\begin{aligned} \partial_t (v_0(t, x, y) + \varepsilon v_1(t, x, y) + \dots) \\ = b(x, y, u_0, v_0) + \varepsilon^2 (\partial_u b(x, y, u_0, v_0) u_1(t, x, y) + \partial_v b(x, y, u_0, v_0) v_1(t, x, y)) \\ + R_\Gamma(v_0(t, x, y)) + \varepsilon R'_\Gamma(v_0(t, x, y)) v_1(t, x, y) + \dots, \end{aligned} \quad (5.21)$$

Further, as in Section 3.2 we obtain (see (3.16) and (3.16))

$$\begin{aligned} u_0(x, y) &= u_0(x) \quad (\text{no } y\text{-dependence}), \text{ and} \\ u_1(x, y) &= \tilde{u}_1(x) + \sum_{j=1}^d w^j(x, y) \partial_{x_j} u_0(x), \end{aligned}$$

with  $w^j$  solving the cell problems  $(P_j^{-1})$  defined in (3.15), and (recall (5.10))

$$\left\{ \begin{array}{l} \partial_t u_0(t, x) + \nabla_x \cdot (\vec{q}_0(x, y) u_0(t, x)) + \nabla_y \cdot (\vec{q}_0(x, y) u_1(t, x, y) + \vec{q}_1(x, y) u_0(t, x)) \\ \quad = \{ \nabla_x \cdot (a(y) (\nabla_x u_0(t, x) + \nabla_y u_1(t, x, y))) \\ \quad \quad \quad + \nabla_y \cdot (a(y) (\nabla_x u_1(t, x, y) + \nabla_y u_2(t, x, y))) \} + R(u_0), \text{ in } \mathcal{P} \\ -\nu \cdot \{ a(y) (\nabla_x u_1(t, x, y) + \nabla_y u_2(t, x, y)) \} = b(x, y, u_0(t, x), v_0(t, x, y)), \text{ on } \Gamma \\ \partial_t v_0(t, x, y) = b(x, y, u_0, v_0) + R_\Gamma(v_0(t, x, y)), \text{ on } \Gamma \end{array} \right.$$

where both  $u_2$  and  $v_0$  are  $Y$ -periodic.

Integrating the first equation over  $\mathcal{P}$  gives (see also (5.11))

$$\left\{ \begin{array}{l} \partial_t u_0 + \nabla_x \cdot (\vec{q} u_0) + \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} \nabla_y \cdot (\vec{q}_0 u_1 + \vec{q}_1 u_0) dy \\ \quad = \nabla_x \cdot \left\{ \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} a(y) dy \cdot \nabla_x u_0 \right\} + \frac{1}{|\mathcal{P}|} \nabla_x \cdot \left( \int_{\mathcal{P}} a(y) \nabla_y u_1 dy \right) \\ \quad \quad \quad + \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} \nabla_y \cdot \{ a(y) (\nabla_x u_1 + \nabla_y u_2) \} dy + \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} R(u_0) dy, \end{array} \right. \quad (5.22)$$

$\vec{q}$  being the Darcy velocity. We proceed now by incorporating the new boundary conditions on  $\Gamma$ .

First, proceeding as for (4.10), the last integral on the left in (5.22) vanishes. Moreover, the first two integrals on the right give the homogenized diffusion tensor (recall the approach in Section 3.2). The only difference appears due to the third integral on the right. for this we use the boundary conditions and obtain

$$\begin{aligned} & \int_{\mathcal{P}} \nabla_y \cdot \{ a(y) (\nabla_x u_1 + \nabla_y u_2) \} dy \\ &= \int_{\partial Y} a(y) \vec{\nu} \cdot (\nabla_x u_1 + \nabla_y u_2) d\sigma_y + \int_{\Gamma} a(y) \vec{\nu} \cdot (\nabla_x u_1 + \nabla_y u_2) d\sigma_y \\ &= 0 - \int_{\Gamma} b(x, y, u_0(t, x), v_0(t, x, y)) d\sigma_y, \end{aligned}$$

where for the integral on  $\partial Y$  we have used the  $Y$ -periodicity of all integration arguments.

The last equation remains unchanged, thus the upscaled variables  $U := u_0$ ,  $V := v_0$ ,

$\vec{q}$  and  $p$  solve the effective model

$$\left\{ \begin{array}{ll} \vec{q}(x) = -\frac{1}{\mu} \mathbf{K} \nabla p(x) & \text{in } \Omega, \\ \nabla \cdot \vec{q}(x) = 0 & \text{in } \Omega, \\ \partial_t U(t, x) + \frac{1}{|\overline{p}|} \int_{\Gamma} b(x, y, U(t, x), V(t, x, y)) d\sigma_y \\ = \nabla \cdot (A^* \nabla U(t, x)) - \nabla \cdot (\vec{q}(x) U(t, x)) + R(U), & \text{in } (0, T] \times \Omega, \\ \partial_t V(t, x, y) = b(x, y, U(t, x), V(t, x, y)) + R_{\Gamma}(V(t, x, y)), & \text{on } (0, T] \times \Omega \times \Gamma, \end{array} \right. \quad (5.23)$$

where  $A^*$  and  $\mathbf{K}$  are obtained in Sections 3.2 and 4.1.

Note that at each macro-scale point  $x \in \Omega$ , the upscaled model includes micro-scale components. These are encountered explicitly, through the last equation in (5.23), and implicitly through the cell problems (5.9) - or (3.15) - and (4.6). This means that the micro-scale components have to be solved for every  $x \in \Omega$ . As discussed in Remark 3.2.1, this still has advantages towards the full problem, as the micro-scale effects are only coupled to the macro-scale. Whenever homogeneous reactions are considered, the situation is much more simplified. In this case the adsorption/desorption rate  $b$  does not depend on the fast variable  $y$ . If the same holds for the reactions at the grain boundaries (as considered here), then  $V$  - the effective concentration of the adsorbed species - is  $y$ -independent as well and the last equation in (5.23) becomes

$$\partial_t V(t, x) = b(x, U(t, x), V(t, x)) + R_{\Gamma}(V(t, x)), \text{ on } (0, T] \times \Omega,$$

leading to the effective model

$$\left\{ \begin{array}{ll} \vec{q}(x) = -\frac{1}{\mu} \mathbf{K} \nabla p(x) & \text{in } \Omega, \\ \nabla \cdot \vec{q}(x) = 0 & \text{in } \Omega, \\ \partial_t U(t, x) + \frac{|\Gamma|}{|\overline{p}|} b(x, U(t, x), V(t, x)) \\ = \nabla \cdot (A^* \nabla U(t, x)) - \nabla \cdot (\vec{q}(x) U(t, x)) + R(U), & \text{in } (0, T] \times \Omega, \\ \partial_t V(t, x) = b(x, U(t, x), V(t, x)) + R_{\Gamma}(V(t, x)), & \text{on } (0, T] \times \Omega, \end{array} \right. \quad (5.24)$$

As for the cell problems providing  $A^*$  and  $\mathbf{K}$ , the local problem for  $V$  has to be solved only once.

### 5.3 Exercises

- 1 Consider the micro-scale model in Section 5.2, but with a different (scaling of the processes at the adsorption-desorption processes (equilibrium kinetics)). Specifically, replace the last two equations of (5.18) by

$$\begin{cases} -a(y)\vec{\nu} \cdot \nabla u^\varepsilon(t, x) = \varepsilon \partial_t v^\varepsilon, & \text{on } (0, T] \times \Gamma^\varepsilon, \\ \partial_t v^\varepsilon = \frac{1}{\varepsilon} b^\varepsilon(x, u^\varepsilon, v^\varepsilon), & \text{on } (0, T] \times \Gamma^\varepsilon. \end{cases}$$

Redo the steps of this chapter and determine the effective model in this case.

- 2 For the model of Section 5.2 assume that the adsorption-desorption rate function is given by

$$b^\varepsilon(x, u^\varepsilon, v^\varepsilon) = f(u^\varepsilon) - v^\varepsilon,$$

and consider  $R_\Gamma \equiv 0$  (no reactions on  $\Gamma^\varepsilon$ ). Note that  $b\varepsilon$  does not depend on the location explicitly. Derive the corresponding homogenized model and show that the adsorbed species  $V$  can be eliminated from the model.



## Chapter 6

# Scaling in reactive porous media flow models

The equations discussed in the other chapters are written in a dimensionless form, involving dimensionless parameters (including  $\varepsilon$ , expressing the ratio of two scales). In this chapter we consider a fairly standard model for reactive flow in a porous medium. For the sake of simplicity we still consider an ideal medium consisting of solid grains surrounded by voids, distributed in a periodic structure. We emphasize that the assumption of periodicity is only made for the ease of presentation, as the scaling analysis done here does not require such a structure.

The model presented here is given at the pore (micro) scale and includes dimensions. The aim of this chapter is to present the steps involved in bringing the model to a dimensionless form, including the definition of  $\varepsilon$ , and discuss the possibility of having different regimes. To focus on these aspects we consider a simple, but fairly representative chemical process (adsorption and desorption) and do not discuss any specific application that may be more involved and realistic, but could affect the readability. Having obtained the pore scale model in the dimensionless form, one can proceed by applying the techniques presented in Chapters 2, 3, 4 and 5 to derive the approximating models at the macro scale.

## 6.1 The mathematical model

We consider a porous medium at the pore scale occupying the volume  $\tilde{\Omega}$  in the 3-dimensional space and consisting of solid grains surrounded by voids (the pores). We assume that the grains are uniform and periodically distributed within the medium. In this way the volume  $\tilde{\Omega}$  is divided into two parts:  $\tilde{\Omega}_P$ , the void space (the pores), and  $\tilde{\Omega}_G$ , the solid matrix (the grains). We are mainly interested in the pore space, which is occupied by a fluid. The boundary of  $\tilde{\Omega}_P$  has two parts:  $\tilde{\Gamma}$ , the outer boundary of the volume  $\tilde{\Omega}$ , and  $\tilde{\Gamma}_G$ , the internal boundary, which is the interface between the fluid and the grains (the pore walls).

Assume that a species ( $M_S$ ) is dissolved in the fluid and has a (bulk) concentration  $c_S$  [ $\frac{\text{kg}}{\text{m}^3}$ ]. This species may be adsorbed at the surface of the grains, forming a species ( $M_I$ ) that is attached to this surface and thus becomes immobile. The reverse process of desorption is also possible. We assume that the fluid properties (including the dynamic viscosity  $\tilde{\mu} > 0$  [Pas]) and the pore volumes are not affected by the adsorption and desorption processes. This can be understood as follows. First, the solute is assumed to have a low concentration in the fluid, so any change in this quantity being not perceptible. Second, the adsorbed species ( $M_I$ ) forms a layer having a thickness that can be neglected when compared to the pore size (or diameter). This means that the chemical processes do not affect the pore configuration, or the eventual modifications are negligible. Therefore the immobile species is modeled through its (surface) concentration  $c_I$  [ $\frac{\text{kg}}{\text{m}^2}$ ]. In particular, no clogging effects are encountered.

The flow is described by the Stokes equations relating the fluid velocity  $\tilde{\mathbf{q}}$  [ $\frac{\text{m}}{\text{s}}$ ] and fluid pressure  $\tilde{p}$  [Pa]:

$$\left. \begin{aligned} \mu \Delta \tilde{\mathbf{q}} &= \nabla \tilde{p}, \\ \nabla \cdot \tilde{\mathbf{q}} &= 0, \end{aligned} \right\} \text{ in } \tilde{\Omega}_P. \quad (6.1)$$

The derivatives are in terms of the dimensional spatial variable  $\tilde{x}$  [m]. Note that using the Navier-Stokes model for the fluid flow would lead to similar results. Along the internal

grain boundary we assume a no-slip condition, implying

$$\tilde{\mathbf{q}} = 0 \quad \text{along } \tilde{\Gamma}_G. \quad (6.2)$$

With  $\tilde{D}$  being the diffusion coefficient [ $\frac{\text{m}^2}{\text{s}}$ ], mass conservation for ( $M_S$ ) gives

$$\partial_{\tilde{t}} c_S + \nabla \cdot (\tilde{\mathbf{q}} c_S - \tilde{D} \nabla c_S) = 0, \quad \text{in } \tilde{\Omega}_P, \quad (6.3)$$

where  $\tilde{t}$  is the dimensional time [s]. Note the absence of bulk reaction terms, which can be included without any difficulty.

On the interior boundary  $\tilde{\Gamma}_G$  one can write two equations. First, the flux of  $c_S$  is proportional to the changes in the adsorbed species  $c_I$ . By (6.2), on  $\tilde{\Gamma}_G$  we have

$$\partial_{\tilde{t}} c_I = -\frac{1}{n} \tilde{D} \vec{\nu} \cdot \nabla c_S, \quad (6.4)$$

where  $\vec{\nu}$  denotes the normal unit vector pointing into the grains, and  $n$  is a dimensionless number related to the stoichiometry of the reaction (e.g. the number of ( $M_S$ ) molecules entering in the composition of a ( $M_I$ ) molecule). A second equation on  $\tilde{\Gamma}_G$  describes the adsorption and desorption processes

$$\partial_{\tilde{t}} c_I = R_S - R_I. \quad (6.5)$$

The adsorption and desorption rate functions (isotherms)  $R_I$  and  $R_S$  (both [ $\frac{\text{kg}}{\text{m}^{d-1}\text{s}}$ ]) depend on the concentrations  $c_I$  and  $c_S$ ; their particular form is model specific. In the simplest situation these functions are linear,

$$R_I = k_I c_I. \quad (6.6)$$

Here  $k_I$  [ $\frac{1}{\text{s}}$ ] is the adsorption rate constant. The desorption rate can be defined similarly. Including nonlinear isotherms (like *Monod*, *Langmuir*, or *Freundlich*), or even multivalued ones is straightforward

## 6.2 The dimensionless form

To bring the model to a dimensionless form we consider reference values for the quantities involved in the model. Specifically, we consider a reference time  $\hat{T}$ , length  $\hat{L}$ , fluid pressure  $\hat{P}$  and velocity  $\hat{Q}$ . Note that, in fact, the model includes two scales: the macro-scale, which can be associated to the size of the medium, and the micro-scale, which is a typical pore length. Here by  $\hat{L}$  we mean the macro-scale, and the micro-scale is denoted by  $\hat{\ell}$ . This immediately allows defining the small parameter

$$\varepsilon = \frac{\hat{\ell}}{\hat{L}}. \quad (6.7)$$

An alternative interpretation of the parameter  $\varepsilon$  is discussed in Remark 6.2.2 below.

When deciding on the reference quantities  $\hat{T}$ ,  $\hat{L}$  and  $\hat{Q}$ , a natural assumption is

$$\hat{L} = \hat{Q}\hat{T}. \quad (6.8)$$

This can be seen as choosing the fluid transport time as reference time. Now we can rescale the space and time variables and the velocity and the pressure as

$$t := \frac{\tilde{t}}{\hat{T}}, \quad x := \frac{1}{\hat{L}}\tilde{x}, \quad \vec{q} := \frac{1}{\hat{Q}}\tilde{\mathbf{q}}, \quad p := \frac{\tilde{p}}{\hat{P}}, \quad \mu = \frac{1}{\varepsilon^2} \frac{\tilde{\mu}\hat{Q}}{\hat{P}\hat{L}}. \quad (6.9)$$

To justify the presence of the factor  $\varepsilon^{-2}$  in the definition of  $\mu$  we recall the discussion in Section 4.1. Specifically, the fluid viscosity is in balance with the fluid pressure and its velocity. In this way, the friction of the fluid with the solid pore boundaries does not lead to a totally blocked flow profile.

Having introduced the dimensionless time and space, the derivatives are transformed correspondingly,

$$\frac{\partial}{\partial \tilde{t}} = \frac{1}{\hat{T}} \frac{\partial}{\partial t}, \quad \frac{\partial}{\partial \tilde{x}_k} = \frac{1}{\hat{L}} \frac{\partial}{\partial x_k} \quad (k = 1, \dots, d). \quad (6.10)$$

Note that the quantities defined in (6.9) are dimensionless. Clearly, the same rescaling can be applied to the flow domain and the grain boundaries

$$\Omega := \frac{1}{\hat{L}}\tilde{\Omega}, \quad \Omega_P^\varepsilon := \frac{1}{\hat{L}}\tilde{\Omega}_P \quad \text{and} \quad \Gamma_G^\varepsilon := \frac{1}{\hat{L}}\tilde{\Gamma}_G, \quad (6.11)$$

where by the multiplication of a scalar  $m$  with a set  $\mathcal{M}$  we understand the set obtained by multiplying all elements of  $\mathcal{M}$  with  $m$ . The superscript  $\varepsilon$  indicates that the dimensionless flow domain and the total grain surface are still complex, as these are determined by the space of all (dimensionless) pores. Having assumed that the typical length of the porous medium  $\tilde{\Omega}$  is  $\hat{L}$  and that the typical pore size is  $\hat{\ell}$ , the number of grains in  $\tilde{\Omega}$  is of order  $\varepsilon^{-d} = \left(\frac{\hat{L}}{\hat{\ell}}\right)^d$ . The surface of a grain being of order  $\hat{\ell}^{d-1}$ , the total surface of  $\tilde{\Gamma}_G$  and the void volume  $\tilde{\Omega}_P$  are related by,

$$\varepsilon \hat{L} |\tilde{\Gamma}_G| \approx |\tilde{\Omega}_P|. \quad (6.12)$$

This, in fact, gives an alternative definition of a typical pore size and of  $\varepsilon$ , namely

$$\hat{\ell} := \frac{|\tilde{\Omega}_P|}{|\tilde{\Gamma}_G|} \quad \text{and} \quad \varepsilon := \frac{|\tilde{\Omega}_P|}{\hat{L} |\tilde{\Gamma}_G|}. \quad (6.13)$$

Also recall that by rescaling, the volumes of  $\Omega$  and of  $\Omega_P$  are brought to an order  $O(1)$ . Then, as above, we get  $|\Gamma^\varepsilon| \approx \varepsilon^{-1} |\Omega_P^\varepsilon|$ .

Next, let  $\hat{c}_S$  and  $\hat{c}_I$  be reference values for the concentrations of the solute  $c_S$  and the adsorbed species. We further assume that both adsorption and desorption isotherms are of similar order and let  $\hat{k}$  be a characteristic value for these functions (for example  $\hat{k} = k_I$  in (6.6)) and define

$$u := \frac{c_S}{\hat{c}_S}, \quad v := \frac{c_I}{\hat{c}_I}, \quad D := \frac{\tilde{D}}{\hat{L} \hat{Q}}, \quad k := \frac{\hat{k} \hat{L}}{\hat{Q} \hat{c}_I} \quad \text{and} \quad r_\alpha := \frac{1}{\hat{k}} R_\alpha \quad (\alpha \in \{S, I\}). \quad (6.14)$$

Observe that the functions  $r_I$  and  $r_S$  are dimensionless.

**Remark 6.2.1** *By (6.8), the reference time is a transport time, which can be seen as the time needed for a particle to be transported over the distance  $\hat{L}$  by the fluid flowing with the velocity  $\hat{Q}$ . However, at least two different time scales can be identified in the model:*

$$\begin{aligned} \hat{T}_D &= \frac{\hat{L}^2}{\tilde{D}} && \text{the diffusion time scale,} \\ \hat{T}_C &= \frac{\hat{c}_I}{\hat{k}} && \text{the adsorption time scale.} \end{aligned} \quad (6.15)$$

For  $T_D$  the interpretation is similar to  $\hat{T}$ : the time needed for a particle to move over the distance  $\hat{L}$  by diffusion, whereas  $\hat{T}_C$  is the time within  $\hat{c}_I L^{d-1}$  moles are adsorbed at the grain boundary. These time scales define two dimensionless numbers,

$$\begin{aligned} Pe &:= \frac{\hat{T}_D}{\hat{T}} = \frac{\hat{L}\hat{Q}}{\hat{D}} && \text{(the Peclet number)} \\ Da &:= \frac{\hat{T}}{\hat{T}_C} = \frac{\hat{k}\hat{L}}{\hat{c}_I\hat{Q}} && \text{(the Damköhler number).} \end{aligned} \tag{6.16}$$

Note that  $Pe$  is the reciprocal of the dimensionless diffusion  $D$  in (6.14). Up to now we have tacitly assumed that these numbers are moderate w.r.t  $\varepsilon$ , meaning that all time scales are in balance. A similar analysis can be done for different regimes, leading to Taylor dispersion models (for numbers  $Pe = O(\varepsilon^{-1})$ ) or equilibrium kinetics/fast reaction models (for  $Da = O(\varepsilon^{-1})$ ).

**Remark 6.2.2** *It seems natural to choose the reference values  $\hat{c}_S$  and  $\hat{c}_I$  such that, at reference state, the system contains about the same number of moles for both solute and adsorbed species. Mathematically this is expressed by*

$$\hat{c}_I |\tilde{\Gamma}_G| = \hat{c}_S |\tilde{\Omega}_P|. \tag{6.17}$$

Using (6.7) or (6.13), we find

$$\varepsilon = \frac{\hat{c}_I}{\hat{L}\hat{c}_S}. \tag{6.18a}$$

In fact this is another way to introduce the parameter  $\varepsilon$ . Assuming (6.17), after the scaling (6.11) this gives

$$\varepsilon |\Gamma_G^\varepsilon| = |\Omega_P^\varepsilon|, \tag{6.18b}$$

implying in particular that  $\varepsilon |\Gamma_G^\varepsilon|$  is uniformly bounded with respect to  $\varepsilon$ , as happening in the case of a periodic distribution of grains. Clearly, when upscaling to a macroscopic model, the total internal surface goes to infinity as  $\varepsilon \searrow 0$ , which justifies the appearance of  $\varepsilon$  in the boundary flux in (6.22) below, allowing to control this growth.

Recalling (6.10), we rewrite (6.1) and (6.3) in the scaled domain  $\Omega_P^\varepsilon$  as

$$\begin{cases} \frac{\tilde{\mu}\hat{Q}}{\hat{L}^2} \Delta \vec{q} = \frac{\hat{P}}{\hat{L}} \nabla p, \\ \frac{\hat{Q}}{\hat{L}} \nabla \cdot \vec{q} = 0, \\ \frac{\hat{c}_S}{\hat{T}} \partial_t u = \frac{\hat{c}_S \tilde{D}}{\hat{L}^2} \Delta u - \frac{\hat{c}_S \hat{Q}}{\hat{L}} \nabla \cdot (\vec{q}u). \end{cases} \quad (6.19)$$

On the scaled interior boundary  $\Gamma_G^\varepsilon$ , (6.2), (6.4) and (6.5) become

$$\begin{cases} \hat{Q} \vec{q} = \bar{0}, \\ -\frac{\hat{c}_S \tilde{D}}{n \hat{L}} \vec{\nu} \cdot \nabla u = \frac{\hat{c}_I}{\hat{T}} \partial_t v, \\ \frac{\hat{c}_I}{\hat{T}} \partial_t v = \hat{k}(r_I - r_S). \end{cases} \quad (6.20)$$

By (6.8) and using the definition of  $\mu$  in (6.9) and  $D$  in (6.14),

$$\begin{cases} \varepsilon^2 \mu \Delta \vec{q} = \nabla p, \\ \nabla \cdot \vec{q} = 0, \\ \partial_t u = D \Delta u - \nabla \cdot (\vec{q}u). \end{cases} \quad (6.21)$$

On the scaled interior boundary  $\Gamma_G$  we have

$$\begin{cases} \vec{q} = \bar{0}, \\ -D \vec{\nu} \cdot \nabla u = \varepsilon n \partial_t v, \\ \partial_t v = D_a(r_I - r_S). \end{cases} \quad (6.22)$$

Having determined the dimensionless form of the model, one can apply the asymptotic expansion methods discussed in the previous chapters to derive a homogenized model, valid at the core scale.

# Chapter 7

## A reaction-dispersion model in a simple geometry

Up to now we have considered a periodic, but fairly general geometry at the pore scale. In this chapter we investigate a reactive flow model in a simplified context: a long and thin pore. The upscaling technique is quite simple: an *anisotropic* asymptotic expansion, followed by a transversal averaging. The underlying model is inspired by the reactive flow in Chapters 5 and 6, but now we work in the transport dominated regime. In other words, the Peclet number is large, leading to an effective model similar to Taylor dispersion.

Taking a simple geometry, simplifies the presentation, as many of the quantities can be calculated explicitly. However, similar results are obtained in more general situations; the upscaled model in a simplified geometry features most of the characteristics of the upscaled models in general domains.

### 7.1 The mathematical model

With  $\varepsilon > 0$  being a small parameter, the domain of interest is a two dimensional, long and thin strip,

$$\Omega_\varepsilon := \{(x, z) \in \mathbb{R}^2 \mid 0 < x < 1, -\varepsilon < z < \varepsilon\} \quad (7.1)$$



Note that now  $x$  and  $z$  simply denote one dimensional (horizontal, resp. vertical) variables. Similar to the grain boundaries in the previous chapters, adsorption/desorption processes are encountered at  $\Gamma_\varepsilon$ , the lateral boundaries of  $\Omega_\varepsilon$ ,

$$\Gamma_\varepsilon := \{(x, z) | 0 \leq x \leq 1, z \in \{-\varepsilon, \varepsilon\}\}. \quad (7.2)$$

the domain also has an inflow boundary

$$\Gamma_i := \{(x, z) | x = 0, -\varepsilon \leq z \leq \varepsilon\}, \quad (7.3)$$

and the outflow boundary  $\Gamma_o$ ,

$$\Gamma_o := \{(x, z) | x = 1, -\varepsilon \leq z \leq \varepsilon\}. \quad (7.4)$$

Without explaining the modelling details and the steps leading to a dimensionless model we consider the following system of equations that describe the flow, diffusion and reaction in  $\Omega_\varepsilon$ . The water velocity  $\vec{q}^\varepsilon$  is given by

The Stokes flow:

$$\begin{cases} \varepsilon^2 \mu \Delta \vec{q}^\varepsilon = \nabla p^\varepsilon, & \text{in } \Omega_\varepsilon \\ \nabla \cdot \vec{q}^\varepsilon = 0, & \text{in } \Omega_\varepsilon \\ \vec{q}^\varepsilon = 0, & \text{on } \Gamma_\varepsilon, \\ \vec{q}^\varepsilon = \vec{q}_b, & \text{on } \Gamma_i \cup \Gamma_o. \end{cases} \quad (7.5)$$

As before,  $p^\varepsilon$  is the pressure inside water,  $\mu$  its dimensionless viscosity, whereas  $\vec{q}_b$  is the in- and outflow velocity (for simplicity considered the same). At the lateral boundaries no slip is encountered. As in Chapter 6 we assume that the fluid is containing a solute of concentration  $u^\varepsilon$ , which is undergoing transport and diffusion. Further, an immobile species of concentration  $v^\varepsilon$  is encountered on  $\Gamma_\varepsilon$ , as the result of adsorption and desorption.

The chemistry:

$$\left\{ \begin{array}{ll} u_t^\varepsilon = \nabla \cdot (\varepsilon D \nabla u^\varepsilon - \bar{q}^\varepsilon u^\varepsilon), & \text{in } (0, T] \times \Omega_\varepsilon, \\ v_t^\varepsilon = f(u^\varepsilon, v^\varepsilon) & \text{on } (0, T] \times \Gamma_\varepsilon, \\ -\nu \cdot \varepsilon D \nabla u^\varepsilon = \varepsilon v_t^\varepsilon & \text{on } (0, T] \times \Gamma_\varepsilon, \\ u^\varepsilon = u_{b_i}, & \text{on } (0, T] \times \Gamma_i, \\ \nu \cdot \nabla u^\varepsilon = 0, & \text{on } (0, T] \times \Gamma_o, \\ u^\varepsilon = u_0, & \text{in } \Omega_\varepsilon, \text{ for } t = 0, \\ v^\varepsilon = v_0, & \text{in } \Gamma_\varepsilon, \text{ for } t = 0. \end{array} \right. \quad (7.6)$$

Note the factor  $\varepsilon$  multiplying the diffusion coefficient  $D$ , which means that we are working in the transport dominated regime. Referring to the definition of the Peclet number in (6.16) and the relation with the diffusion coefficient in (6.14), having a diffusion coefficient of order  $\varepsilon$  means in fact that the diffusion time scale  $T_D$  is much larger than the transport time scale. In the above we have given the initial and boundary conditions explicitly, and considered a general term  $f$  including both adsorption and desorption effects.

In contrast to the expansion in the other chapters, we consider here only a rescaling in the vertical direction. Specifically, we simply define  $y = z/\varepsilon$ , and redefine the domain and its boundaries in (7.1)–(7.4) accordingly

$$\Omega := (0, 1) \times (-1, 1), \Gamma := (0, 1) \times \{-1, 1\}, \Gamma_i := \{0\} \times (-1, 1), \Gamma_o := \{1\} \times (-1, 1). \quad (7.7)$$

Recalling that the vertical derivative  $\partial_z$  becomes now  $\varepsilon^{-1}\partial_y$ , we rewrite the model as

$$u_t^\varepsilon + \nabla \cdot (\bar{q}^\varepsilon u^\varepsilon) - \varepsilon D (\partial_{xx} u^\varepsilon + \varepsilon^{-2} \partial_{yy} u^\varepsilon) = 0, \quad \text{in } (0, T] \times \Omega \quad (7.8)$$

$$\mu \begin{pmatrix} \varepsilon^2 \partial_{xx} q^{(1)\varepsilon} + \partial_{yy} q^{(1)\varepsilon} \\ \varepsilon^2 \partial_{xx} q^{(2)\varepsilon} + \partial_{yy} q^{(2)\varepsilon} \end{pmatrix} = \begin{pmatrix} \partial_x p^\varepsilon \\ \varepsilon^{-1} \partial_y p^\varepsilon \end{pmatrix}, \quad \text{in } (0, T] \times \Omega \quad (7.9)$$

$$\partial_x q^{(1)\varepsilon} + \varepsilon^{-1} \partial_y q^{(2)\varepsilon} = 0, \quad \text{in } (0, T] \times \Omega \quad (7.10)$$

$$v_t^\varepsilon = f(u^\varepsilon, v^\varepsilon) \quad \text{on } (0, T] \times \Gamma, \quad (7.11)$$

$$-\nu \cdot \varepsilon D (\partial_x u^\varepsilon, \varepsilon^{-1} \partial_y u^\varepsilon) = \varepsilon v_t^\varepsilon \quad \text{on } (0, T] \times \Gamma, \quad (7.12)$$

$$\bar{q}^\varepsilon = 0, \quad \text{on } \Gamma. \quad (7.13)$$

We observe that the particular form of  $\Gamma$  implies  $\nu = (0, 1)^T$  on the upper part, resp.  $\nu = (0, -1)^T$  in the lower part, allowing to rewrite the normal solute flux as

$$-\nu \cdot \varepsilon D(\partial_x u^\varepsilon, \varepsilon^{-1} \partial_y u^\varepsilon) = \pm D \partial_y u^\varepsilon,$$

where the sign on the right is  $-$  in the upper part of  $\Gamma$ , and  $+$  in the lower part.

In the above,  $q^{(i)\varepsilon}$  ( $i = 1, 2$ ) are the two components the velocity  $\vec{q}^\varepsilon$ . As before, the Stokes equation (7.9)-(7.10) with the no-slip boundary condition (7.13) can be decoupled from the other equations of the model. To simplify the presentation, we assume that  $\vec{q}_b = (q_b^1, 0)$ , with  $q_b^1$  having a parabolic profile. This leads to a Poiseuille flow

$$q^{(1)\varepsilon}(y) = Q(1 - y^2), \quad q^{(2)\varepsilon} = 0,$$

where  $Q > 0$  is a given constant depending on the pressure gradient.

Assuming that the boundary and initial conditions are symmetric w.r.t.  $y = 0$ , this symmetry is then inherited by the model. In particular, it holds along the  $x$  axis

$$\partial_y u^\varepsilon = 0, \quad \text{for } x \in (0, 1) \text{ and } y = 0,$$

allowing to reduce the problem to the unit square  $(0, 1)^2$ , the upper half of the domain  $\Omega$ . The in- and outflow boundaries are reduced then accordingly, whereas for  $\Gamma$  we only consider its upper part  $[0, 1] \times \{1\}$ .

Further we assume the following asymptotic expansion for  $u^\varepsilon$  and  $v^\varepsilon$

$$\begin{aligned} u^\varepsilon &= u_0 + \varepsilon u_1 + O(\varepsilon^2), \\ v^\varepsilon &= v_0 + \varepsilon v_1 + O(\varepsilon^2). \end{aligned}$$

This gives

$$f(u^\varepsilon, v^\varepsilon) = f(u_0, v_0) + \varepsilon(\partial_1 f(u_0, v_0)u_1 + \partial_2 f(u_0, v_0)u_2) + O(\varepsilon^2),$$

where  $\partial_1 f$  is the partial derivative of  $f$  w.r.t. the first variable  $u$ , and similarly for  $\partial_2 f$ .

Using the expansion above in the convection-diffusion equation (7.8) gives

$$\begin{aligned}\partial_t u_0 + \varepsilon \partial_t u_1 &= \varepsilon D \partial_{xx} u_0 + \varepsilon^{-1} D \partial_{yy} u_0 + \varepsilon^2 D \partial_{xx} u_1 + D \partial_{yy} u_1 \\ &\quad - Q(1 - y^2) \partial_x (u_0 + \varepsilon u_1) + O(\varepsilon^2),\end{aligned}\tag{7.14}$$

for  $t \in (0, T]$  and  $x, y \in (0, 1)$ , whereas along  $y = 1$ , by (7.11), (7.12) one has

$$\begin{aligned}D(\partial_y u_0 + \varepsilon \partial_y u_1) &= \varepsilon \partial_t v_0 + \varepsilon^2 \partial_t v_1 + O(\varepsilon^3), \\ \partial_t v_0 + \varepsilon \partial_t v_1 &= f(u_0, v_0) + \varepsilon(\partial_1 f(u_0, v_0) u_1 + \partial_2 f(u_0, v_0) u_2) + O(\varepsilon^2).\end{aligned}\tag{7.15}$$

Finally, the symmetry along  $y = 0$  translates into

$$\partial_y u_0 + \varepsilon \partial_y u_1 + O(\varepsilon^2) = 0.\tag{7.16}$$

Now we proceed again by equating the terms having a similar order, which gives

- $\varepsilon^{-1}$  in (7.14) and  $\varepsilon^0$  in (7.15), (7.16):

$$\begin{aligned}D \partial_{yy} u_0 &= 0, \\ D \partial_y u_0 &= 0, \quad \text{along } y = 0 \text{ and } y = 1.\end{aligned}$$

Hence for  $u_0$  one gets

$$u_0(x, y, t) = u_0(x, t).$$

- $\varepsilon^0$  term in (7.14) and  $\varepsilon^1$  in (7.15), (7.16):

$$\partial_t u_0 - D \partial_{yy} u_1 + Q(1 - y^2) \partial_x u_0 = 0,\tag{7.17}$$

$$-D \partial_y u_1 = \partial_t v_0, \quad \text{along } y = 1,\tag{7.18}$$

$$\partial_t v_0 = f(u_0, v_0), \quad \text{along } y = 1,\tag{7.19}$$

$$\partial_y u_1 = 0, \quad \text{along } y = 0.\tag{7.20}$$

Integrating the first equation from  $y = 0$  to 1, and using the boundary conditions, (7.18) and (7.20) gives

$$\begin{aligned}\partial_t u_0 + \partial_t v_0 + \frac{2}{3} Q \partial_x u_0 &= 0, \\ \partial_t v_0 &= f(u_0, v_0),\end{aligned}\tag{7.21}$$

for all  $t \in (0, T]$  and  $x \in (0, 1)$ .

Note that (7.21) is in fact an upscaled equation for  $u_0$  and  $v_0$ , the first approximations of  $u^\varepsilon$  and  $v^\varepsilon$ . Since in the original model we have assumed that the diffusion is of order  $\varepsilon$ , the diffusive effects are not present in the upscaled model above, this having a hyperbolic type. Such an approximation is sufficiently good whenever  $\varepsilon$  is very small, i.e. if the scales are properly separated. Whenever  $\varepsilon$  is not small enough, the upscaled model in 7.21 provides an approximation of poor quality, and the higher order terms  $u_1$  and  $v_1$  have to be taken into account to improve the model. As will be seen below, this leads to an upscaled model that is similar to the Taylor dispersion, but includes the effects of the reactions.

To obtain an expression for  $u_1$ , we eliminate  $\partial_t u_0$  from equation (7.17). Subtracting (7.21) from (7.17) gives

$$-D\partial_{yy}u_1 + Q\left(\frac{1}{3} - y^2\right)\partial_x u_0 - \partial_t v_0 = 0. \quad (7.22)$$

Integrating the above with respect to  $y$  gives

$$u_1(x, y, t) = \frac{Q}{D} \left( \frac{y^2}{6} - \frac{y^4}{12} + C_0(x, t) \right) \partial_x u_0 + \frac{1}{D} \left( \frac{-y^2}{2} + C_1(x, t) \right) \partial_t v_0, \quad (7.23)$$

where  $C_0, C_1$  are expressions in  $x$  and  $t$  appearing due to integration. As will be seen later, there is no need for specifying any specific form for  $C_0$  and  $C_1$ , since these will cancel in the averaging process.

- $\varepsilon^1$  term in (7.14) and  $\varepsilon^2$  in (7.15), (7.16):

$$\partial_t u_1 - D(\partial_{xx}u_0 + \partial_{yy}u_2) + Q(1 - y^2)\partial_x u_1 = 0, \quad (7.24)$$

$$-D\partial_y u_2 = \partial_t v_1. \quad (7.25)$$

Integrating (7.24) from  $y = 0$  to  $y = 1$  and using the boundary conditions at  $y = 1$  and the symmetry at  $y = 0$  gives

$$\partial_t \int_0^1 u_1 - D\partial_{xx}u_0 + k\partial_t v_1 + Q \int_0^1 (1 - y^2)\partial_x u_1 dy = 0. \quad (7.26)$$

Defining

$$\bar{u}_1 = \int_0^1 u_1 dy,$$

(7.26) becomes

$$\partial_t \bar{u}_1 - D \partial_{xx} u_0 + \partial_t v_1 + Q \partial_x \bar{u}_1 = Q \int_0^1 y^2 \partial_x u_1 dy. \quad (7.27)$$

Adding (7.27) and (7.21) gives

$$\begin{aligned} & \partial_t(u_0 + \varepsilon \bar{u}_1) - \varepsilon D \partial_{xx} u_0 + \partial_t(v_0 + \varepsilon v_1) + \frac{2}{3} Q \partial_x(u_0 + \varepsilon \bar{u}_1) \\ &= \varepsilon Q \left( \int_0^1 y^2 \partial_x \bar{u}_1 dy - \frac{1}{3} \int_0^1 \partial_x \bar{u}_1 dy \right), \end{aligned} \quad (7.28)$$

With the effective concentrations

$$u_e = u_0 + \varepsilon \bar{u}_1,$$

$$v_e = v_0 + \varepsilon v_1,$$

(7.28) becomes

$$\partial_t(u_e + v_e) - \varepsilon D \partial_{xx} u_e + \frac{2}{3} Q \partial_x u_e = -\varepsilon^2 D \partial_{xx} \bar{u}_1 + \varepsilon Q \int_0^1 \left( y^2 - \frac{1}{3} \right) \partial_x \bar{u}_1. \quad (7.29)$$

To compute the  $\int_0^1 (y^2 - \frac{1}{3}) \partial_x \bar{u}_1$ , we can use the expression for  $u_1$  as obtained in equation (7.23). Basically, we need to compute the following integrals

$$\int_0^1 \left( y^2 - \frac{1}{3} \right) \left( \frac{y^2}{6} - \frac{y^4}{12} + C_0 \right) dy = \frac{8}{945},$$

and

$$\int_0^1 \left( y^2 - \frac{1}{3} \right) \left( C_1 - \frac{y^2}{2} \right) dy = \frac{-2}{45}.$$

We do not give any specific expressions for  $C_0, C_1$  as they will be eliminated later. Substituting in (7.29) the value of  $\int_0^1 (y^2 - \frac{1}{3}) \partial_x \bar{u}_1$  and using the integrals computed above leads to

$$\partial_t(u_e + v_e) - \varepsilon D \partial_{xx} u_e + \frac{2Q}{3} \partial_x u_e = -\varepsilon^2 D \partial_{xx} \bar{u}_1 + \frac{8\varepsilon}{945} \frac{Q^2}{D} \partial_{xx} u_0 - \frac{\varepsilon Q}{D} \frac{2}{45} \partial_{xt} v_0. \quad (7.30)$$

Hence, the upscaled equation takes the form,

$$\begin{aligned}
\partial_t(u_e + v_e) - \varepsilon D \partial_{xx} u_e + \frac{2Q}{3} \partial_x u_e &= -\varepsilon^2 D \partial_{xx} \bar{u}_1 \\
&+ \frac{8\varepsilon}{945} \frac{Q^2}{D} \partial_{xx} u_0 + \varepsilon^2 \frac{8}{945} \frac{Q^2}{D} \partial_{xx} \bar{u}_1 \\
&- \varepsilon^2 \frac{8}{945} \frac{Q^2}{D} \partial_{xx} \bar{u}_1 - \frac{\varepsilon Q}{D} \frac{2}{45} \partial_{xt} v_0 \\
&- \varepsilon^2 \frac{Q}{D} \frac{2}{45} \partial_{xt} v_1 + \varepsilon^2 \frac{Q}{D} \frac{2}{45} \partial_{xt} v_1.
\end{aligned}$$

Up to an error of order  $O(\varepsilon^2)$  this can be then rewritten as

$$\begin{aligned}
\partial_t(u_e + v_e) - \varepsilon D \partial_{xx} u_e + \frac{2Q}{3} \partial_x u_e &= -\varepsilon^2 D \partial_{xx} \bar{u}_1 \\
&+ \frac{8\varepsilon}{945} \frac{Q^2}{D} (\partial_{xx}(u_0 + \varepsilon \bar{u}_1)) \\
&- \varepsilon^2 \frac{8}{945} \frac{Q^2}{D} \partial_{xx} u_1 - \varepsilon \frac{Q}{D} \frac{2}{45} (\partial_{xt}(v_0 + \varepsilon v_1)) \\
&+ \varepsilon^2 \frac{Q}{D} \frac{2}{45} \partial_{xt} v_1.
\end{aligned}$$

For  $v_e$ , we can have, formally, by using Taylor expansion of  $f(u^\varepsilon, v^\varepsilon)$  around  $(u_e, v_e)$ ,

$$\begin{aligned}
\partial_t v_e = f(u^\varepsilon, v^\varepsilon) &= f(u_0 + \varepsilon \bar{u}_1, v_0 + \varepsilon v_1) + \varepsilon (u_1|_{y=1} - \bar{u}_1) \partial_1 f(u_0 + \varepsilon \bar{u}_1, v_0 + \varepsilon v_1) + O(\varepsilon^2) \\
&= f(u_e, v_e) + \varepsilon (u_1|_{y=1} - \bar{u}_1) \partial_1 f(u_e, v_e) + O(\varepsilon^2). \tag{7.31}
\end{aligned}$$

Further, recalling the expression for  $u_1$  and using (7.23), we have

$$\begin{aligned}
u_1(y=1) - \bar{u}_1 &= \frac{Q}{D} \left( \frac{1}{12} + C_0 - \frac{7}{180} - C_0 \right) \partial_x u_0 + \frac{1}{D} \left( C_1 - \frac{1}{2} - C_1 + \frac{1}{6} \right) \\
&= \left\{ \frac{Q}{D} \frac{2}{45} \partial_x u_0 - \frac{1}{3} \frac{1}{D} \partial_t v_0 \right\}. \tag{7.32}
\end{aligned}$$

Once again, we note that the values of  $C_0, C_1$  are unimportant. Finally, (7.31) and (7.32) give the final equation for  $v_e$ ,

$$\partial_t v_e = f(u_e, v_e) + \varepsilon \left\{ \frac{Q}{D} \frac{2}{45} \partial_x u_0 - \frac{1}{3} \frac{1}{D} \partial_t v_0 \right\} \partial_1 f(u_e, v_e).$$

Including the average velocity

$$\bar{q}_e = \int_0^1 q^{(1)\varepsilon}(y) dy = \int_0^1 Q(1 - y^2) dy = \frac{2}{3}Q,$$

we obtain the effective model for the transport dominated regime ( $Pe = O(\varepsilon^{-1})$ )

$$\begin{aligned} \partial_t(u_e + v_e) &= \partial_x \left\{ -u_e \bar{q}_e + \varepsilon D \left( 1 + \frac{2\bar{q}_e^2}{105D^2} \right) \partial_x u_e - \varepsilon \frac{1}{15} \frac{\bar{q}_e}{D} f(u_e, v_e) \right\} \\ \partial_t v_e &= f(u_e, v_e) + \varepsilon \left( -\frac{1}{3D} \partial_t v_e + \frac{1}{15D} \bar{q}_e \partial_x u_e \right) \partial_1 f(u_e, v_e). \end{aligned}$$

This model includes terms of order  $\varepsilon$ , so is an  $O(\varepsilon^2)$  approximation of the original model.