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HOMOGENIZATION OF COMPLEX FLOWS IN POROUS MEDIA AND APPLICATIONS

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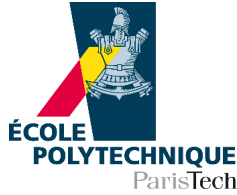
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Thesis submitted to obtain the title of

Doctor of École Polytechnique

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Homogenization of complex flows in porous media and applications

by

Harsha HUTRIDURGA RAMAIAH

under the supervision of

Grégoire ALLAIRE

defended publicly on 17 September 2013 in front of the jury composed of

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Prepared at

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HOMOGENIZATION OF COMPLEX FLOWS IN POROUS MEDIA AND APPLICATIONS

Harsha HUTRIDURGA RAMAIAH

Douter de tout ou tout croire, ce sont deux solutions également commodes, qui l'une et l'autre nous dispensent de réfléchir.

- Henri Poincaré.

To my parents
Shylaja & Ramaiah

and to my sister
Prathima

In the loving memory of
my grandmother *Lakshmiddevamma*
and my uncle *Suresh*

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Abstract

Our work is a contribution to the understanding of transport of solutes in a porous medium. It has applications in groundwater contaminant transport, CO₂ sequestration, underground storage of nuclear waste, oil reservoir simulations. We derive expressions for the effective Taylor dispersion taking into account convection, diffusion, heterogeneous geometry of the porous medium and reaction phenomena. Microscopic phenomena at the pore scale are upscaled to obtain effective behaviour at the observation scale. Method of two-scale convergence with drift from the theory of homogenization is employed as an upscaling technique. In the first part of our work, we consider reactions of mass exchange type, adsorption/desorption, at the fluid-solid interface of the porous medium. Starting with coupled convection-diffusion equations for bulk and surface concentrations of a single solute, coupled via adsorption isotherms, at a microscopic scale we derive effective equations at the macroscopic scale. We consider the microscopic system with highly oscillating coefficients in a strong convection regime i.e., large Péclet regime. The presence of strong convection in the microscopic model leads to the induction of a large drift in the concentration profiles. Both linear and nonlinear adsorption isotherms are considered and the results are compared. In the second part of our work we generalize our results on single component flow to multicomponent flow in a linear setting. In the latter case, the effective parameters are obtained using Factorization principle and two-scale convergence with drift. The behaviour of effective parameters with respect to Péclet number and Damköhler number are numerically studied. Freefem++ is used to perform numerical tests in two dimensions.

Keywords: Homogenization, Porous media, Periodic structures, Two-scale convergence, Dispersion Tensor, Reactive flows, Adsorption isotherms, Multicomponent flow.

Résumé

Ce travail est une contribution pour mieux comprendre le transport de solutés dans un milieu poreux. Ce phénomène se rencontre dans de nombreux domaines: transport de contaminants dans les eaux souterraines, séquestration du CO₂, stockage souterrain des déchets nucléaires, simulations de réservoirs pétroliers. On obtient la dispersion effective de Taylor en tenant compte de la convection, de la diffusion, de la géométrie du milieu poreux et des réactions chimiques. Le but de la théorie d'homogénéisation est, à partir d'équations microscopiques, de dériver un modèle effectif à l'échelle macroscopique. Ici, on applique la méthode de convergence à deux échelles avec dérive pour arriver au comportement effectif. Dans un premier temps, on considère les réactions de type adsorption à la surface des pores. À l'échelle microscopique, le phénomène de transport est modélisé par des équations couplées de type advection-diffusion, une pour la concentration dans le fluide et l'autre pour la concentration à la surface de milieu poreux. Le couplage est fait par les isothermes d'adsorption. Le système microscopique avec des coefficients fortement oscillants est étudié dans un régime de forte convection i.e., dans un régime de grand nombre de Péclet. La présence de forte convection dans le modèle microscopique se traduit par l'apparition d'une large dérive dans les profils de concentrations. On considère à la fois l'isotherme linéaire et l'isotherme non linéaire et les résultats ainsi obtenus sont comparés. Dans la deuxième partie, on généralise nos résultats concernant le transport réactif d'un seul soluté à ceux de plusieurs solutés dans un cadre linéaire. Dans ce cas, les paramètres effectifs sont obtenus en utilisant le principe de Factorisation et la convergence à deux échelles avec dérive. On étudie numériquement le comportement des paramètres effectifs par rapport au nombre de Péclet et au nombre de Damköhler. On utilise Freefem++ pour effectuer des tests numériques en dimension deux.

Mots clefs: Homogénéisation, Milieux poreux, Structures périodiques, Convergence à deux échelles, Tenseur de dispersion, Écoulements réactifs, Isothermes d'adsorption.

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Chapter 1

Introduction

This thesis is a contribution to the study of reactive flows in porous media. This general introduction to the thesis recalls some of the historical aspects regarding the study of the dispersion of dissolved solutes. We present the progress that has been made in the field of reactive transport. Some of the well known results are recounted. From Section 1.12 onwards, the contribution of this thesis is briefly described.

1.1 Historical background

It all started with [157] where Sir Geoffrey Taylor studied the spreading of a soluble substance dissolved in water flowing through a tube. The interplay between molecular diffusion and the variations in fluid velocity across a cross section of the tube were studied. The phenomenon of spreading is usually referred as “Dispersion”. Neither a simple molecular diffusion nor a simple convection can account for the effective mixing of solutes. Fick’s law states that the molecular diffusion is proportional to the concentration gradient i.e., the diffusive flux is always from the region of higher concentration to that of the lower concentration. So the diffusion is more pronounced only in presence of sharp concentration gradients. In case of pure convection, if the velocity were constant then the solutes are transported from one region to other with no change in distribution. In case of non constant velocity, however, the solute distribution is distorted. Thus, the presence of both convection and diffusion makes the study of dispersion of solutes very interesting. In [157], a fluid flowing through a tube is considered in which a solute is dissolved. Taking u to be the concentration of the dissolved solute, we can write the following advection-diffusion equation for the transport of solutes in the tube:

$$\frac{\partial u}{\partial t} + b(t, x) \cdot \nabla u - \operatorname{div}(D \nabla u) = 0 \quad \text{in } \mathbb{R}^+ \times \Omega \quad (1.1)$$

where Ω is the tube, b is the fluid velocity and D is the molecular diffusion. Through some heuristic arguments it is shown formally in [157] that the effective dispersion is given by

$$\mathcal{D} = D \left(1 + c \mathbf{Pe}^2 \right) \quad (1.2)$$

where $c \ll 1$ is some positive constant, D is the molecular diffusion and \mathbf{Pe} is a dimensionless number called the “Péclet number”. In the context of mass transport, the Péclet number is defined as

$$\mathbf{Pe} = \frac{L B}{\mathbf{D}} \quad (1.3)$$

where L is the characteristic length of the medium, B is the characteristic velocity and \mathbf{D} the characteristic diffusion. The expression (1.2) for the effective dispersion suggests that for large

Pe the dispersion is greater than the simple molecular diffusion. In [157], a Poiseuille flow was considered for the fluid flow in a tube and the solutes are considered to be inert i.e., absence of chemical reactions. Taylor, in [158], has even tried to obtain expression for the effective dispersion upon replacing Poiseuille flow of [157] by a turbulent flow. Since the seminal works of G.I. Taylor [157, 158, 159], the effective dispersion has come to be called “Taylor Dispersion” in the literature (In fact it was H. Brenner, in [47], who coined the term “Taylor Dispersion” as a tribute to the pioneering work of Taylor). As stated earlier, the results of Taylor were very formal. R. Aris, in [30], tried to make the theory of Taylor Dispersion more mathematically sound by using the method of moments. In the works [157, 30] of Taylor and Aris only a simple Poiseuille flow was considered for the fluid velocity. Since their works, there have been thousands of scientific articles that have been produced in relation to Taylor Dispersion owing to its importance in many applications ranging from flow in porous media to transport in arrays of regular convection cells, in plasma physics, and in the study of turbulence.

Solute transport in porous media is of paramount importance in chemical engineering, soil sciences, petroleum engineering, geology [95, 40] e.g., groundwater contaminant transport, carbon sequestration, underground storage of nuclear waste, oil reservoir simulations. In the 50’s as the dispersion theory of Taylor was gaining popularity, it was adapted to study the spreading of solutes in porous media. The porous media were modelled as networks of capillaries [146]. The geometrical characteristics of a porous medium are more complex than a simple network of capillaries. Also the Dispersion theory due to Taylor-Aris was conceived for unidirectional flows in a tube. P.G. Saffman in [146] applied the Taylor-Aris approach to study the dispersion of solutes in a porous medium assuming that the local velocity field is everywhere parallel to the mean velocity field in the domain. This is indeed the case for the Poiseuille flow in a capillary tube. A very good discussion on the drawbacks of this approach of supposing a porous medium as a network of capillaries is found in [47]. The study of dispersion in porous medium saw some new directions in the 70’s and 80’s. Remarkable contributions being the method of asymptotic analysis applied in the case of no net macroscopic convection [41] and the method of moments (borrowed from [30]) applied to the case of spatially periodic porous medium [46, 47, 48]. The crucial idea in the cited references being the consideration of convection-diffusion phenomena at the pore scale and averaging them over the entire porous medium, via asymptotic expansions in [41], and via the method of moments in [47]. This viewpoint of starting with pore scale phenomena followed by an averaging technique had appeared in [163, 164] in the context of volume averaging techniques.

1.2 Developments in Homogenization theory

The study of flows in porous media has been around for over 150 years. The first valuable discovery was realized by H. Darcy [72]. Based on some filtration experiments with a packed sand column, Darcy empirically formulated that the flow rate is proportional to the balance of forces including the pressure. This observation came to be known as “Darcy’s law”. For its enormous utility in petroleum engineering and groundwater hydrology, Darcy’s law has been heavily used in the industry since its discovery. Even though this was just an empirical result, only in the 60’s was some interest shown in justifying Darcy’s law via some theoretical analysis. A significant advancement was made in this direction by S. Whitaker in [164]. The analysis in [164] starts with a pore scale description followed by the averaging over a representative volume of the porous medium. The equivalent description for the pore scale description was found to be the well-known Darcy’s law. This conception of finding equivalent descriptions for highly heterogeneous phenomena gained attention of the scientific community and since then there has been a wave of new techniques to obtain these equivalent description in various contexts. In the

mechanics literature, these techniques are universally nomenclatured as “upscaling techniques”. The method of asymptotic expansions of [41] and the method of moments of [30, 47] qualify as some of those upscaling techniques. In mathematics literature, these techniques are referred to as “Homogenization”. Chapter 2 recounts some of the techniques in the theory of periodic homogenization. The method of volume averaging is a formal method as there is no prescribed rule on choosing a proper representative elementary volume. Also, during the analysis one has to close the systems of equations through some heuristic arguments. The method of volume averaging is frequently called “Representative Elementary Volume (REV) method”. This method is very well documented in the book of S. Whitaker [165].

Another prominent upscaling technique in the periodic regime is the method of two-scale asymptotic expansions. Let l denote the length scale of the heterogeneities present in the medium and L be the observation length scale. Under the assumption of scale separation, we define a scale parameter $\varepsilon = l/L \ll 1$. In a periodic setting, the period would be of $\mathcal{O}(\varepsilon)$. Under periodicity assumptions, the system of equations representing the physical phenomena in a medium usually takes the form

$$L_\varepsilon u_\varepsilon = f \quad \text{in } \Omega, \quad (1.4)$$

where L_ε is a partial differential operator with periodic coefficients, f is a source term and u_ε is the solution to the partial differential equation. As an effective equation, we wish to replace (1.4) by a continuum model posed in an equivalent macroscopic medium:

$$\bar{L} u = f \quad \text{in } \Omega, \quad (1.5)$$

where \bar{L} is the homogenized operator and u is the homogenized limit of u_ε . In a nutshell, the method of asymptotic expansions begins with an assumption that the solution u_ε to the partial differential equation (1.4) can be written in the form of an asymptotic expansion in terms of the period ε i.e.,

$$u_\varepsilon(t, x) = u_0\left(t, x, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(t, x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(t, x, \frac{x}{\varepsilon}\right) + \dots \quad (1.6)$$

where the coefficient functions $u_i(t, x, y)$ are Y -periodic with respect to the variable y . This approach was hinted at in [147, 36, 37, 103, 41, 38]. The method of two-scale asymptotic expansions was employed in [148, 115] to derive Darcy’s law as the effective model. Starting with steady Stokes equations at the pore scale, Darcy’s law is derived using the formal method of asymptotic expansions. Like the REV method and the method of moments, the method of asymptotic expansions is also a formal method as there is no guarantee as to why the postulated ansatz (1.6) holds. But this method has an added advantage as the results obtained by asymptotic expansions can be made mathematically rigorous using the theory of periodic homogenization. In Section 2.2 of Chapter 2, the method of two-scale asymptotic expansions is briefly depicted and is elucidated by applying it to the upscaling of steady incompressible Stokes equations in a periodic porous medium. Proposition 2.2.2 gives the homogenization result. This is just a reproduction of the result obtained in [148, 115].

As stated before, the formal method of asymptotic expansions can be made rigorous. L. Tartar proposed the “method of oscillating test functions” [153] (English translation in [55]) as a means to justifying the homogenization process. In loose terms this method aims at proving the convergence of u_ε , the solution to (1.4), to u , solution to (1.5), in a proper function space. It goes via choosing of proper test functions (thus the name) in the variational formulation of the microscopic partial differential equation (1.4) and passing to the limit as $\varepsilon \rightarrow 0$ to arrive at

a variational formulation for (1.5). The test functions are built using solutions to the so-called cell problems that we encounter in the asymptotic analysis. Tartar applied his method in justifying the upscaling of steady Stokes equations to Darcy’s law in [155] with a restriction on the solid part of the periodic porous medium that it is disconnected. G. Allaire in [3], using Tartar’s method, generalized this result even in the presence of connected solid part in a periodic porous medium. Tartar’s method, however, was introduced in the context of H-convergence [153, 131] (English translations in [55]) and is not very specific for the upscaling problems in periodic regimes. Any robust approach should take into account the periodic nature of the coefficients in (1.4). This breakthrough was found by G. Nguetseng in [132] where he introduced a compactness phenomenon suitable for periodic homogenization. This phenomenon was coined “Two-scale convergence” and was further developed by G. Allaire in [5]. Section 2.3 of Chapter 2 defines the notion of two-scale convergence and recalls some of the compactness results. In [115], the homogenization of unsteady incompressible Stokes equations in a periodic porous medium was undertaken. It was shown, formally, that the effective equation is a generalized Darcy’s law with memory terms. This result was formal as it used the two-scale asymptotic expansions method. G. Allaire in [4] employed the theory of “two-scale convergence” from [132, 5] to rigorously justify the upscaling done in [115]. Theorem 2.3.7 recalls the result obtained in [4].

Tartar’s Energy Method was introduced in the context of H-convergence where ‘H’ stands for Homogenization. In the literature, there has been a notion of G-convergence dedicated to the study of convergence associated to the sequence of symmetric operators [151]. The ‘G’ in G-convergence stands for Green as the convergence here, loosely speaking, corresponds to the convergence of the associated Green functions. H-convergence is a generalization of G-convergence to incorporate non-symmetric operators. We shall not be giving any more information on these two notions of convergence.

Quite recently, a new notion of upscaling technique called “Periodic unfolding” has been developed [58, 60, 59]. This method uses the dilation operator defined in [29]. This dilation operator has been employed by Lenczner and collaborators in the study of electrical networks [112, 113]. This notion of “Periodic unfolding” and its relation to the two-scale convergence is briefly recalled in Section 2.4 of Chapter 2.

1.3 Passive transport: Different mixing regimes

Simultaneously during all the above developments in the theory of periodic homogenization in the context of fluid flows in porous media and elasticity, there were quite a few results that were obtained in the theory of dispersion in porous media borrowing ideas from asymptotic analysis. It is to be noted that S. Whitaker did apply the theory of REV to upscale the dispersion phenomena in porous media [164]. The study of the dispersion of solutes can be widely categorized as

- Diffusion dominated mixing.
- Taylor dispersion mediated mixing.
- Chaotic advection.

The first category of “diffusion dominated mixing”, as the name suggests, considers the study of physical phenomena of transport where the diffusion is more pronounced at the microscopic scale. The second category of “Taylor dispersion mediated mixing” refers to the models where both convection and diffusion are important at the microscopic scale. In the final category “Chaotic

advection”, the turbulent effects at the microscopic scale for the velocity field are taken into account. This final category is quite complicated and is not well understood. A very good survey on the known results in the area of turbulent diffusion can be found in [120]. We shall content ourselves with the first two regimes in relation to transport phenomena in periodic porous media.

Let Ω_f denote the fluid part of the porous medium and Ω_s the solid part. Using the scale parameter ε , we define an ε -periodic porous medium as

$$\Omega_\varepsilon = \varepsilon \Omega_f \quad \text{and} \quad \partial\Omega_\varepsilon = \varepsilon \partial\Omega_s.$$

Let $Y =]0, 1[^d$ be the unit cell which is a disjoint union of Y^0 , the fluid part, and Σ^0 , the solid part.

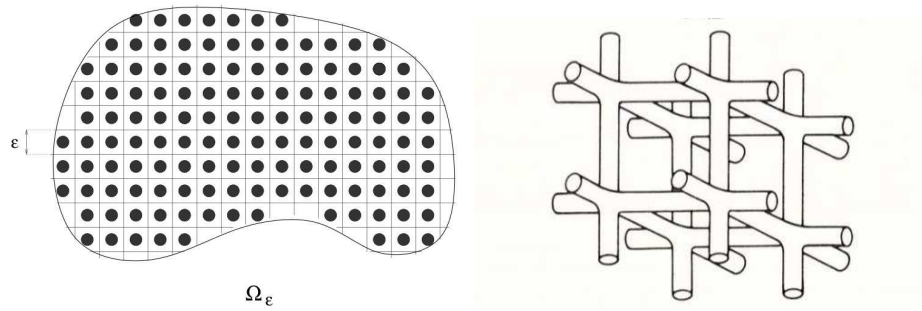


Figure 1.1: Schematics of porous media: Left, in two dimensions; Right, in three dimensions

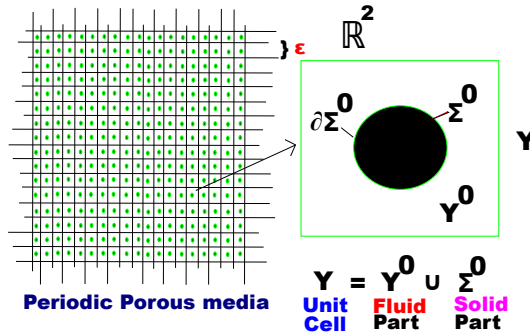


Figure 1.2: Schematics of an unbounded porous medium in two dimensions

To study the transport of the dissolved solutes, we consider the following convection-diffusion equation:

$$\begin{cases} \frac{\partial u}{\partial t} + b \cdot \nabla u - \operatorname{div}(D \nabla u) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ D \nabla u \cdot n = 0 & \text{on } (0, T) \times \partial\Omega_\varepsilon, \\ u(0, x) = u^{in}(x) & \text{in } \Omega_\varepsilon. \end{cases} \quad (1.7)$$

Associated with (1.7) there are the following time scales:

$$\begin{aligned}\tau_1 &= \frac{l}{B}, & \tau_2 &= \frac{l^2}{\mathbf{D}}, \\ \tau_3 &= \frac{L}{B}, & \tau_4 &= \frac{L^2}{\mathbf{D}},\end{aligned}\tag{1.8}$$

where B is the characteristic velocity and \mathbf{D} is the characteristic diffusion. The non dimensional numbers, local and global Péclet numbers, are defined respectively as

$$\mathbf{Pe}_l = \frac{\tau_2}{\tau_1}, \quad \mathbf{Pe}_g = \frac{\tau_4}{\tau_3}.\tag{1.9}$$

Upon dimensional analysis, we arrive at

$$\begin{cases} \frac{\partial u_\varepsilon}{\partial t} + \mathbf{Pe}_g b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ D_\varepsilon \nabla u_\varepsilon \cdot n = 0 & \text{on } (0, T) \times \partial\Omega_\varepsilon, \\ u_\varepsilon(0, x) = u^{in}(x) & \text{in } \Omega_\varepsilon, \end{cases}\tag{1.10}$$

where the unknown $u_\varepsilon(t, x) = u(\tau, y)$. The velocity field b_ε is governed by the Stokes equations, upon neglecting inertial and transient terms in the Navier-Stokes equations, at the pore scale:

$$\begin{cases} \nabla p_\varepsilon - \varepsilon^2 \mu \Delta b_\varepsilon = f & \text{in } \Omega_\varepsilon, \\ \operatorname{div} b_\varepsilon = 0 & \text{in } \Omega_\varepsilon, \\ b_\varepsilon = 0 & \text{on } \partial\Omega_\varepsilon. \end{cases}\tag{1.11}$$

1.4 Global Péclet regimes of $\mathcal{O}(\varepsilon)$ and $\mathcal{O}(1)$

In the literature, different scales are considered for \mathbf{Pe}_g . When $\mathbf{Pe}_g = \mathcal{O}(\varepsilon)$ and $\mathbf{Pe}_g = \mathcal{O}(1)$, we are in the ‘‘diffusion dominated mixing’’ regime. In [33] both these cases are considered. We shall state here a result in the regime $\mathbf{Pe}_g = \mathcal{O}(\varepsilon)$ due to Auriault and Adler.

Proposition 1.4.1. [33] *Let $\mathbf{Pe}_g = \mathcal{O}(\varepsilon)$ in (1.10). Under the assumption (1.6) on the solute concentration u_ε , the solution u_ε of (1.10) satisfy*

$$u_\varepsilon(t, x) \approx u_0(t, x) + \varepsilon u_1\left(t, x, \frac{x}{\varepsilon}\right)\tag{1.12}$$

where u_1 can be decomposed as

$$u_1(t, x, y) = \sum_{i=1}^d \omega_i(y) \frac{\partial u_0}{\partial x_i}(t, x)$$

and ω_i satisfy the following cell problem

$$\begin{cases} \operatorname{div}_y \left(D \left(\nabla_y \omega_i + e_i \right) \right) = 0 & \text{in } Y^0, \\ D \left(\nabla_y \omega_i + e_i \right) \cdot n = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow \omega_i(y) & Y\text{-periodic.} \end{cases}\tag{1.13}$$

The u_0 in (1.12) satisfies the following homogenized diffusion equation

$$\frac{\partial u_0}{\partial t} - \operatorname{div}(\mathcal{D} \nabla u_0) = 0 \quad \text{in } (0, T) \times \Omega.\tag{1.14}$$

The diffusion tensor \mathcal{D} is given in terms of the cell solution ω_i :

$$\mathcal{D}_{ij} = \int_{Y^0} D \left(\nabla_y \omega_i + e_i \right) \cdot \left(\nabla_y \omega_j + e_j \right) dy. \quad (1.15)$$

Remark that the velocity field b_ε in (1.10) does not appear in the cell problem (1.13), thus implying that the velocity field doesn't play much of a role in the transport phenomena at the pore scale. Also, it is interesting to note that the velocity plays no role in the homogenized equation (1.14) either. The regime $\mathbf{Pe}_g = \mathcal{O}(\varepsilon)$ is where the diffusion is predominant. Hence we can ignore the convection in (1.10).

Next interesting case in the category of "diffusion dominated mixing" is when $\mathbf{Pe}_g = \mathcal{O}(1)$. As the convection term didn't affect the upscaling process in the previous regime ($\mathbf{Pe}_g = \mathcal{O}(\varepsilon)$), we didn't see the impact of the homogenized velocity associated at the Darcy scale for (1.11). As both the fluid flow and the transport of solutes are coupled, we have to simultaneously homogenize both the equations (1.10) and (1.11). Similar to the ansatz for u_ε from (1.6), let us consider the following ansatz for the velocity and pressure fields.

$$b_\varepsilon(x) = b_0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon b_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 b_2\left(x, \frac{x}{\varepsilon}\right) + \dots \quad (1.16)$$

$$p_\varepsilon(x) = p_0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon p_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 p_2\left(x, \frac{x}{\varepsilon}\right) + \dots \quad (1.17)$$

We state below the upscaling result.

Proposition 1.4.2. [33] *Let $\mathbf{Pe}_g = \mathcal{O}(1)$ in (1.10). Under the assumption (1.6) on the solute concentration u_ε , the solution u_ε of (1.10) satisfies*

$$u_\varepsilon(t, x) \approx u_0(t, x) + \varepsilon u_1\left(t, x, \frac{x}{\varepsilon}\right) \quad (1.18)$$

where u_1 can be decomposed as

$$u_1(t, x, y) = \sum_{i=1}^d \omega_i(y) \frac{\partial u_0}{\partial x_i}(t, x)$$

and ω_i satisfy the following cell problem

$$\begin{cases} \operatorname{div}_y \left(D \left(\nabla_y \omega_i + e_i \right) \right) = 0 & \text{in } Y^0, \\ D \left(\nabla_y \omega_i + e_i \right) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \omega_i(y) & Y\text{-periodic.} \end{cases} \quad (1.19)$$

The u_0 in (1.18) satisfies the following homogenized convection-diffusion equation

$$\frac{\partial u_0}{\partial t} + \bar{b} \cdot \nabla u_0 - \operatorname{div}(\mathcal{D} \nabla u_0) = 0 \quad \text{in } (0, T) \times \Omega, \quad (1.20)$$

where

$$\bar{b}(x) = \int_{Y^0} b_0(x, y) dy \quad (1.21)$$

is the Darcy velocity that satisfies

$$\begin{cases} \bar{b}(x) = -\frac{1}{\mu} K \nabla p(x) & \text{in } \Omega, \\ \operatorname{div} \bar{b} = 0 & \text{in } \Omega, \\ \bar{b} \cdot n = 0 & \text{on } \partial\Omega, \end{cases} \quad (1.22)$$

with $p(x) \equiv p_0(x, y)$. The diffusion tensor \mathcal{D} in (1.20) is given in terms of the cell solution ω_i :

$$\mathcal{D}_{ij} = \int_{Y^0} D \left(\nabla_y \omega_i + e_i \right) \cdot \left(\nabla_y \omega_j + e_j \right) dy. \quad (1.23)$$

Let us point out that the cell problem (1.19) obtained in the regime $\mathbf{Pe}_g = \mathcal{O}(1)$ is still independent of the convection terms. Thus the diffusion is dominant at the pore scale. Also the cell problem (1.19) is the same as the cell problem (1.13) obtained in the regime $\mathbf{Pe}_g = \mathcal{O}(\varepsilon)$. The main distinction between the two regimes is with regard to the homogenized equations. The effective equation (1.14) in the regime $\mathbf{Pe}_g = \mathcal{O}(\varepsilon)$ is a pure diffusion equation. In the regime $\mathbf{Pe}_g = \mathcal{O}(1)$, however, we get a convection-diffusion equation (1.20) as a homogenized model. The convection being contributed by the Darcy velocity (1.21). A while ago, we remarked that the upscaling is done simultaneously. It just means that the asymptotic expansion (1.16) for b_ε is plugged in (1.10) and the asymptotic analysis is carried out. The details on the upscaling of Stokes equations (1.11) to arrive at Darcy law (1.22) is given in Section 2.2 of Chapter 2.

1.5 Global Péclet regime of $\mathcal{O}(\varepsilon^{-1})$

In both of the two regimes ($\mathbf{Pe}_g = \mathcal{O}(\varepsilon)$ or $\mathcal{O}(1)$) considered so far, the convective terms haven't appeared in the cell problems i.e., at the pore scale, thus diffusion playing a dominant role. The next regime of interest is where $\mathbf{Pe}_g = \mathcal{O}(\varepsilon^{-1})$. This regime is studied in [123, 145, 124, 33]. The contrast between the approach of [33, 124] and that of [123, 145] is the choice of the velocity fields. As pointed out before, in the Propositions 1.4.1 and 1.4.2, the upscaling is done with a velocity b_ε given by Stokes equations (1.11). So, there is a simultaneous upscaling. In [123], however, one of the cases studied is where the velocity field is assumed to be given and purely periodic. The governing equations for the velocity field aren't considered. As a result of this hypothesis, the velocity field $b_\varepsilon(x)$ takes the form $b(x/\varepsilon)$ implying no dependence on the slow variable. Consider a convection diffusion equation in a dominant Péclet regime i.e., $\mathbf{Pe}_g = \mathcal{O}(\varepsilon^{-1})$:

$$\frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) = 0. \quad (1.24)$$

Let b^* be the average of $b(y)$ over the fluid part of the unit cell Y^0 :

$$b^* = \frac{1}{|Y^0|} \int_{Y^0} b(y) dy. \quad (1.25)$$

In [123], an assumption is made that the velocity field $b(y)$ is of zero mean i.e., $b^* = 0$. Now we state a result due to McLaughlin, Papanicolaou and Pironneau.

Proposition 1.5.1. [123] *Under the assumption that the velocity field is of mean zero, the solution u_ε of (1.24) can be approximated as*

$$u_\varepsilon(t, x) \approx u_0(t, x) + \varepsilon \sum_{i=1}^d \omega_i \left(\frac{x}{\varepsilon} \right) \frac{\partial u_0}{\partial x_i}(t, x) \quad (1.26)$$

where ω_i satisfy the following cell problem, for every $1 \leq i \leq d$,

$$\begin{cases} b(y) \cdot (\nabla_y \omega_i + e_i) - \operatorname{div}_y (D(y) (\nabla_y \omega_i + e_i)) = 0 & \text{in } Y^0, \\ D(\nabla_y \omega_i + e_i) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \omega_i & Y\text{-periodic.} \end{cases} \quad (1.27)$$

Further the zero order approximation, $u_0(t, x)$, in (1.26) satisfies the following diffusion equation:

$$\begin{cases} \frac{\partial u_0}{\partial t} - \operatorname{div}(\mathcal{D} \nabla u_0) = 0 & \text{in } (0, T) \times \mathbb{R}^d, \\ u_0(0, x) = u^{in}(x) & x \in \mathbb{R}^d, \end{cases} \quad (1.28)$$

with a dispersion matrix \mathcal{D} given in terms of the cell solutions ω_i .

Note that the cell problem (1.27) has contributions both from the convective field and the diffusion. The assumption that $b^* = 0$ helps us deduce the solvability of the cell problem. The proof of the above Proposition 1.5.1 can be detailed using the formal method of two-scale asymptotic analysis. However, the mean zero condition on the fluid field is quite restrictive.

In [44], convection-diffusion equation in this regime of $\mathbf{Pe}_g = \mathcal{O}(\varepsilon^{-1})$ is studied. Homogenization procedure in [44] involves the upscaling of both the convection-diffusion equation and the fluid equations simultaneously. The convection-diffusion equation studied in [44] is

$$\frac{\partial u_\varepsilon}{\partial t} + b_\varepsilon \cdot \nabla u_\varepsilon - \varepsilon \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) = 0, \quad (1.29)$$

where the convection is driven by Darcy velocity b_ε which fluctuates according to the permeability fluctuations:

$$\begin{cases} b_\varepsilon = -K\left(\frac{x}{\varepsilon}\right) \nabla p_\varepsilon, \\ \operatorname{div} b_\varepsilon = 0. \end{cases} \quad (1.30)$$

The microscopic model (1.29) studied in [44] is quite different from the microscopic model (1.24) studied in [123]. Starting with

$$\frac{\partial u_\varepsilon}{\partial \tau} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) = 0 \quad (1.31)$$

and making the change of time variable: $\tau = \varepsilon^{-1} t$, we arrive at (1.29). This enables us to study the small time behaviour of the transport model in large Péclet regime. The classical asymptotic expansion (1.6) for u_ε that we have been considering has only one time scale and two space scales: x and $y = x/\varepsilon$. In [44], in addition to the two space scales, two time scales t and τ are also considered i.e.,

$$u_\varepsilon(t, x) = u_0(t, \tau, x, y) + \varepsilon u_1(t, \tau, x, y) + \varepsilon^2 u_2(t, \tau, x, y) \cdots \quad (1.32)$$

Taking the following asymptotic expansion for the pressure p_ε in (1.30)

$$p_\varepsilon(x) = p_0(x) + \varepsilon p_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 p_2\left(x, \frac{x}{\varepsilon}\right) + \cdots,$$

an asymptotic expansion for the Darcy velocity b_ε is obtained

$$b_\varepsilon \approx b_0 + \varepsilon b_1 + \varepsilon^2 b_2 + \cdots \quad (1.33)$$

We state a result from [44] that approximates the dispersion in this regime. The analysis in [44] is quite involved as it considers the effect of boundary layers. The following statement is intended to give a loose account of the results due to A. Bourgeat, M. Jurak and A.L. Piatnitski.

Proposition 1.5.2. [44] *Let us assume the asymptotic expansion (1.32) for the solute concentration u_ε , the solution of (1.29). The zero order concentration approximation, $u_0(t, x)$, satisfies the following transport equation:*

$$\frac{\partial u_0}{\partial t} + \bar{b}_0(x) \cdot \nabla u_0 = 0 \quad (1.34)$$

where \bar{b} is the mean of the zero order Darcy velocity

$$\bar{b}_0(x) = \int_{Y^0} b_0(x, y) dy. \quad (1.35)$$

Further the sum of first two non-oscillating terms of the expansion (1.32) i.e., $\mathcal{U}(t, x; \varepsilon) = u_0(t, x) + \varepsilon \bar{u}_1(t, x)$ satisfies

$$\frac{\partial \mathcal{U}}{\partial t} + (\bar{b}_0 + \bar{b}_1)(x) \cdot \nabla \mathcal{U} - \varepsilon \operatorname{div}(\mathcal{D}(x) \nabla \mathcal{U}) = \mathcal{O}(\varepsilon^2) \quad (1.36)$$

where \mathcal{D} is given in terms of solutions to a so-called cell problem:

$$\begin{cases} b_0 \cdot \nabla_y \omega_i - \operatorname{div}_y \left(D \left(\nabla_y \omega_i + e_i \right) \right) = (\bar{b}_0 - b_0) \cdot e_i & \text{in } Y^0, \\ D \left(\nabla_y \omega_i + e_i \right) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \omega_i(y) & Y\text{-periodic.} \end{cases} \quad (1.37)$$

Unlike the previous two regimes, the cell problem (1.37) has contributions from both convection and diffusion. This regime falls into the category of ‘‘Taylor dispersion mediated mixing’’ as we are considering the interplay between both convection and diffusion at the micro scale (pore scale or cell problem) as was the case with Taylor’s original studies of dispersion in a tube [157]. We remark that the cell solutions ω_i in (1.37) are not independent of the slow variable x . In the regimes $\mathbf{Pe}_g = \mathcal{O}(\varepsilon)$ and $\mathbf{Pe}_g = \mathcal{O}(1)$, the cell solutions were depending only on the fast variable y . The dependency of ω_i on x is due to its dependence on the pressure gradient $\nabla p(x)$. Result similar to Proposition 1.5.2 was also obtained by C.C. Mei in [124], J.L. Auriault and P.M. Adler in [33] but in a less rigorous manner.

1.6 Scaling arguments

The approach of considering different orders of the global Péclet number, as recalled in Sections 1.4 and 1.5, is well-received in the engineering literature. The governing equations in an heterogeneous medium are usually derived via dimensional analysis. In mathematics, one begins with a partial differential equation for the physical phenomena in the unit cell and via some scaling arguments, derives the governing equations for the entire heterogeneous medium. Well known scaling arguments are ‘‘parabolic’’ and ‘‘hyperbolic’’ scaling. These scalings are a simple change of variables. The following is called the hyperbolic scaling:

$$(\tau, y) \rightarrow (\varepsilon^{-1}t, \varepsilon^{-1}x). \quad (1.38)$$

It is so named because if we take a typical hyperbolic equation, say an advection equation in (τ, y) :

$$\frac{\partial u}{\partial \tau} + b \cdot \nabla_y u = 0 \quad (1.39)$$

and make the change of variables as in (1.38), the advection equation remains invariant i.e., we get an advection equation in (t, x) :

$$\frac{\partial u}{\partial t} + b \cdot \nabla_x u = 0. \quad (1.40)$$

The following is called the parabolic scaling:

$$(\tau, y) \rightarrow (\varepsilon^{-2}t, \varepsilon^{-1}x). \quad (1.41)$$

It is so named because if we take a typical parabolic equation, say a diffusion equation in (τ, y) :

$$\frac{\partial u}{\partial \tau} - \Delta_{yy} u = 0 \quad (1.42)$$

and make the change of variables as in (1.41), the diffusion equation remains invariant i.e., we get a diffusion equation in (t, x) :

$$\frac{\partial u}{\partial t} - \Delta_{xx} u = 0. \quad (1.43)$$

Now let us consider a convection-diffusion equation in the fluid part Ω_f of the porous medium. Let the convective field $b(y)$ be Y -periodic and the diffusion matrix $D(y)$ be Y -periodic.

$$\frac{\partial u}{\partial \tau} + b(y) \cdot \nabla_y u - \operatorname{div}_y(D(y)\nabla_y u) = 0 \quad \text{in } (0, \zeta) \times \Omega_f. \quad (1.44)$$

If we employ the hyperbolic scaling (1.38) in the above convection-diffusion equation, then we arrive at

$$\frac{\partial u_\varepsilon}{\partial t} + b_\varepsilon(x) \cdot \nabla_x u_\varepsilon - \varepsilon \operatorname{div}_x(D_\varepsilon(x)\nabla_x u_\varepsilon) = 0 \quad \text{in } (0, T) \times \Omega_\varepsilon. \quad (1.45)$$

This corresponds to the small time behaviour stated in Proposition 1.5.2. Remark that the scaling in the space variable resulted in a scaled domain Ω_ε which is nothing but the ε -periodic porous medium. Also note that the Y -periodic coefficients in (1.44) become ε -periodic in (1.45) as the space variable is scaled. The scaling parameter ε gets next to the diffusion term. The scaled equation (1.45) is similar to the transport equation (1.29) studied in [44]. The time scaling in (1.38) corresponds to the study for short times. On the other hand the time scaling in (1.41) corresponds to longer times. The scaled equation (1.45) can be homogenized by the classical two-scale asymptotic expansions [41, 148]. The homogenized equation corresponding to (1.45) is an advection equation of the type (1.34).

1.7 Two-scale asymptotics with drift

Let us scale the convection diffusion equation (1.44) using the parabolic change of variables (1.41):

$$\frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon(x) \cdot \nabla_x u_\varepsilon - \operatorname{div}_x(D_\varepsilon(x)\nabla_x u_\varepsilon) = 0 \quad \text{in } (0, T) \times \Omega_\varepsilon. \quad (1.46)$$

This is indeed the convection-diffusion equation (1.31) that we considered in the dominant global Péclet regime i.e., with $\mathbf{Pe}_g = \mathcal{O}(\varepsilon^{-1})$. This regime is also referred to as the “strong convection regime” due to the large convection term in (1.46).

Remark 1.7.1. *The final time T in (1.46) is related to the final time in (1.44) as $T = \varepsilon^2 \zeta$. Since $\zeta = \mathcal{O}(\varepsilon^{-2})$, the final time $T = \mathcal{O}(1)$.*

In Proposition 1.5.1 we cited a result from [123] treating zero mean flow fields. This situation was generalized a little bit in [121, 76, 25] by considering incompressible periodic flows with non zero mean i.e., we choose $b(y) \in L^\infty_{\#}(\Omega_f; \mathbb{R}^d)$ such that

$$\operatorname{div}_y b = 0 \text{ in } Y^0, \quad b \cdot n = 0 \text{ on } \partial \Sigma^0 \quad \text{and} \quad b^* = \frac{1}{|Y^0|} \int_{Y^0} b(y) dy. \quad (1.47)$$

Remark 1.7.2. *All through this thesis, the subscript $\#$ indicates a space of Y -periodic functions. Recall that Y^0 and Σ^0 are thought as subsets of the unit cell Y , identified with the unit torus \mathbb{T}^d i.e., Y^0 and Σ^0 are periodic subsets of \mathbb{R}^d .*

It is shown in [121, 76, 25] that the convection-diffusion equation (1.46) can still be upscaled by using a variant of the two-scale asymptotic expansions method. The authors in [121, 76, 25] consider the following ansatz for the solution of (1.46):

$$u_\varepsilon(t, x) = u_0\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) + \dots \quad (1.48)$$

If $b^* = 0$ in (1.48), the above ansatz falls back to the classical asymptotic expansion. This is called the method of ‘‘Two-scale asymptotic expansions with drift’’. This method is briefly recalled in Section 2.6 of Chapter 2 where we implement this method in the context of homogenizing the following advection-diffusion equation in a porous medium:

$$\begin{cases} \frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b\left(\frac{x}{\varepsilon}\right) \cdot \nabla u_\varepsilon - \operatorname{div}\left(D\left(\frac{x}{\varepsilon}\right) \nabla u_\varepsilon\right) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ D\left(\frac{x}{\varepsilon}\right) \nabla u_\varepsilon \cdot n = 0 & \text{on } (0, T) \times \partial \Omega_\varepsilon, \\ u_\varepsilon(0, x) = u^{in}(x) & x \in \Omega_\varepsilon. \end{cases} \quad (1.49)$$

As in any method of asymptotic analysis, we need to plug the postulated ansatz into the partial differential equation under consideration. While plugging (1.48), we need to keep in mind the following chain rule for differentiation:

$$\begin{cases} \frac{\partial}{\partial t} \left[\phi\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) \right] = \left[\frac{\partial \phi}{\partial t} - \frac{b^*}{\varepsilon} \cdot \nabla_x \phi \right] \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right), \\ \nabla \left[\phi\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) \right] = \left[\nabla_x \phi + \frac{1}{\varepsilon} \nabla_y \phi \right] \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right). \end{cases} \quad (1.50)$$

We shall state below a formal result on the homogenization of (1.49) using the method of two-scale asymptotic expansions with drift. The details of the proof are found in Section 2.6.

Proposition 1.7.3. *Under the assumption (1.48), the solution for (1.49) formally satisfies*

$$u_\varepsilon(t, x) \approx u_0\left(t, x - \frac{b^* t}{\varepsilon}\right) + \varepsilon u_1\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) \quad (1.51)$$

where the first order corrector u_1 can be written as

$$u_1(t, x, y) = \sum_{i=1}^d \omega_i(y) \frac{\partial u_0}{\partial x_i}(t, x) \quad (1.52)$$

and the zero order term u_0 in (1.51) satisfies the following effective diffusion equation:

$$\begin{cases} |Y^0| \frac{\partial u_0}{\partial t} = \operatorname{div}(\mathcal{D}\nabla u_0) & \text{in } (0, T) \times \mathbb{R}^d, \\ u_0(0, x) = u^{in}(x) & x \in \mathbb{R}^d. \end{cases} \quad (1.53)$$

The elements of the dispersion tensor \mathcal{D} are given by

$$\mathcal{D}_{ij} = \int_{Y^0} D(y) (\nabla_y \omega_i + e_i) \cdot (\nabla_y \omega_j + e_j) dy \quad (1.54)$$

where ω_i in (1.54) and (1.52) satisfy the following cell problem, for each $1 \leq i \leq d$,

$$\begin{cases} b(y) \cdot (\nabla_y \omega_i + e_i) - \operatorname{div}_y (D(y) (\nabla_y \omega_i + e_i)) = b^* \cdot e_i & \text{in } Y^0, \\ D(y) (\nabla_y \omega_i + e_i) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \omega_i & Y\text{-periodic.} \end{cases} \quad (1.55)$$

As expected, both the convection and diffusion play role in the cell problem (1.55). This was indeed the case in the cell problem (1.37). The dispersion tensor \mathcal{D} is symmetric positive definite.

Remark 1.7.4. *The asymptotic expansion (1.48) can handle the upscaling of (1.49) only if the velocity field b_ε is purely periodic which in turn guarantees that the drift b^* is a constant. The chain rule differentiation given in (1.50) no longer holds if b^* were not a constant. The supposition of pure periodicity for the velocity field is quite restrictive. Stokes equations (1.11) posed in a porous medium spits out purely periodic velocity fields only if the forces, including the pressure gradients, remain constant over the entire domain Ω_ε .*

Remark 1.7.5. *From Proposition 1.7.3, we gather that the effective equation is a diffusion equation. This is resulted because of our choice of the ansatz (1.48) where each of the u_i 's are written in moving coordinates with respect to the slow variable x . Let us define a new effective concentration:*

$$\tilde{u}_\varepsilon(t, x) = u_0 \left(t, x - \frac{b^* t}{\varepsilon} \right) \quad (1.56)$$

which satisfies the following convection diffusion equation

$$|Y^0| \frac{\partial \tilde{u}_\varepsilon}{\partial t} + |Y^0| \frac{b^*}{\varepsilon} \cdot \nabla \tilde{u}_\varepsilon - \operatorname{div}(\mathcal{D}\nabla \tilde{u}_\varepsilon) = 0 \quad \text{in } (0, T) \times \mathbb{R}^d \quad (1.57)$$

with the same initial condition as in (1.53). So the assumed ansatz (1.48) in moving coordinates makes sure that the observer gets to see only the diffusion due to \mathcal{D} . For a purely periodic velocity field b_ε , the Darcy scale velocity is $|Y^0|b^*$. So the above upscaling is as though we homogenized both the transport and fluid equations simultaneously.

This notion of taking asymptotic expansions in moving coordinates was first suggested by A. Piatnitski in [140]. Homogenization of (1.49) with a macroscopically modulated velocity b_ε i.e., of the form $b(x, x/\varepsilon)$ is still an open problem.

1.8 Reactive transport: Different mixing regimes

Earlier works on Taylor Dispersion in porous media were concerned with inert solutes as was the assumption in Taylor's original work [157]. In many natural phenomena and industrial applications involving transport of solutes, we have to consider the chemical reactions. The practical applications of the reactive flows and their mathematical modeling were given by J. Rubin in [144]. The qualitative properties of the Reaction-Diffusion equations taken from [144] were studied in [73]. As in the study of passive scalar transport, we can consider different scales for the different phenomena in reactive flows too. Thus the reactive flows in porous media could also be studied under different categories.

- Diffusion dominated mixing.
- Taylor dispersion mediated mixing.
- Chaotic advection.

1.9 Diffusion dominated mixing: Adsorption reactions

The regime of "Diffusion dominated mixing" were studied in the 90's and the theory related to it is very well developed. Adsorption reaction represents the exchange of mass between the fluid bulk and the surface. The adsorption reactions are characterized by the associated isotherms. Isotherms express the relationship between the bulk concentration and the adsorbed concentration, at a constant temperature, when the reaction is in equilibrium. Let u be the solute concentration in the bulk and v be the adsorbed solute concentration on the surface. In the literature, there are the following well known isotherms:

$$\left\{ \begin{array}{lll} \text{Henry's isotherm} & v = K u & \text{with } K > 0, \\ \text{Langmuir's isotherm} & v = \frac{\alpha u}{1 + \beta u} & \text{with } \alpha, \beta > 0, \\ \text{Freundlich's isotherm} & v = \gamma u^\delta & \text{with } \gamma > 0 \text{ and } 0 < \delta < 1. \end{array} \right. \quad (1.58)$$

Taking $f(u)$ to be one of the isotherms in (1.58), in the non-equilibrium regime we can write the following governing equations for the solute concentrations (u, v) :

$$\left\{ \begin{array}{ll} \frac{\partial u}{\partial \tau} + b \cdot \nabla u - \operatorname{div}(D \nabla u) = 0 & \text{in } (0, \zeta) \times \Omega_f \\ -D \nabla u \cdot n = \frac{\partial v}{\partial \tau} = \kappa (f(u) - v) & \text{on } (0, \zeta) \times \partial \Omega_s \\ u(0) = u^{in} \text{ in } \Omega_f, \quad v(0) = v^{in} \text{ on } \partial \Omega_s, \end{array} \right. \quad (1.59)$$

where κ is the reaction rate. Note that an ordinary differential equation is considered for the adsorbed concentration. In [78], the mathematical justification of the isotherms (1.58) is shown. Travelling wave solutions are shown to exist for (1.59). Apart from the explicit expressions for the nonlinear isotherms in (1.58), a classification of isotherms is done in [78]. They classify the nonlinear isotherms as concave and convex isotherms. An isotherm is called "convex" if f is strictly convex near 0. In the category of "concave isotherms", two sub-categories are considered namely

$$\text{Langmuir type if } f \text{ is strictly concave near } 0 \text{ and } f'(0+) < +\infty \quad (1.60)$$

and

$$\text{Freundlich type if } f \text{ is strictly concave near } 0 \text{ and } f'(0+) = +\infty. \quad (1.61)$$

The explicit expressions for Langmuir and Freundlich isotherms given in (1.58) do fall into their respective categories. The qualitative analysis of (1.59) is also undertaken in [77, 78, 79, 80]. The study of (1.59) falls under the regime of ‘‘Diffusion dominated mixing’’ as only diffusion plays a major role at the pore scales. In [97], the ordinary differential equation for v in (1.59) is replaced by a diffusion equation, the diffusion being modelled by the Laplace Beltrami operator on the surface. Also the linear isotherm is considered to represent the adsorption phenomenon. The microscopic model studied in [97] is

$$\left\{ \begin{array}{ll} \nabla p_\varepsilon - \varepsilon^2 \Delta b_\varepsilon = f & \text{in } \Omega_\varepsilon, \\ \operatorname{div} b_\varepsilon = 0 & \text{in } \Omega_\varepsilon, \\ b_\varepsilon = 0 & \text{on } \partial\Omega_\varepsilon, \\ \frac{\partial u_\varepsilon}{\partial t} + b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ -D_\varepsilon \nabla u_\varepsilon \cdot n = \varepsilon g_\varepsilon(t, x) & \text{on } (0, T) \times \partial\Omega_\varepsilon, \\ \frac{\partial v_\varepsilon}{\partial t} - \varepsilon^2 \operatorname{div}^s(D_\varepsilon^s \nabla^s v_\varepsilon) + a_\varepsilon(x) v_\varepsilon = g_\varepsilon(t, x) & \text{on } (0, T) \times \partial\Omega_\varepsilon, \\ u(0, x) = u^{in}(x) \text{ in } \Omega_\varepsilon, \quad v(0, x) = v^{in}(x) \text{ on } \partial\Omega_\varepsilon. \end{array} \right. \quad (1.62)$$

where ∇^s and div^s represent the tangential gradient and tangential divergence respectively. Taking the projection matrix on the tangent hyperplane to the surface $\partial Y^0 = \partial \Sigma^0$ as

$$G(y) = \operatorname{Id} - n(y) \otimes n(y), \quad (1.63)$$

the tangential gradient is defined as

$$\nabla^s = G(y) \nabla \quad (1.64)$$

and the tangential divergence for any vector field $\Psi(y) : \Omega_f \rightarrow \mathbb{R}^d$ as

$$\operatorname{div}^s \Psi = \operatorname{div}(G(y) \Psi). \quad (1.65)$$

The adsorption reaction in (1.62) is modelled as

$$g_\varepsilon(t, x) = g\left(t, x, \frac{x}{\varepsilon}\right) \text{ with } g(t, x, y) = c(y)u(t, x) - d(y)v(t, x). \quad (1.66)$$

Remark 1.9.1. *The scale parameter ε next to the boundary condition in the fifth line of (1.62) just means that the reaction is considered to be weak in comparison to other transport phenomena like the diffusion and convection. The ε^2 next to the surface diffusion term means that it is very small compared to the bulk diffusion.*

The velocity field b_ε in (1.62) is governed by the steady Stokes equations. It is proved in [97] that the effective equation corresponding to (1.62) is the following:

$$\left\{ \begin{array}{ll} b_0(x) = -K \nabla p(x) & \text{in } \Omega, \\ \operatorname{div} b_0(x) = 0 & \text{in } \Omega, \\ |Y^0| \frac{\partial u_0}{\partial t} + b_0 \cdot \nabla u_0 - \operatorname{div}(D \nabla u_0) + \int_{\partial \Sigma^0} g(t, x, y) d\sigma(y) = 0 & \text{in } (0, T) \times \Omega, \\ \frac{\partial v_0}{\partial t} - \operatorname{div}^s(D^s \nabla^s v_0) + a(y)v_0 = g(t, x, y) & \text{on } (0, T) \times \Omega \times \partial \Sigma^0, \end{array} \right. \quad (1.67)$$

where the effective bulk and surface diffusions \mathcal{D} and \mathcal{D}^s are given in terms of the so-called cell problems that are just diffusion equations. In (1.67) b_0 is the effective Darcy velocity, K is the permeability tensor and $p(x)$ is the effective pressure. The zero order approximation $u_0(t, x)$ for the bulk concentration is independent of the fast variable. But the zero order approximation $v_0(t, x, y)$ of the surface concentration has both the slow and fast variables.

Remark 1.9.2. *Note that the coupled nature of the microscopic equation (1.62) continues on to the homogenized equation (1.67).*

Tartar’s method of “oscillating test functions” is employed in [97] to arrive at the homogenized limit. It is to be noted that the regime of “Diffusion dominated mixing” can be studied in bounded porous media. So the microscopic equation (1.62) is supplemented with appropriate boundary data on the exterior boundary of the porous medium. As there are sequences defined on the porous skeleton, we have to be careful while applying the standard compactness results of functional analysis.

[98] is another interesting reference where a similar phenomena of convection diffusion in the bulk and diffusion on the surfaces is studied. In [98], the non-penetrating condition for the velocity field on the porous skeleton is lifted i.e., the porous skeleton is semi-permeable. The solutes that enter the permeable solid in the porous medium are considered to be diffusing inside the semi-permeable solid medium. Here again, function sequences defined on surfaces have to be considered to obtain the effective limit of the microscopic model. We remarked earlier in Section 1.2 that the Tartar’s method can be replaced by a more adapted “Two-scale convergence” in a periodic setting. The extension of the notion of “Two-scale convergence” to function sequences defined on periodic surfaces was achieved in [14, 134]. This extension of two-scale convergence is recounted in Section 2.5 of Chapter 2. It is to be noted that this notion of compactness for sequences on periodic surfaces can simplify the analysis in [97, 98] to a great extent.

It is to be noted that Cioranescu and Donato had approached the homogenization of steady state problems in perforated domain with non-homogeneous boundary data in [61]. This article was written before the notion of two-scale convergence appeared in the literature. In [61], they use the variational approach via Tartar’s Energy Method. To handle the surface integral terms in the variational formulation, they introduce an auxiliary problem which helps transform the surface integral into a volume integral. Then, the proof of Homogenization utilizes information from the convergence in the associated linear forms. For precise details, do refer [61].

The mathematical modelling in [98] has very close ties to the double porosity model of [29]. The double porosity model was formulated to study the flow in fractured porous media. The transport model considered in [98] also falls under the category of “Diffusion dominated mixing”. Homogenization in this regime, even in the presence of nonlinear reaction terms, is well understood. This is demonstrated in [98] in case of semi-permeable porous media, in [81] with regard to adsorption reactions, in [69, 68, 64] in the context of pure steady diffusion equation with Langmuir adsorption on the surfaces. As in the case of passive transport, this regime of “Diffusion dominated mixing” in the context of reactive flows has seen enormous progress in the last two decades.

1.10 Reactive transport: Taylor dispersion mediated mixing

The next regime that we wish to consider is that of “Taylor dispersion mediated mixing”. We remarked earlier in the case of passive transport, this regime is the richest regime as it takes into account both convection and diffusion at the micro scale. In the context of reactive flows, we

shall consider the reaction in addition to convection and diffusion at the pore scale. R. Mauri in [122] studied the homogenization of a convection-diffusion-reaction phenomena in this regime:

$$\begin{cases} \frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ D_\varepsilon \nabla u_\varepsilon \cdot n + \frac{\kappa}{\varepsilon} u_\varepsilon = 0 & \text{on } (0, T) \times \partial\Omega_\varepsilon, \\ u_\varepsilon(0, x) = u^{in}(x) & \text{in } \Omega_\varepsilon. \end{cases} \quad (1.68)$$

The system (1.68) of [122] was generalized in [25] by considering a large lower order term in the bulk equation representing the bulk reactions. So the new model looks like

$$\begin{cases} \frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) + \frac{1}{\varepsilon^2} c_\varepsilon u_\varepsilon = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ D_\varepsilon \nabla u_\varepsilon \cdot n + \frac{\kappa}{\varepsilon} u_\varepsilon = 0 & \text{on } (0, T) \times \partial\Omega_\varepsilon, \\ u_\varepsilon(0, x) = u^{in}(x) & \text{in } \Omega_\varepsilon. \end{cases} \quad (1.69)$$

The velocity field in (1.69) is considered to be periodic and no further assumptions are made. In [25], the following spectral problem associated with (1.69) is considered:

$$\begin{cases} b(y) \cdot \nabla_y \phi - \operatorname{div}_y(D(y) \nabla_y \phi) + c(y) \phi = \lambda \phi & \text{in } Y^0, \\ D(y) \nabla_y \phi \cdot n + \kappa \phi = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow \phi(y) & Y\text{-periodic.} \end{cases} \quad (1.70)$$

The adjoint of (1.70) is

$$\begin{cases} -\operatorname{div}_y(b(y) \phi^*) - \operatorname{div}_y(D(y) \nabla_y \phi^*) + c(y) \phi^* = \lambda \phi^* & \text{in } Y^0, \\ D(y) \nabla_y \phi^* \cdot n + b(y) \cdot n \phi^* + \kappa \phi^* = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow \phi^*(y) & Y\text{-periodic.} \end{cases} \quad (1.71)$$

To perform the upscaling, a slight variant of the asymptotic ansatz (1.48) for the unknown concentration u_ε in (1.69) is considered:

$$u_\varepsilon(t, x) = \exp(-\lambda t / \varepsilon^2) \sum_{i \geq 0} \varepsilon^i u_i \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \quad (1.72)$$

The homogenization result for (1.69) due to G. Allaire and A.L. Raphael is summarized below.

Proposition 1.10.1. [25] *Under the assumption (1.72), the solution for the microscopic model satisfies*

$$u_\varepsilon(t, x) \approx \exp(-\lambda t / \varepsilon^2) \phi\left(\frac{x}{\varepsilon}\right) \left(v\left(t, x - \frac{b^* t}{\varepsilon}\right) + \varepsilon \sum_{i=1}^d \frac{\partial v}{\partial x_i} \left(t, x - \frac{b^* t}{\varepsilon}\right) \omega_i\left(\frac{x}{\varepsilon}\right) \right), \quad (1.73)$$

with (λ, ϕ) being the first eigenpair associated with (1.70). The components $(\omega_i)_{1 \leq i \leq d}$ satisfy the following cell problem:

$$\begin{cases} \tilde{b}(y) \cdot (\nabla_y \omega_i + e_i) - \operatorname{div}_y(\tilde{D}(\nabla_y \omega_i + e_i)) = \phi \phi^* b^* \cdot e_i & \text{in } Y^0, \\ \tilde{D}(\nabla_y \omega_i + e_i) \cdot n = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow \omega_i & Y\text{-periodic,} \end{cases} \quad (1.74)$$

where the convective field $\tilde{b}(y)$ and the diffusion matrix $\tilde{D}(y)$ are given in terms of the original velocity field $b(y)$, diffusion matrix $D(y)$ and the eigenfunctions $\phi(y)$ and $\phi^*(y)$:

$$\begin{aligned}\tilde{b}(y) &= \phi\phi^*b(y) + \phi D\nabla_y\phi^* - \phi^* D\nabla_y\phi, \\ \tilde{D}(y) &= \phi\phi^*D(y).\end{aligned}\tag{1.75}$$

The effective drift in (1.73) is given by

$$b^* = \int_{Y^0} \tilde{b}(y) dy.\tag{1.76}$$

Further, the zero order concentration approximation $v(t, x)$ satisfies the following diffusion equation:

$$\begin{cases} \frac{\partial v}{\partial t} = \operatorname{div}(D\nabla u) & \text{in } (0, T) \times \mathbb{R}^d, \\ v(0, x) = \frac{u^{in}(x)}{\phi(x/\varepsilon)} & \text{in } \mathbb{R}^d, \end{cases}\tag{1.77}$$

where the dispersion matrix \mathcal{D} is given in terms of the cell solutions:

$$\mathcal{D}_{ij} = \int_{Y^0} \tilde{D}(\nabla_y\omega_i + e_i) \cdot (\nabla_y\omega_j + e_j) dy.\tag{1.78}$$

We took a modified asymptotic expansion (1.72) for the unknown concentration. This idea of performing time renormalization in terms of the first eigenvalue of the spectral problem was identified in [12, 76]. We can also perform a change of unknowns in the spirit of Factorization principle:

$$v_\varepsilon(t, x) = \exp(\lambda t/\varepsilon^2) \frac{u_\varepsilon(t, x)}{\phi(x/\varepsilon)}.\tag{1.79}$$

Writing down the equation satisfied by v_ε we can perform the asymptotic analysis with “Two-scale asymptotic expansions with drift”. The Factorization principle has been around in the theory of homogenization since the 80’s [161]. Section 2.8 of Chapter 2 details the Factorization principle when applied to the eigenvalue problems and also to the case of convection-diffusion equations in strong convection regime with a bulk reaction term.

The “Two-scale convergence method” was conceived to justify the upscaling results obtained via the formal method of two-scale asymptotic analysis. Section 2.3 of Chapter 2 explains the “Two-scale convergence” approach in deriving effective Darcy law for the unsteady incompressible Stokes equations. In the same spirit, a new notion of compactness was developed by Marusic-Paloka and Piatnitski in [121]. This new conception of [121] is coined as “Two-scale convergence with drift”. As the name suggests, it tries to justify the homogenization results obtained through “Two-scale asymptotic expansions with drift”. We briefly explain the concepts involved with “Two-scale convergence with drift” in Section 2.6 of Chapter 2. This notion of compactness is used in rigorously justifying the result of the above Proposition 1.10.1 in [25].

1.11 Taylor-Aris regime: Adsorption via isotherms

In (1.69), the bulk reaction is modelled by a lower order term, $c_\varepsilon u_\varepsilon$, and the surface reaction is modelled via $k u_\varepsilon$ appearing as a Neumann data for the flux. The particular reactions of adsorption type have been studied exhaustively in the regime of “Diffusion dominated mixing”.

Very important references being [77, 97, 78, 79, 80, 81, 69, 68, 64]. In all these cited references, except for [69, 68, 64], in order to study the adsorption models, two concentrations are introduced: one for the concentration in the fluid bulk and the other for the concentration of the adsorbed solutes on the surface. In [10, 20], coupled convection-diffusion-reaction equations are considered for the solute concentrations (u, v) :

$$\begin{cases} \frac{\partial u}{\partial \tau} + b(y) \cdot \nabla u - \operatorname{div}(D(y)\nabla u) = 0 & \text{in } (0, T) \times \Omega_f, \\ -D(y)\nabla u \cdot n = \frac{\partial v}{\partial \tau} = \kappa \left(u - \frac{v}{K} \right) & \text{on } (0, T) \times \Omega_s. \end{cases} \quad (1.80)$$

The above model is supplemented with initial data for u and v . The adsorption is modelled in (1.80) using the linear isotherm from (1.58). Upon parabolic scaling, (1.80) leads to

$$\begin{cases} \frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ -\frac{1}{\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot n = \frac{\partial v_\varepsilon}{\partial t} = \frac{\kappa}{\varepsilon^2} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right) & \text{on } (0, T) \times \Omega_\varepsilon, \\ u_\varepsilon(0, x) = u^{in}(x) & x \in \Omega_\varepsilon, \\ v_\varepsilon(0, x) = v^{in}(x) & x \in \partial\Omega_\varepsilon. \end{cases} \quad (1.81)$$

In [10], the formal method of two-scale asymptotic expansions with drift is used to upscale the microscopic model (1.81). Note that the governing equation for v_ε in the coupled system (1.81) is just an ordinary differential equation. Consider the following asymptotic expansions for the concentrations:

$$\begin{aligned} u_\varepsilon(t, x) &= \sum_{i \geq 0} \varepsilon^i u_i \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \\ v_\varepsilon(t, x) &= \sum_{i \geq 0} \varepsilon^i v_i \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \end{aligned} \quad (1.82)$$

Proposition 1.11.1. [10], [20] *Under the assumption (1.82), the solution $(u_\varepsilon, v_\varepsilon)$ of (1.81) satisfies*

$$\begin{aligned} u_\varepsilon(t, x) &\approx u_0 \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon u_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \\ v_\varepsilon(t, x) &\approx K u_0 \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon v_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \end{aligned} \quad (1.83)$$

where b^* is the effective drift given by

$$b^* = \left(|Y^0| + K |\partial\Sigma^0| \right)^{-1} \int_{Y^0} b(y) dy. \quad (1.84)$$

The first order correctors u_1 and v_1 in (1.83) satisfy

$$\begin{aligned} v_1(t, x, y) &= K u_1(t, x, y) + \frac{K^2}{\kappa} b^* \cdot \nabla_x u_0(t, x) \\ u_1(t, x, y) &= \sum_{i=1}^d \omega_i(y) \frac{\partial u_0}{\partial x_i}(t, x) \end{aligned} \quad (1.85)$$

where ω_i satisfies, for each $1 \leq i \leq d$,

$$\begin{cases} b(y) \cdot \nabla_y \omega_i - \operatorname{div}_y(D(\nabla_y \omega_i + e_i)) = (b^* - b) \cdot e_i & \text{in } Y^0, \\ -D(\nabla_y \omega_i + e_i) \cdot n = K b^* \cdot e_i & \text{on } \partial \Sigma^0, \\ y \rightarrow \omega_i(y) & Y\text{-periodic.} \end{cases} \quad (1.86)$$

Further, the zero order concentration approximation $u_0(t, x)$ in (1.83) satisfies the following diffusion equation:

$$\begin{cases} \left(|Y^0| + K|\partial \Sigma^0| \right) \frac{\partial u_0}{\partial t} = \operatorname{div}(\mathcal{D} \nabla u_0) & \text{in } (0, T) \times \mathbb{R}^d, \\ u_0(0, x) = \left(|Y^0| + K|\partial \Sigma^0| \right)^{-1} \left(|Y^0| u^{in}(x) + |\partial \Sigma^0| v^{in}(x) \right) & x \in \mathbb{R}^d, \end{cases} \quad (1.87)$$

with the dispersion tensor \mathcal{D} given by

$$\mathcal{D}_{ij} = \frac{K^2}{\kappa} |\partial \Sigma^0| b_i^* b_j^* + \int_{Y^0} D(y) (\nabla_y \omega_i + e_i) \cdot (\nabla_y \omega_j + e_j) dy. \quad (1.88)$$

The above result is proved formally in [10] using the two-scale asymptotic expansions with drift. In [20] the above result is made rigorous in the following sense.

Proposition 1.11.2. [20] *The sequence $\{u_\varepsilon, v_\varepsilon\}$ of solutions to (1.81) satisfies*

$$\begin{aligned} u_\varepsilon(t, x) &= u_0 \left(t, x - \frac{b^* t}{\varepsilon} \right) + r_\varepsilon^u(t, x), \\ v_\varepsilon(t, x) &= K u_0 \left(t, x - \frac{b^* t}{\varepsilon} \right) + r_\varepsilon^v(t, x). \end{aligned} \quad (1.89)$$

where the residual functions r_ε^u and r_ε^v vanish as $\varepsilon \rightarrow 0$ and the limit u_0 satisfies the effective diffusion equation (1.87).

The cell problem (1.86) has contributions from convection, diffusion and reaction as we are in the ‘‘Taylor dispersion mediated mixing regime’’.

Remark 1.11.3. *The contribution from the reaction at the pore scale is via the equilibrium constant K and not the reaction rate κ . In the limit $K \rightarrow 0$, we recover the cell problem and the homogenized limit corresponding to the convection-diffusion equation in the strong convection regime with homogeneous Neumann boundary condition on the pore boundaries. In the other limit $K \rightarrow \infty$, it follows from the expression for the drift velocity (1.84) that $b^* = 0$.*

Remark 1.11.4. *The reaction rate κ does appear in the expression for the dispersion tensor (1.88). In the limit $\kappa \rightarrow 0$, the dispersion \mathcal{D} blows up but the limit case $\kappa = 0$ in (1.81) corresponds to the regime with no chemical reaction i.e., homogeneous Neumann boundary condition on the pore boundaries. So the homogenization doesn’t commute with the limit as κ goes to zero. On the other hand, when $\kappa \rightarrow \infty$ the first term in the dispersion (1.88) goes to zero and the limit corresponds to the study of the adsorption phenomena in porous media which are in equilibrium.*

1.12 Our contribution: Linear isotherm

The contribution of this thesis is in the context of reactive flows in the strong convection regime. To begin with, we consider a coupled convection-diffusion equations. The coupling is through

a reaction term similar to the one in (1.81). In (1.81), the surface concentration v_ε is governed by an ordinary differential equation. As remarked earlier, in [97] surface diffusion is considered for the adsorbed concentration. We generalize the microscopic model (1.81) by considering both surface convection and surface diffusion for the adsorbed concentration. Taking $b^s(y)$ as a Y -periodic velocity field on the pore surface and $D^s(y)$ as a Y -periodic diffusion matrix associated with surface diffusion, the model we consider is the following:

$$\begin{cases} \frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ -\frac{1}{\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot n = \frac{\partial v_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon - \operatorname{div}^s(D_\varepsilon^s \nabla^s v_\varepsilon) = \frac{\kappa}{\varepsilon^2} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right) & \text{on } (0, T) \times \Omega_\varepsilon, \\ u_\varepsilon(0, x) = u^{in}(x) & x \in \Omega_\varepsilon, \\ v_\varepsilon(0, x) = v^{in}(x) & x \in \partial\Omega_\varepsilon. \end{cases} \quad (1.90)$$

To perform formal upscaling of (1.90), we postulate asymptotic expansions for the bulk and surface concentrations u_ε and v_ε as in (1.82). The homogenization result concerning (1.90) is given below.

Proposition 1.12.1. *Under the assumption (1.82), the solution $(u_\varepsilon, v_\varepsilon)$ of (1.90) formally satisfy*

$$\begin{aligned} u_\varepsilon(t, x) &\approx u_0 \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon u_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \\ v_\varepsilon(t, x) &\approx K u_0 \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon v_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \end{aligned}$$

with the effective drift

$$b^* = \left(|Y^0| + K |\partial\Sigma^0| \right)^{-1} \left(\int_{Y^0} b(y) dy + K \int_{\partial\Sigma^0} b^s(y) d\sigma(y) \right) \quad (1.91)$$

and u_0 the solution of the homogenized problem

$$\begin{cases} \left(|Y^0| + K |\partial\Sigma^0| \right) \frac{\partial u_0}{\partial t} - \operatorname{div}_x(\mathcal{D} \nabla_x u_0) = 0 & \text{in } (0, T) \times \mathbb{R}^d, \\ \left(|Y^0| + K |\partial\Sigma^0| \right) u_0(0, x) = |Y^0| u^{in}(x) + |\partial\Sigma^0| v^{in}(x) & x \in \mathbb{R}^d. \end{cases} \quad (1.92)$$

where the dispersion tensor \mathcal{D} is given by

$$\begin{aligned} \mathcal{D}_{ij} &= \int_{Y^0} D(y) (\nabla_y \chi_i + e_i) \cdot (\nabla_y \chi_j + e_j) dy + \kappa \int_{\partial\Sigma^0} \left(\chi_i - \frac{\omega_i}{K} \right) \left(\chi_j - \frac{\omega_j}{K} \right) d\sigma(y) \\ &\quad + K^{-1} \int_{\partial\Sigma^0} D^s(y) (K e_i + \nabla_y^s \omega_i) \cdot (K e_j + \nabla_y^s \omega_j) d\sigma(y) \end{aligned} \quad (1.93)$$

with $(\chi, \omega) = (\chi_i, \omega_i)_{1 \leq i \leq d}$ being the solution of the cell problem such that

$$u_1(t, x, y) = \sum_{i=1}^d \chi_i(y) \frac{\partial u_0}{\partial x_i}(t, x), \quad v_1(t, x, y) = \sum_{i=1}^d \omega_i(y) \frac{\partial u_0}{\partial x_i}(t, x) \quad (1.94)$$

and the cell problem is

$$\begin{cases} b(y) \cdot \nabla_y \chi_i - \operatorname{div}_y(D(\nabla_y \chi_i + e_i)) = (b^* - b) \cdot e_i & \text{in } Y^0, \\ b^s(y) \cdot \nabla_y^s \omega_i - \operatorname{div}_y^s(D^s(\nabla_y^s \omega_i + K e_i)) = K(b^* - b^s) \cdot e_i + \kappa(\chi_i - K^{-1} \omega_i) & \text{on } \partial \Sigma^0, \\ -D(\nabla_y \chi_i + e_i) \cdot n = \kappa(\chi_i - K^{-1} \omega_i) & \text{on } \partial \Sigma^0, \\ y \rightarrow (\chi_i, \omega_i) & Y\text{-periodic.} \end{cases} \quad (1.95)$$

The coupling in the microscopic model (1.90) is carried on to the cell problem (1.95). In the absence of the surface convection and surface diffusion, the first order correctors for the surface concentration were given in terms of the first order correctors for the bulk concentration as in (1.85). So, we would like to see if we get back the upscaling result obtained in [10, 20] in the limit $b^s \rightarrow 0$, $D^s \rightarrow 0$. The effective drift velocity (1.91) depends on both the bulk and surface velocity fields. It is the weighted average of both the velocity fields with the equilibrium constant K as the weight on the pore surface. In the limit $b^s \rightarrow 0$, the effective drift (1.91) matches with the effective drift (1.84). The first order correctors for the concentrations u_ε , v_ε are given in terms of solutions (χ_i, ω_i) to a coupled steady problem in the unit cell (1.95). In the limit $b^s \rightarrow 0$, $D^s \rightarrow 0$, we recover a decoupled cell problem only for χ_i as in (1.86) and the surface corrector is given in terms of the bulk correctors via the following algebraic relation:

$$\omega_i = K \chi_i - \frac{K^2}{\kappa} b^* \cdot e_i \quad (1.96)$$

The above expression (1.96) is nothing but the expression for v_1 in (1.85). Also the expression for the dispersion \mathcal{D} in (1.93) matches with that of (1.88) in the limit $b^s \rightarrow 0$, $D^s \rightarrow 0$. Thus we recover the results obtained in [10, 20].

When $\kappa \rightarrow 0$, the equations for u_ε and v_ε are decoupled, thus making the cell problem (1.95) ill-posed with the effective drift (1.91). So, we always assume $\kappa > 0$. Formally, when κ tends to $+\infty$, the two concentrations are fully coupled in the sense that $v_\varepsilon = K u_\varepsilon$. On the other hand, when $K = 0$, it formally yields that $v_\varepsilon = 0$ and the only remaining unknown u_ε satisfies a homogeneous Neumann boundary condition on $\partial \Omega_\varepsilon$. However, if K tends to $+\infty$, then u_ε and v_ε are again decoupled in the limit, with a Fourier-type boundary condition $-D_\varepsilon \nabla u_\varepsilon \cdot n = \kappa u_\varepsilon / \varepsilon$ on $\partial \Omega_\varepsilon$. The governing model in this limit is actually (1.68), the one studied in [122, 25].

So our model generalizes some of the linear adsorption models that were studied in the regime of strong convection. A formal proof, using the two-scale asymptotic expansions with drift, of the result announced in the above Proposition 1.12.1 is found in Section 3.7 of Chapter 3. Sections 3.8, 3.9, 3.10 of Chapter 3 are concerned with the rigorous justification of the above formal result in the sense of Proposition 1.11.2.

In the ansatz (1.82) for the unknown concentrations u_ε and v_ε , a common drift b^* was chosen. Even if we start off with different drifts, say b_1^* and b_2^* , for the two unknowns, during the formal upscaling procedure for (1.90) we deduce that $b_1^* = b_2^*$. In the microscopic model (1.90), convection-diffusion and reaction are pronounced at the pore scale as is evident from the cell problem (1.95). Taking cues from some of the works on reactive flows in ‘‘Diffusion dominated’’ regime [81, 109], we shall consider the following microscopic model where convection and diffusion are dominant at the pore scale but not the reaction:

$$\left\{ \begin{array}{ll} \frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div} (D_\varepsilon \nabla u_\varepsilon) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ -\frac{1}{\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot n = \frac{\partial v_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon - \operatorname{div}^s (D_\varepsilon^s \nabla^s v_\varepsilon) = \kappa \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right) & \text{on } (0, T) \times \Omega_\varepsilon, \\ u_\varepsilon(0, x) = u^{in}(x) & x \in \Omega_\varepsilon, \\ v_\varepsilon(0, x) = v^{in}(x) & x \in \partial\Omega_\varepsilon. \end{array} \right. \quad (1.97)$$

Mathematically speaking, the above model is obtained from (1.90) upon scaling the reaction rate as $\kappa \rightarrow \varepsilon^2 \kappa$. The homogenization result concerning (1.97) is very different from the one announced in Proposition 1.12.1. Consider two constants $b_1^*, b_2^* \in \mathbb{R}^d$:

$$b_1^* = \frac{1}{|Y^0|} \int_{Y^0} b(y) dy \quad \text{and} \quad b_2^* = \frac{1}{|\partial\Sigma^0|} \int_{\partial\Sigma^0} b^s(y) d\sigma(y). \quad (1.98)$$

Depending upon whether the bulk and surface drifts (1.98) are equal or not, different effective behaviour for (1.97) is obtained. The results regarding the upscaling are found in Section 3.11 of Chapter 3. The values of the two drifts play an interesting role in determining whether the homogenized equation of the coupled system (1.97) stays coupled or not. The two constants b_1^* and b_2^* shall be of interest in Chapter 4 where we study the upscaling of a nonlinear adsorption model.

In the linear adsorption models (1.90) and (1.97) that we have considered so far, the velocity fields are considered incompressible. In Section 3.12 of Chapter 3, we consider a convection-diffusion equation with homogeneous Neumann boundary conditions and compressible velocity fields. In the context of homogenization of convection-diffusion equations, the presence of compressible flows manifests as if there were bulk reactions in the fluid. With the consideration of the compressible flows, we have worked with all possible scenarios for a convection-diffusion-reaction equations with periodic coefficients that model linear adsorption phenomena on the pore boundaries. Chapter 3 contains proofs and detailed analysis of the linear adsorption models. Some of the results from Chapter 3 are published in [17].

1.13 Our contribution: Nonlinear isotherms

In Chapter 4, we generalize our results from Chapter 3 on linear isotherms to nonlinear isotherms. The nonlinear isotherm that we consider is the one due to Langmuir and is given by

$$f(u) = \frac{\alpha u}{1 + \beta u}. \quad (1.99)$$

The microscopic model that we consider is the following:

$$\left\{ \begin{array}{ll} \frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div} (D_\varepsilon \nabla u_\varepsilon) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ -\frac{1}{\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot n = \frac{\partial v_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon - \operatorname{div}^s (D_\varepsilon^s \nabla^s v_\varepsilon) = \frac{\kappa}{\varepsilon^2} \left(\frac{\alpha u_\varepsilon}{1 + \beta u_\varepsilon} - v_\varepsilon \right) & \text{on } (0, T) \times \Omega_\varepsilon, \\ u_\varepsilon(0, x) = u^{in}(x) & x \in \Omega_\varepsilon, \\ v_\varepsilon(0, x) = v^{in}(x) & x \in \partial\Omega_\varepsilon. \end{array} \right. \quad (1.100)$$

In the previous section while presenting the slow reaction model (1.97), we pointed out the importance of the bulk and surface drifts:

$$b_1^* = \frac{1}{|Y^0|} \int_{Y^0} b(y) dy \quad \text{and} \quad b_2^* = \frac{1}{|\partial\Sigma^0|} \int_{\partial\Sigma^0} b^s(y) d\sigma(y). \quad (1.101)$$

The presence of the nonlinear term in the microscopic model (1.100) forces to assume that the bulk and surface drifts in (1.101) are equal i.e.,

$$\frac{1}{|Y^0|} \int_{Y^0} b(y) dy = \frac{1}{|\partial\Sigma^0|} \int_{\partial\Sigma^0} b^s(y) d\sigma(y) = b^*. \quad (1.102)$$

Such an assumption was not necessary in the linear case [10, 20, 17] but is the price to pay for extending our previous results to the nonlinear case of the Langmuir isotherm. The upscaling result regarding the nonlinear model (1.100) is as follows.

Proposition 1.13.1. *The solution $(u_\varepsilon, v_\varepsilon)$ of the coupled convection-diffusion-reaction system (1.100) is approximatively given by the ansatz*

$$\begin{aligned} u_\varepsilon(t, x) &\approx u_0\left(t, x - \frac{b^*t}{\varepsilon}\right) + \varepsilon u_1\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right), \\ v_\varepsilon(t, x) &\approx f(u_0)\left(t, x - \frac{b^*t}{\varepsilon}\right) + \varepsilon v_1\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right), \end{aligned} \quad (1.103)$$

where f is the Langmuir isotherm given in (1.99) and b^* is the effective drift given by (1.102). Further, the zero order approximation u_0 in (1.103) is the solution of the following macroscopic nonlinear monotone diffusion equation:

$$\begin{cases} \left[|Y^0| + \frac{\alpha|\partial\Sigma^0|}{(1+\beta u_0)^2} \right] \frac{\partial u_0}{\partial t} - \operatorname{div}_x(\mathcal{D}(u_0)\nabla_x u_0) = 0 & \text{in } (0, T) \times \mathbb{R}^d, \\ \left[|Y^0|u_0 + \frac{|\partial\Sigma^0|\alpha u_0}{1+\beta u_0} \right] (0, x) = |Y^0|u^{in}(x) + |\partial\Sigma^0|v^{in}(x) & \text{in } \mathbb{R}^d, \end{cases} \quad (1.104)$$

and the correctors (u_1, v_1) in (1.103) are defined by

$$\begin{aligned} u_1(t, x, y) &= \sum_{i=1}^d \chi_i(y, u_0(t, x)) \frac{\partial u_0}{\partial x_i}(t, x) \\ v_1(t, x, y) &= \frac{\alpha}{(1+\beta u_0(t, x))^2} \sum_{i=1}^d \omega_i(y, u_0(t, x)) \frac{\partial u_0}{\partial x_i}(t, x) \end{aligned} \quad (1.105)$$

where $(\chi_i, \omega_i)_{1 \leq i \leq d}$ is the solution of the cell problem:

$$\begin{cases} -b^* \cdot e_i + b(y) \cdot (e_i + \nabla_y \chi_i) - \operatorname{div}_y(D(e_i + \nabla_y \chi_i)) = 0 & \text{in } Y^0, \\ -D(e_i + \nabla_y \chi_i) \cdot n = \frac{\alpha \kappa}{(1+\beta u_0)^2} (\chi_i - \omega_i) & \text{on } \partial\Sigma^0, \\ -b^* \cdot e_i + b^s(y) \cdot (e_i + \nabla_y^s \omega_i) - \operatorname{div}_y^s(D^s(e_i + \nabla_y^s \omega_i)) = \kappa (\chi_i - \omega_i) & \text{on } \partial\Sigma^0, \\ y \rightarrow (\chi_i(y), \omega_i(y)) & Y\text{-periodic.} \end{cases} \quad (1.106)$$

The dispersion tensor $\mathcal{D}(u_0)$ in (1.104) is given in terms of the cell solutions χ_i, ω_i as

$$\begin{aligned}
\mathcal{D}_{ij}(u_0) = & \int_{Y^0} D(y) (\nabla_y \chi_i + e_i) \cdot (\nabla_y \chi_j + e_j) dy + \frac{\alpha \kappa}{(1 + \beta u_0)^2} \int_{\partial \Sigma^0} [\chi_i - \omega_i] [\chi_j - \omega_j] d\sigma(y) \\
& + \frac{\alpha}{(1 + \beta u_0)^2} \int_{\partial \Sigma^0} D^s(y) (\nabla_y^s \omega_i + e_i) \cdot (\nabla_y^s \omega_j + e_j) d\sigma(y) \\
& + \int_{Y^0} D(y) (\nabla_y \chi_j \cdot e_i - \nabla_y \chi_i \cdot e_j) dy \\
& + \frac{\alpha}{(1 + \beta u_0)^2} \int_{\partial \Sigma^0} D^s(y) (\nabla_y^s \omega_j \cdot e_i - \nabla_y^s \omega_i \cdot e_j) d\sigma(y) \\
& + \int_{Y^0} (b(y) \cdot \nabla_y \chi_i) \chi_j dy + \frac{\alpha}{(1 + \beta u_0)^2} \int_{\partial \Sigma^0} (b^s(y) \cdot \nabla_y^s \omega_i) \omega_j d\sigma(y).
\end{aligned} \tag{1.107}$$

Note that the cell solution (χ_i, ω_i) depends not only on y but also on the value of $u_0(t, x)$. Furthermore, the technical assumption (1.102) is precisely the compatibility condition for solving the cell problem for any value of $u_0(t, x)$. In the linear case, the dispersion tensor we obtain is always symmetric and constant. But in the above nonlinear case, $\mathcal{D}(u_0)$ is neither symmetric nor constant. The proof of the above Proposition 1.13.1 is given in Chapter 4. Observe that as $\beta \rightarrow 0$, we fall back to the linear model and we recover the results from Chapter 4. The requirement of the effective drift to be independent of the slow variable x results in the technical assumption (1.102). The method of two-scale asymptotic expansions with drift cannot handle the homogenization of (1.100) for any purely periodic velocity fields b and b^s unless they satisfy (1.102).

A rigorous justification of the above Proposition 1.13.1 is undertaken in Chapter 4 using “Two-scale convergence with drift”. The presence of nonlinearity in (1.100) demands some strong compactness of the sequence of solutions in order to pass to the limit. Following the ideas of [121, 24], we first show that, in a moving frame of reference, a uniform localization of solutions holds. Then a time equicontinuity type result allows us to gain compactness. These technical results are not straightforward extensions of those in [121, 24]. There are a number of additional difficulties, including the perforated character of the domain, the nonlinearity of the equations and more importantly the fact that there are two unknowns u_ε and v_ε .

1.14 Our contribution: Multicomponent reactive flows

Chapter 5 is concerned with the homogenization of multicomponent reactive flows. We consider the following system of convection-diffusion-reaction equations, for every $1 \leq \alpha \leq N$,

$$\begin{cases} \rho_\alpha^\varepsilon \frac{\partial u_\alpha^\varepsilon}{\partial t} + \frac{1}{\varepsilon} b^\varepsilon \cdot \nabla u_\alpha^\varepsilon - \operatorname{div}(D_\alpha^\varepsilon \nabla u_\alpha^\varepsilon) + \frac{1}{\varepsilon^2} \sum_{\beta=1}^N \Pi_{\alpha\beta} u_\beta^\varepsilon = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ D_\alpha^\varepsilon \nabla u_\alpha^\varepsilon \cdot n = 0 & \text{on } (0, T) \times \partial \Omega_\varepsilon, \\ u_\alpha^\varepsilon(0, x) = u_\alpha^{in}(x) & x \in \mathbb{R}^d. \end{cases} \tag{1.108}$$

where the coupling matrix Π models the chemical reactions between the solutes in the fluid. The homogenization of parabolic systems with large lower order terms was studied in [12] where the Factorization principle is employed. We assume that the nondiagonal entries of the coupling matrix Π is not positive. This assumption is borrowed from [152] and from the following references

where neutronic diffusion problems are studied [11, 53]. We too will be using the Factorization principle to homogenize our weakly coupled system (1.108). As usual, we pass via the associated spectral problems. Let us consider the following asymptotic ansatz for the solution u_α^ε :

$$u_\alpha^\varepsilon(t, x) = \exp(-\lambda t/\varepsilon^2) \sum_{i \geq 0} \varepsilon^i u_{i,\alpha} \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \quad \text{for every } 1 \leq \alpha \leq N. \quad (1.109)$$

The upscaling result linked to (1.108) can be summarized as follows.

Proposition 1.14.1. *If the ansatz for the solution (u_α^ε) of (1.108) given in (1.109) is true, then the solution formally satisfies*

$$u_\alpha^\varepsilon(t, x) \approx \exp(-\lambda t/\varepsilon^2) \varphi_\alpha \left(\frac{x}{\varepsilon} \right) \left(v \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon \sum_{i=1}^d \frac{\partial v}{\partial x_i} \left(t, x - \frac{b^* t}{\varepsilon} \right) \omega_{i,\alpha} \left(\frac{x}{\varepsilon} \right) \right), \quad (1.110)$$

with $(\lambda, \varphi_\alpha)$ being the first eigenpair associated with a spectral cell problem. The components $(\omega_{i,\alpha})_{1 \leq \alpha \leq N}$, for every $1 \leq i \leq d$, satisfy a so-called cell problem.

$$\left\{ \begin{array}{ll} \tilde{b}_\alpha(y) \cdot (\nabla_y \omega_{i,\alpha} + e_i) - \operatorname{div}_y (\tilde{D}_\alpha (\nabla_y \omega_{i,\alpha} + e_i)) \\ + \sum_{\beta=1}^N \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (\omega_{i,\beta} - \omega_{i,\alpha}) = \varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* \cdot e_i & \text{in } Y^0, \\ \tilde{D}_\alpha (\nabla_y \omega_{i,\alpha} + e_i) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \omega_{i,\alpha} & Y\text{-periodic,} \end{array} \right. \quad (1.111)$$

where the drift velocity b^* is given by

$$b^* = \frac{1}{\rho^*} \sum_{\alpha=1}^N \int_{Y^0} \tilde{b}_\alpha(y) dy, \quad (1.112)$$

where the effective porosity, ρ^* , is given by

$$\rho^* = \sum_{\alpha=1}^N \int_{Y^0} \varphi_\alpha \varphi_\alpha^* \rho_\alpha(y) dy \quad (1.113)$$

with φ_α^* the first eigenfunction associated with an adjoint spectral cell problem. The modified velocity fields \tilde{b}_α and the diffusion matrices \tilde{D}_α are given in terms of the velocity fields b_α and diffusion matrices D_α of (1.108) and the eigenfunctions $(\varphi_\alpha, \varphi_\alpha^*)$.

Further, v in (1.110) satisfies the following scalar homogenized equation:

$$\left\{ \begin{array}{ll} \rho^* \frac{\partial v}{\partial t} - \operatorname{div}(\mathcal{D} \nabla v) = 0 & \text{in } (0, T) \times \mathbb{R}^d, \\ v(0, x) = \sum_{\alpha=1}^N u_\alpha^{in}(x) \int_{Y^0} \varphi_\alpha^*(y) dy & \text{in } \mathbb{R}^d. \end{array} \right. \quad (1.114)$$

where \mathcal{D} is defined by

$$\begin{aligned} \mathcal{D}_{ij} &= \sum_{\alpha=1}^N \int_{Y^0} \tilde{D}_\alpha (\nabla_y \omega_{i,\alpha} + e_i) \cdot (\nabla_y \omega_{j,\alpha} + e_j) dy \\ &\quad - \frac{1}{2} \sum_{\alpha,\beta=1}^N \int_{Y^0} \varphi_\alpha^* \varphi_\beta \Pi_{\alpha\beta} (\omega_{i,\alpha} - \omega_{i,\beta}) (\omega_{j,\alpha} - \omega_{j,\beta}) dy. \end{aligned} \quad (1.115)$$

We have also worked with surface reactions in the context of multicomponent flows. The microscopic model (1.108) is slightly modified by taking the reaction term due to the coupling matrix Π as a Neumann boundary condition on the pores boundaries. The results regarding this boundary reaction model are found in Sections 5.7 and 5.8 of Chapter 5. Adsorption phenomena are also incorporated into the multicomponent model in Section 5.9. Homogenization of this adsorption model is undertaken in Section 5.10.

Publications

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Under preparation

[18] Allaire G, Hutridurga H. *Upscaling nonlinear adsorption in periodic porous media - Homogenization approach*.

[19] Allaire G, Hutridurga H. *Homogenization of multispecies transport in porous media*.

Chapter 2

Theory of Periodic Homogenization

2.1 Introduction

In this chapter we prepare the ground work for the homogenization theory that we will be using in the following chapters where we wish to study the upscaling of the transport equations governing the spreading of solutes dissolved in a fluid filling a periodic porous medium. More often than not, multiscale phenomena are encountered in nature. The presence of heterogeneities in a domain complicates the mathematical modelling of the physical phenomena present in the given domain. Consider l to be the heterogeneities' (microscopic) length scale and L as the observation (macroscopic) length scale. We make the separation of scales assumption i.e., $l/L = \varepsilon \ll 1$. We consider two space variables: macroscopic slow variable x and microscopic fast variable $y = x/\varepsilon$. The idea of upscaling is to determine an equivalent macroscopic medium, a continuous medium which behaves "on average" like the heterogeneities that are present. Beginning with the governing equations at the heterogeneities's length scale, we want to replace it with a continuum model posed in an equivalent macroscopic medium.

In the mechanics literature, Representative Elementary Volume (REV) method [165] is a popular upscaling technique where REV is chosen of $\mathcal{O}(h)$ with $l \ll h \ll L$. Another popular approach is the method of moments [46, 47]. In a periodic setting, the period is of $\mathcal{O}(\varepsilon)$. A well-known technique in the periodic setting has been the multiple scale expansions [41, 148]. Heuristic arguments to this approach were presented in [147, 103]. When the separation of scales assumption isn't met, there is a continuum of non separated length scales. Percolation Theory has been used in this context. Percolation theory in the context of fluid mechanics in porous media is presented by K. M. Golden in Chapter 2 of [96]. All through the thesis we will be working with periodic porous media and transport equations with periodically oscillating coefficients. So this chapter is dedicated to refresh some of the known theories in periodic homogenization.

Let us consider a partial differential equation with periodically oscillating coefficients of period ε :

$$L_\varepsilon u_\varepsilon = f \quad \text{in } \Omega, \quad (2.1)$$

where f is the source term. The above partial differential equation is supplemented with appropriate boundary conditions and initial data (in case of evolution equations). Using some upscaling technique, the objective is to find an effective equation:

$$\bar{L} u_0 = f \quad \text{in } \Omega. \quad (2.2)$$

In a periodic porous medium, the system of equations representing the physical phenomena usually takes the form (2.1). The principle of asymptotic expansion is to postulate an ansatz

for the solution u_ε of (2.1) in terms of the period ε and Y -periodic coefficient functions in the fast variable y :

$$u_\varepsilon(x) = u_0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(x, \frac{x}{\varepsilon}\right) + \dots$$

A classical result where this method was successfully applied is to obtain the famous Darcy's law starting from fluid equations in microscale. Darcy's law is a filtration law that was empirically obtained by H. Darcy [72]. Darcy's law states that the flow rate u is proportional to the balance of forces including the pressure. Starting with steady Stokes equations, Darcy's law has been derived using the formal method of asymptotic expansions in [148, 115]. In Section 2.2, we illustrate the method of two-scale asymptotic expansions applying it to the upscaling of steady Stokes equations to arrive at Darcy's law. This homogenization result is presented in Proposition 2.2.2.

The method of two-scale asymptotic expansion is a formal method that can only guess the effective behavior. To rigorously justify the Homogenization process, L. Tartar proposed the "method of oscillating test functions" [153]. Tartar's method is also coined as "Energy Method" in [41]. In loose terms, Energy method is to prove the convergence of u_ε , the solution of (2.1), to u_0 , solution of (2.2), in a proper function space. It goes via choosing of proper test functions in the variational formulation of the microscopic partial differential equation (2.1) and passing to the limit as $\varepsilon \rightarrow 0$. The test functions are built using solutions to the so-called cell problems. Energy method was introduced in a general context of H -convergence [153, 131]. This method isn't very specific for the homogenization problems in periodic setting. Ngutseng introduced a compactness phenomenon suitable for periodic homogenization in [132]. This phenomenon was coined as "Two-scale convergence" and was further developed by G. Allaire in [5]. Section 2.3 deals with this phenomenon of two-scale convergence. We recall some of the standard results and apply the same to homogenize unsteady Stokes equations (2.23) in a periodic porous medium. Theorem 2.3.7 gives the homogenization result related to the Stokes equations in the unsteady case. The effective equation is shown to be a two-scale equation (2.30). This result was obtained formally in [115, 148, 104] and later rigorously justified in [155, 4]. In (2.32) the homogenized equation in only slow variable is given. The homogenized equation (2.32) turns out to be an integro-differential equation. This generalizes the usual Darcy's law.

In Section 2.5, we present the notion of "Two-scale convergence on periodic surfaces". This adaptation of two-scale convergence to function sequences defined on surfaces was done in [14, 134]. This helps us treat different kinds of boundary data and diffusion phenomena on surfaces as illustrated in Section 2.5. As we remarked in the general Introduction (Chapter 1), there have been other approaches to handle the function sequences on the surfaces. In [61], Cioranescu and Donato homogenize steady state problems in perforated domains with non-homogeneous boundary data. Loosely speaking, their approach passes via the introduction of an auxiliary problem which helps transform surface integrals in the variational formulation into volume integrals. Please refer to [61] for precise details.

The study of convection-diffusion equations governing the movement of dissolved solutes has been a long-standing question [157, 158, 159, 30, 46, 47, 145]. The interplay between the flow (fluid equations), the solute transport (convection-diffusion equation) and the geometry of the porous medium is quite a challenging problem. Let us consider the following convection diffusion equation for the solute concentration in the fluid part Ω_f of the porous medium:

$$\frac{\partial u}{\partial \tau} + b \cdot \nabla u - \operatorname{div}(D \nabla u) = 0.$$

In Section 1.6 we introduced various scaling techniques. Among them, when global Péclet

number is of $\mathcal{O}(\varepsilon^{-1})$, the two-scale asymptotic analysis recalled in Section 2.2 isn't able to homogenize the above convection diffusion equation without imposing zero mean condition on the velocity field as demonstrated in the beginning of the Section 2.6. This handicap of the two-scale asymptotic method is overcome by the introduction of "two-scale asymptotic analysis with drift" in (2.44). This variant introduces a drift in the second variable of the coefficient functions in the ansatz:

$$u_\varepsilon(t, x) = u_0\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) + \dots$$

This concept of effective drift in the concentration profile was first introduced in [140]. This notion of effective drift also has appeared in the context of turbulent diffusion as "Ballistic velocity" [162, 94]. Section 2.6 presents the method of two-scale asymptotic expansion with drift via its application to upscaling the above convection-diffusion equation under the supposition of global Péclet number being of $\mathcal{O}(\varepsilon^{-1})$. After an overview of the formal asymptotic method, we get into the rigorous justification of using "Two-scale convergence with drift", definition of which is given in Definition 2.6.2. This notion was introduced in [121]. A pedagogical review of this method is given by G. Allaire in [7] (See also [137]). Compactness results related to drift are recalled in Section 2.6. Theorem 2.6.9 gives a rigorous justification of the homogenization of convection-diffusion equation in large global Péclet regime. This justifies the formal homogenized equation (2.50) obtained in the beginning of Section 2.6.

In [58, 60, 59], a new upscaling notion of "Periodic Unfolding" has been developed. This method is briefly recalled in Section 2.4. Taking lead from [14, 134], we generalize the notion of two-scale convergence to function sequences defined on surfaces in Section 2.5. On same lines, we generalize the notion of two-scale convergence with drift to function sequences defined on surfaces in Section 2.7. As far as we know, this new notion of convergence in Section 2.7 is introduced for the first time in this thesis.

In some cases we obtain two-scale homogenized equation i.e., the presence of both fast and slow variables. This is demonstrated in Theorem 2.3.7 where we obtain a two pressure model (2.30) as an effective model for the unsteady incompressible Stokes equations. It is of paramount importance to eliminate the fast variable, if possible, in the homogenized model. This was addressed by M. Vanninathan in [161] in the context of elliptic eigenvalue problems. Loosely speaking, the idea is to factor out the oscillations from the solution sequences and then pass to the limit. Section 2.8 recalls this "Factorization principle". The results obtained in [161] are presented followed by the application of the Factorization principle to convection-diffusion-reaction equation in periodic porous media [25]. This method of factorization is quite popular in the literature [51, 11, 53, 12, 76]. We will be using this approach in dealing with compressible flows in Section 3.12 of Chapter 3 and in Chapter 5 in relation to spreading of multiple solutes in periodic porous media.

2.2 Two-scale asymptotics

This formal method begins with an assumption that the solution u_ε to the partial differential equation (2.1) can be written in the form of an asymptotic expansion in terms of the period ε :

$$u_\varepsilon(x) = u_0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(x, \frac{x}{\varepsilon}\right) + \dots$$

where the coefficient functions $u_i(x, y)$ are Y -periodic with respect to the variable y . We plug the above expansion for u_ε in the partial differential equation (2.1) keeping in mind the following

chain rule for differentiation:

$$\nabla \left[\phi \left(x, \frac{x}{\varepsilon} \right) \right] = \left[\nabla_x \phi + \frac{1}{\varepsilon} \nabla_y \phi \right] \left(x, \frac{x}{\varepsilon} \right). \quad (2.3)$$

Upon inserting the proposed ansatz for the solution u_ε in (2.1), we arrive at a cascade of equations as coefficients of different powers of ε . Usually we integrate the equation for u_0 over the unit cell Y to arrive at the homogenized equation (2.2). The form of \bar{L} is obtained using the so-called cell problems posed in the unit cell Y . This formal method has been very popular in the literature regarding the upscaling of partial differential equations. To name a few good references, among many others, where this method is documented are [41, 148, 62, 6].

To illustrate the method of asymptotic expansions, we will be giving an example of homogenizing the following incompressible steady Stokes equations:

$$\begin{cases} \nabla p_\varepsilon - \varepsilon^2 \mu \Delta u_\varepsilon = f & \text{in } \Omega_\varepsilon, \\ \operatorname{div} u_\varepsilon = 0 & \text{in } \Omega_\varepsilon, \\ u_\varepsilon = 0 & \text{on } \partial\Omega_\varepsilon, \end{cases} \quad (2.4)$$

where u_ε and p_ε denote the velocity and pressure fields associated with the fluid filling the porous medium. The positive μ is the viscosity. We further assume that the porous medium Ω_ε is a bounded convex domain.

Remark 2.2.1. *In (2.4), the viscosity μ is scaled by ε^2 . As is well known from [148, 115, 4], this is the actual scaling which gives a non zero limit for the velocity u_ε as $\varepsilon \rightarrow 0$.*

We take the forcing term $f \in L^2(\Omega)^d$. It follows, consult [160] if necessary, that the system (2.4) admits a unique solution

$$u_\varepsilon \in H_0^1(\Omega_\varepsilon)^d, \quad p_\varepsilon \in L^2(\Omega_\varepsilon)/\mathbb{R}. \quad (2.5)$$

As explained above, we shall postulate the following ansatz for the unknowns u_ε and p_ε :

$$u_\varepsilon(x) = u_0 \left(x, \frac{x}{\varepsilon} \right) + \varepsilon u_1 \left(x, \frac{x}{\varepsilon} \right) + \varepsilon^2 u_2 \left(x, \frac{x}{\varepsilon} \right) + \dots \quad (2.6)$$

$$p_\varepsilon(x) = p_0 \left(x, \frac{x}{\varepsilon} \right) + \varepsilon p_1 \left(x, \frac{x}{\varepsilon} \right) + \varepsilon^2 p_2 \left(x, \frac{x}{\varepsilon} \right) + \dots \quad (2.7)$$

Proposition 2.2.2. *[148, 115] The homogenized model for the Stokes problem (2.4) is given by*

$$\begin{cases} u(x) = \frac{1}{\mu} K \left(f(x) - \nabla p(x) \right) & \text{in } \Omega, \\ \operatorname{div} u = 0 & \text{in } \Omega, \\ u \cdot n = 0 & \text{on } \partial\Omega, \end{cases} \quad (2.8)$$

where $u(x)$ is the homogenized velocity given as the average of the first term of the ansatz (2.6) for u_ε :

$$u(x) = \int_{Y^0} u_0(x, y) dy. \quad (2.9)$$

The homogenized pressure $p(x) = p_0(x, y)$, the first term of the ansatz (2.7) for p_ε , independent of y . The permeability tensor K is symmetric, positive definite and is given by

$$K_{ij} = \int_{Y^0} \nabla_y w_i \cdot \nabla_y w_j dy \quad (2.10)$$

in terms of the solutions $w_i \in H_{\#}^1(Y^0)^d$ to the following cell problem:

$$\begin{cases} \nabla_y q_i - \Delta_{yy} w_i = e_i & \text{in } Y^0, \\ \operatorname{div}_y w_i(y) = 0 & \text{in } Y^0, \\ w_i(y) = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow w_i(y) & Y\text{-periodic.} \end{cases} \quad (2.11)$$

Furthermore, the second term in the ansatz (2.7) is given in terms of the cell pressure q_i :

$$p_1(x, y) = \sum_{i=1}^d q_i(y) \left(f - \frac{\partial p}{\partial x_i} \right)(x). \quad (2.12)$$

Proof. Plugging (2.6)-(2.7) into (2.4) yields

$$\varepsilon^{-1} \nabla_y p_0 \left(x, \frac{x}{\varepsilon} \right) + \varepsilon^0 \left[\nabla_x p_0 + \nabla_y p_1 - \mu \Delta_{yy} u_0 \right] \left(x, \frac{x}{\varepsilon} \right) + \mathcal{O}(\varepsilon) = f(x) \quad (2.13)$$

$$\varepsilon^{-1} \operatorname{div}_y u_0 \left(x, \frac{x}{\varepsilon} \right) + \varepsilon^0 \left[\operatorname{div}_x u_0 + \operatorname{div}_y u_1 \right] \left(x, \frac{x}{\varepsilon} \right) + \mathcal{O}(\varepsilon) = 0 \quad (2.14)$$

At order ε^{-1} , the corresponding momentum equation is

$$\begin{cases} \nabla_y p_0 = 0 & \text{in } Y^0, \\ y \rightarrow p_0 & Y\text{-periodic,} \end{cases} \quad (2.15)$$

implying that $p_0(x, y)$ is independent of y . That is, $p_0(x, y) = p(x)$.

Now, at order ε^0 for the momentum equation and at order ε^{-1} for the incompressibility condition, we arrive at

$$\begin{cases} \nabla_y p_1 - \mu \Delta_{yy} u_0 = f(x) - \nabla_x p(x) & \text{in } Y^0, \\ \operatorname{div}_y u_0 = 0 & \text{in } Y^0, \\ u_0 = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow (p_1, u_0) & Y\text{-periodic.} \end{cases} \quad (2.16)$$

By the linearity of (2.16) we deduce that

$$u_0(x, y) = \sum_{i=1}^d w_i(y) \left(f_i - \frac{\partial p}{\partial x_i} \right)(x), \quad p_1(x, y) = \sum_{i=1}^d q_i(y) \left(f_i - \frac{\partial p}{\partial x_i} \right)(x), \quad (2.17)$$

where w_i , the cell velocity, and q_i , the cell pressure, are solutions to the cell problem (2.11).

At order ε^0 , the incompressibility condition leads to

$$\operatorname{div}_x u_0(x, y) + \operatorname{div}_y u_1(x, y) = 0. \quad (2.18)$$

Now we shall integrate the above equation over Y^0 :

$$\operatorname{div}_x \left(\int_{Y^0} u_0 dy \right) + \int_{Y^0} \operatorname{div}_y u_1 dy = 0.$$

The term with u_1 vanishes as it is periodic with respect to the y variable. Taking into consideration the expression for $u_0(x, y)$ from (2.17), the above equation leads to the pressure equation:

$$-\operatorname{div}_x \left(K \left(\nabla_x p - f \right) \right) = 0,$$

where

$$K_{ij} = K e_i \cdot e_j = \int_{Y^0} w_{ji} dy. \quad (2.19)$$

This expression is equivalent to (2.10). To see that, we multiply the cell problem (2.11) for w_i by the cell solution w_j :

$$\int_{Y^0} \nabla_y q_i w_j dy - \int_{Y^0} \Delta_{yy} w_i w_j dy = \int_{Y^0} w_{ji} dy.$$

Integrating by parts, we arrive at

$$\int_{Y^0} \nabla_y w_i \cdot \nabla_y w_j dy = \int_{Y^0} w_{ji} dy,$$

thus the expression (2.10) for the permeability tensor. The symmetry and positive definiteness follows. Defining the homogenized velocity as

$$u(x) = \int_{Y^0} u_0(x, y) dy,$$

we arrive at the homogenized equation (2.8). As for the Neumann boundary condition, it follows from the definition of $u(x)$ that $\operatorname{div}_x u = 0$ in Ω . Application of the Stokes theorem leads to the intended Neumann condition for u on $\partial\Omega$ as in (2.8). \square

Proposition 2.2.2 is a formal result as, a priori, we do not know if the assumed ansatz (2.6) and (2.7) hold. The effective equation (2.8) is the famous Darcy's law which was obtained empirically by Henry Darcy [72].

2.3 Two-scale convergence

This section is about rigorously justifying the homogenization of periodic structures. In the previous section, we managed to arrive at a homogenized equation (2.8) for the steady incompressible Stokes equations (2.4) via a formal method of two-scale asymptotic expansion. This formal approach can be made rigorous using the Energy method introduced by Tartar [153]. In a periodic setting, we can rely on a more robust method of two-scale convergence introduced by Nguetseng in [132] and further developed by Allaire in [5]. Recently, E. Frénod has published a very thorough overview of the method of two-scale convergence [86]. In the sequel of chapters to follow, we intend to work on partial differential equations of evolution type. So, in this section, we shall be trying to prove the homogenization of unsteady incompressible Stokes equation. The notion of two-scale convergence can be easily adopted to time dependent functions. We shall introduce definitions and state propositions that are applicable to the time dependent case.

Definition 2.3.1. [5] *A sequence of functions $u_\varepsilon(t, x)$ in $L^2((0, T) \times \Omega)$ is said to two-scale converge to a limit $u_0(t, x, y) \in L^2((0, T) \times \Omega \times Y)$ if, for any function $\phi(t, x, y) \in C_c^\infty((0, T) \times \Omega; C_\#^\infty(Y))$, we have*

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_\Omega u_\varepsilon(t, x) \phi\left(t, x, \frac{x}{\varepsilon}\right) dx dt = \int_0^T \int_\Omega \int_Y u_0(t, x, y) \phi(t, x, y) dy dx dt. \quad (2.20)$$

We denote this convergence by $u_\varepsilon \xrightarrow{2scale} u_0$.

Please note that the time variable t is just a parameter in the above definition as we aren't considering any oscillations with respect to time in the test functions. The above definition makes sense because of the following compactness result.

Proposition 2.3.2. [5] *For any bounded sequence of functions $u_\varepsilon(x) \in L^2((0, T) \times \Omega)$, i.e., satisfying*

$$\|u_\varepsilon\|_{L^2((0, T) \times \Omega)} \leq C,$$

there exists a limit $u_0(t, x, y) \in L^2((0, T) \times \Omega \times Y)$ and one can extract a subsequence (still denoted by ε) such that this subsequence two-scale converges to u_0 .

In case the sequence $\{u_\varepsilon\}$ has additional bounds, the above compactness result can be improved.

Proposition 2.3.3. [5] *Let $u_\varepsilon(t, x)$ be a bounded sequence in $L^2((0, T); H^1(\Omega))$ that converges weakly to a limit u_0 in $L^2((0, T); H^1(\Omega))$. Then,*

$$\begin{aligned} u_\varepsilon &\xrightarrow{2scale} u_0(t, x), \\ \nabla u_\varepsilon &\xrightarrow{2scale} \nabla_x u_0(t, x) + \nabla_y u_1(t, x, y). \end{aligned} \quad (2.21)$$

for some $u_1 \in L^2((0, T) \times \Omega; H^1_\#(Y))$.

Remark 2.3.4. *Note that the Definition 2.3.1 of two-scale convergence is given for sequences defined in a fixed domain Ω . But, when it comes to periodic porous media, the domain Ω_ε varies with ε too. The main challenge with compactness theorems for functions sequences on Ω_ε is to extend them to the full domain Ω and then apply the standard compactness results of functional analysis. When Σ^0 is strictly contained in Y i.e., isolated solid obstacles, Cioranescu and Saint Jean Paulin in [65] solved this difficulty by giving extension operators. Acerbi et al in [1] further solved this challenge by coming up with extension operators in general case. Here we recall that the extension operator $E_\varepsilon : H^1(\Omega_\varepsilon) \rightarrow H^1(\Omega)$ satisfies the following property: there exists a constant C , independent of ε , such that, for any function $u_\varepsilon \in H^1(\Omega_\varepsilon)$, $E_\varepsilon u_\varepsilon|_{\Omega_\varepsilon} = u_\varepsilon$ and*

$$\|E_\varepsilon u_\varepsilon\|_{L^2(\Omega)} \leq C \|u_\varepsilon\|_{L^2(\Omega_\varepsilon)}, \quad \|\nabla E_\varepsilon u_\varepsilon\|_{L^2(\Omega)} \leq C \|\nabla u_\varepsilon\|_{L^2(\Omega_\varepsilon)}. \quad (2.22)$$

Allaire and Murat in [21] avoided giving any sophisticated extensions. Rather, they gave a version of Rellich compactness theorem in perforated domains. Two-scale convergence, however, avoids the use of any sophisticated extensions. It just takes the trivial extension by zero on the solid part of the porous medium $\Omega \setminus \Omega_\varepsilon$. Proposition 2.3.2 equally applies to a sequence $u_\varepsilon(t, x) \in L^2((0, T) \times \Omega_\varepsilon)$, merely defined in the perforated domain Ω_ε , and satisfying the uniform bound:

$$\|u_\varepsilon\|_{L^2((0, T) \times \Omega_\varepsilon)} \leq C.$$

Indeed, defining an extended function $U_\varepsilon(t, x) = u_\varepsilon(t, x)$ in Ω_ε and $U_\varepsilon(t, x) = 0$ in $\Omega \setminus \Omega_\varepsilon$, we obtain that

$$\int_0^T \int_{\Omega_\varepsilon} u_\varepsilon(t, x) \phi\left(t, x, \frac{x}{\varepsilon}\right) dx dt = \int_0^T \int_{\Omega} U_\varepsilon(t, x) \phi\left(t, x, \frac{x}{\varepsilon}\right) dx dt$$

and the two-scale limit $U_0(t, x, y)$ of U_ε vanishes in Σ^0 so that

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon(t, x) \phi\left(t, x, \frac{x}{\varepsilon}\right) dx dt = \int_0^T \int_{\Omega} \int_{Y^0} U_0(t, x, y) \phi(t, x, y) dy dx dt.$$

We can also extend ∇u_ε by zero on $\Omega \setminus \Omega_\varepsilon$ when we take $u_\varepsilon \in H^1(\Omega_\varepsilon)$. Thus Proposition 2.3.3 can be applied to sequence $u_\varepsilon \in L^2((0, T); H^1(\Omega_\varepsilon))$, merely defined in the perforated domain Ω_ε . Allaire in (Section 2 of [5]) details on how this trivial extension by zero suffices to prove compactness results on function sequences in perforated domains.

To appreciate the method of two-scale convergence, we shall apply it to the upscaling of the unsteady incompressible Stokes equations in a periodic porous medium:

$$\begin{cases} \frac{\partial u_\varepsilon}{\partial t} + \nabla p_\varepsilon - \varepsilon^2 \mu \Delta u_\varepsilon = f & \text{in } (0, T) \times \Omega_\varepsilon, \\ \operatorname{div} u_\varepsilon = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ u_\varepsilon = 0 & \text{on } (0, T) \times \partial\Omega_\varepsilon, \\ u_\varepsilon(0, x) = u_\varepsilon^{in}(x) & \text{in } \Omega_\varepsilon. \end{cases} \quad (2.23)$$

where u_ε and p_ε denote the velocity and pressure fields associated with the fluid filling the porous medium. The viscosity scaling is the same as in the steady Stokes equations (2.4). The force term $f(t, x) \in L^2((0, T) \times \Omega)^d$ and the initial data $u_\varepsilon^{in} \in H_0^1(\Omega_\varepsilon)^d$. Furthermore, we denote the extension of u_ε^{in} by zero on $\Omega/\Omega_\varepsilon$ as u_ε^{in} . We also assume that the extension satisfies

$$\begin{cases} \|u_\varepsilon^{in}\|_{L^2(\Omega)^d} + \varepsilon \|\nabla u_\varepsilon^{in}\|_{L^2(\Omega)^{d \times d}} \leq C, \\ \operatorname{div} u_\varepsilon^{in} = 0 \quad \text{in } \Omega, \\ u_\varepsilon^{in} \xrightarrow{2scale} u^{in}(x, y). \end{cases} \quad (2.24)$$

The wellposedness of the unsteady Stokes system (2.23) follows from the standard theory (refer to [160, 115]). We just state the following proposition.

Proposition 2.3.5. [4] *The unsteady incompressible Stokes system (2.23) admits a unique solution in the following energy space:*

$$u_\varepsilon \in L^2((0, T); H_0^1(\Omega_\varepsilon)^d), \quad p_\varepsilon \in L^2((0, T); L^2(\Omega_\varepsilon)/\mathbb{R}). \quad (2.25)$$

The extension of u_ε by zero on $\Omega/\Omega_\varepsilon$ satisfies the following a priori estimates:

$$\begin{aligned} \|u_\varepsilon\|_{L^\infty((0, T); L^2(\Omega)^d)} + \varepsilon \|\nabla u_\varepsilon\|_{L^\infty((0, T); L^2(\Omega)^{d \times d})} &\leq C, \\ \left\| \frac{\partial u_\varepsilon}{\partial t} \right\|_{L^2((0, T) \times \Omega)} &\leq C. \end{aligned} \quad (2.26)$$

Further, there exists an extension for p_ε defined in the following way (the extension still denoted as p_ε)

$$p_\varepsilon = p_\varepsilon \text{ in } \Omega_\varepsilon \quad \text{and} \quad p_\varepsilon = \frac{1}{|Y_\varepsilon^i|} \int_{Y_\varepsilon^i} p_\varepsilon \text{ in each } \Sigma_\varepsilon^i. \quad (2.27)$$

The extended pressure, p_ε , satisfies the following a priori estimate:

$$\|p_\varepsilon\|_{L^2((0, T); L^2(\Omega)/\mathbb{R})} \leq C. \quad (2.28)$$

Now that we have a priori estimates on the velocity and pressure fields, the idea is to use compactness theorems of the two-scale convergence to extract subsequences that converge. Here we present a compactness lemma suitable to our a priori estimates (2.26) and (2.28) that helps us extract convergent subsequences off the velocity and pressure sequences.

Lemma 2.3.6. [4] *Let u_ε be a bounded sequence in $L^2((0, T) \times \Omega)^d$ such that its divergence in space, $\operatorname{div} u_\varepsilon$, is bounded in $L^2(\Omega)^d$ and $\varepsilon \nabla u_\varepsilon$ is also bounded in $L^2(\Omega)^{d \times d}$. Then, there exists $u_0(t, x, y) \in L^2((0, T) \times \Omega; H_{\#}^1(Y)^d)$ such that $\operatorname{div}_y u_0 = 0$ and*

$$\begin{cases} u_\varepsilon \xrightarrow{2scale} u_0(t, x, y), \\ \varepsilon \nabla u_\varepsilon \xrightarrow{2scale} \nabla_y u_0(t, x, y), \\ \operatorname{div} u_\varepsilon \xrightarrow{2scale} \operatorname{div}_x \left(\int_{Y^0} u_0(t, x, y) dy \right). \end{cases} \quad (2.29)$$

In [115], it was shown using the formal method of asymptotic expansions that the homogenized equation for the unsteady Stokes system (2.23) is a Darcy's law with memory which generalizes the usual Darcy's law (2.8) obtained in the previous section. Now we state the main result regarding the homogenization of the unsteady Stokes system (2.23).

Theorem 2.3.7. [4] *The solution $(u_\varepsilon, p_\varepsilon)$ of the Stokes system (2.23) two-scale converges to the unique solution $(u_0(t, x, y), p(t, x))$ of the two-scale homogenized problem:*

$$\left\{ \begin{array}{ll} \frac{\partial u_0}{\partial t} + \nabla_y p_1 + \nabla_x p - \mu \Delta_{yy} u_0 = f & \text{in } (0, T) \times \Omega \times Y^0, \\ \operatorname{div}_y u_0 = 0 & \text{in } (0, T) \times \Omega \times Y^0, \\ \operatorname{div}_x \left(\int_{Y^0} u_0(x, y) dy \right) = 0 & \text{in } (0, T) \times \Omega, \\ u_0 = 0 & \text{on } (0, T) \times \Omega \times \Sigma^0, \\ \left(\int_{Y^0} u_0(x, y) dy \right) \cdot n = 0 & \text{on } (0, T) \times \partial\Omega, \\ u_0(t=0) = u^{in}(x, y) & \text{in } \Omega \times Y^0, \\ y \rightarrow p_1, u_0 & Y\text{-periodic.} \end{array} \right. \quad (2.30)$$

Proof. Let us consider the a priori estimates from (2.26). Then, Lemma 2.3.6 implies the existence of $u_0 \in L^2((0, T) \times \Omega; H_{\#}^1(Y)^d)$ such that the second, third and fourth lines of (2.30) hold true. Now let us multiply the first line in (2.23) by $\varepsilon \phi(t, x, x/\varepsilon)$ with $\phi(t, x, y) = 0$ on $(0, T) \times \Omega \times \Sigma^0$ and integrate by parts in space leading to

$$\int_0^T \int_{\Omega} p_\varepsilon \operatorname{div}_y \phi \left(t, x, \frac{x}{\varepsilon} \right) dx dt + \mathcal{O}(\varepsilon) = 0.$$

From the a priori estimate (2.28) and the compactness Proposition 2.3.2 we have the existence of $p_0(t, x, y)$ such that

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\Omega} p_\varepsilon \operatorname{div}_y \phi \left(t, x, \frac{x}{\varepsilon} \right) dx dt = \int_0^T \int_{\Omega} \int_Y p_0 \operatorname{div}_y \phi dy dx dt = 0. \quad (2.31)$$

We deduce from the above expression that p_0 is independent of the fast variable y . That is, $p_0(t, x, y) \equiv p(t, x)$.

Next we multiply the first line in (2.23) by $\phi(t, x, x/\varepsilon)$ with further assumptions of $\phi(T) = 0$, $\phi(t, x, y) = 0$ on $(0, T) \times \Omega \times \Sigma^0$ and $\operatorname{div}_y \phi(t, x, y) = 0$ on $(0, T) \times \Omega \times Y$. Integrating by parts lead to

$$\begin{aligned} & - \int_0^T \int_{\Omega} u_\varepsilon \frac{\partial \phi}{\partial t} dx dt - \int_{\Omega} u_\varepsilon^{in} \phi(0) dx - \int_0^T \int_{\Omega} p_\varepsilon \operatorname{div}_x \phi dx dt \\ & + \varepsilon \int_0^T \int_{\Omega} \nabla u_\varepsilon \cdot \nabla_y \phi dx dt + \mathcal{O}(\varepsilon) = \int_0^T \int_{\Omega} f \phi dx dt. \end{aligned}$$

Taking into account (2.31) and that $\phi(t, x, y) = 0$ on $(0, T) \times \Omega \times \Sigma^0$, we pass to the two-scale limit in the above expression:

$$- \int_0^T \int_{\Omega} \int_{Y^0} u_0 \frac{\partial \phi}{\partial t} dy dx dt - \int_{\Omega} \int_{Y^0} u^{in} \phi(0) dy dx - \int_0^T \int_{\Omega} \int_{Y^0} p(t, x) \operatorname{div}_x \phi(t, x, y) dy dx dt$$

$$+ \int_0^T \int_{\Omega} \int_{Y^0} \nabla_y u_0(t, x, y) \cdot \nabla_y \phi(t, x, y) dy dx dt = \int_0^T \int_{\Omega} \int_{Y^0} f(t, x) \phi(t, x, y) dy dx dt.$$

From [154, 160], we know that the orthogonal of divergence free fields are exactly the gradients. So, there exists $p_1 \in L^2((0, T) \times \Omega; H_{\#}^1(Y^0))$ such that

$$\frac{\partial u_0}{\partial t} + \nabla_x p - \mu \Delta_{yy} u_0 - f = \nabla_y p_1 \text{ in } (0, T) \times \Omega \times Y^0.$$

Thus we have the first line of (2.30).

The above observation together with Lemma 2.3.6 leads to the homogenized system (2.30). \square

The homogenized system (2.30) is called a two-scaled homogenized system as there are both the slow variable x and the fast variable y present in (2.30). This two-scale homogenized system (2.30) is sometimes referred to as two pressures Stokes system [115]. The homogenized problem (2.8) that we obtained in Section 2.3 for the steady Stokes system was just in the slow variable x . This, we achieved by defining the homogenized velocity as

$$u(x) = \int_{Y^0} u_0(x, y) dy,$$

thus eliminating the slow variable y . Even in case of the unsteady Stokes system, we can arrive at a homogenized equation with only the slow variable. We shall not give the details on eliminating the fast variable but given below is the homogenized problem that we arrive at after some analysis:

$$\begin{cases} \frac{\partial u}{\partial t}(t, x) = u^{in}(x) + \int_0^t A(t-s) (f(s, x) - \nabla p(s, x)) ds & \text{in } (0, T) \times \Omega, \\ \operatorname{div}_x u(t, x) = 0 & \text{in } (0, T) \times \Omega, \\ u(t, x) \cdot n = 0 & \text{on } (0, T) \times \partial\Omega, \end{cases} \quad (2.32)$$

where the initial data u^{in} is just the average of the two-scale limit in (2.24) over Y^0 , that is,

$$u^{in}(x) = \int_{Y^0} u^{in}(x, y) dy$$

and the pressure $p(t, x)$ is the same as in (2.30). The kernel $A(t)$ in (2.32) is given in terms of the solutions to a cell problem. The explicit expression for $A(t)$ and the cell problem can be found in [115, 4].

2.4 Periodic unfolding

In [29], a dilation operator is utilized to study the homogenization of single phase fluid flow equations. This operator has been used in [112, 113] in relation to the study of electrical networks. Using this dilation technique, in [58] a new notion of upscaling technique was announced. In [58], the dilation operator is coined as the ‘‘unfolding operator’’. Using this operator and incorporating some ideas from finite element approximations to construct scale-splitting operators, a new kind of homogenization technique is presented in [58, 60, 59].

Before we go any further, we shall define the unfolding operator borrowed from [58]. But, first some notations. As usual, let $Y =]0, 1[^d$ be the unit cell. For a $z \in \mathbb{R}^d$, let us take

$$[z]_Y = \sum_i^d k_i e_i \text{ such that } z - [z]_Y \in Y, \quad (2.33)$$

where $k_i \in \mathbb{Z}$. Denote the difference $z - [z]_Y$ by $\{z\}_Y$. For any $z \in \mathbb{R}^d$, $\varepsilon > 0$, we have $z = \varepsilon([z/\varepsilon]_Y + \{z/\varepsilon\}_Y)$. Now we are equipped to give the definition of the unfolding operator.

Definition 2.4.1. *Let $u \in L^2(\Omega)$. The unfolding operator $\mathcal{T}_\varepsilon : L^2(\Omega) \rightarrow L^2(\Omega \times Y)$ is defined as*

$$\mathcal{T}_\varepsilon(u)(x, y) = u\left(\varepsilon[x/\varepsilon]_Y + \varepsilon y\right) \text{ for } x \in \Omega, y \in Y. \quad (2.34)$$

Next we state a result from [58, 60] which sheds some light on the relationship between the unfolding operator \mathcal{T}_ε and the two-scale convergence described in Section 2.3.

Proposition 2.4.2. *Let u_ε be a bounded sequence in $L^2(\Omega)$. The following are equivalent:*

- $\mathcal{T}_\varepsilon(u_\varepsilon) \rightharpoonup u$ in $L^2(\Omega \times Y)$
- $u_\varepsilon \xrightarrow{2scale} u$

The proof of the above result can be found in [60]. The essence of this result being, it replaces two-scale convergence by a weak convergence type notion with the introduction of the unfolding operator. Another important ingredient of this method is the scale-splitting operators. Every $\varphi \in H^1(\Omega)$ is split as

$$\varphi = \mathcal{Q}_\varepsilon(\varphi) + \mathcal{R}_\varepsilon(\varphi), \quad (2.35)$$

where \mathcal{Q}_ε doesn't capture any micro-oscillations and the reminder \mathcal{R}_ε captures the oscillations. $\mathcal{Q}_\varepsilon(\varphi)$ is defined similar to interpolation functions in Finite Element Method. For any sequence $\{u_\varepsilon\} \subset H^1(\Omega)$, weak convergence results are proved for the $\mathcal{Q}_\varepsilon(u_\varepsilon)$ and $\mathcal{T}_\varepsilon(\mathcal{R}_\varepsilon(u_\varepsilon))$ in [60] which help us upscale the equations with periodically oscillating coefficients. This technique has been further developed to handle periodic porous media and also non-homogeneous boundary conditions in [59]. Please refer to the cited references for further information on this technique.

2.5 Two-scale convergence on periodic surfaces

In the examples (2.4) and (2.23) cited in the previous sections, we considered zero Dirichlet conditions for the velocity field on the porous boundary. There are more complex physical phenomena where we work with different kinds of boundary data. Some such models are studied in [67, 63]. Let us consider an example of diffusion equation in the porous medium Ω_ε with Fourier boundary condition on $\partial\Omega_\varepsilon$ that is studied in [14]:

$$\begin{cases} -\Delta u_\varepsilon + u_\varepsilon = f & \text{in } \Omega_\varepsilon, \\ \nabla u_\varepsilon \cdot n + \varepsilon \alpha\left(\frac{x}{\varepsilon}\right) u_\varepsilon = 0 & \text{on } \partial\Omega_\varepsilon, \\ u_\varepsilon = 0 & \text{on } \partial\Omega, \end{cases} \quad (2.36)$$

where $f \in L^2(\Omega)$ and $\alpha \geq 0 \in L^\infty_\#(\Omega)$. Let us consider the variational formulation of (2.36) with ϕ as test function:

$$\int_{\Omega_\varepsilon} \nabla u_\varepsilon \cdot \nabla \phi \, dx + \int_{\Omega_\varepsilon} u_\varepsilon \phi \, dx + \varepsilon \int_{\partial\Omega_\varepsilon} \alpha\left(\frac{x}{\varepsilon}\right) u_\varepsilon \phi \, d\sigma(x) = \int_{\Omega_\varepsilon} f \phi \, dx.$$

If we wish to find the two-scale limit problem for (2.36) using the method of two-scale convergence, we need to pass to the limit in the above variational formulation with properly chosen test function as in the previous section. However, we have a little difficulty posed by the third term of the left hand side in the above variational formulation. Similar surface terms arise while studying surface diffusion and surface chemical processes as demonstrated in [97, 98, 14, 69, 68, 64, 20, 10, 17, 18, 19]. This asks for the development of a notion of two-scale convergence for function sequences defined on periodic surfaces like $\partial\Omega_\varepsilon$. This task is achieved in [14, 134]. Now we define the notion of two-scale convergence on periodic surfaces. This is similar to the Definition 2.3.1.

Definition 2.5.1. [14] Let $u_\varepsilon(x)$ be a sequence in $L^2(\partial\Omega_\varepsilon)$ such that

$$\varepsilon \int_{\partial\Omega_\varepsilon} |u_\varepsilon(x)|^2 d\sigma(x) \leq C.$$

The sequence $\{u_\varepsilon\}$ is said to two-scale converge on surfaces to a limit $u_0 \in L^2(\Omega \times \partial\Sigma^0)$ if, for any function $\phi(x, y) \in C_c^\infty(\Omega; C_\#^\infty(Y))$, we have

$$\lim_{\varepsilon \rightarrow 0} \varepsilon \int_{\partial\Omega_\varepsilon} u_\varepsilon(x) \phi\left(x, \frac{x}{\varepsilon}\right) d\sigma(x) = \int_{\Omega} \int_{\partial\Sigma^0} u_0(x, y) \phi(x, y) d\sigma(y) dx. \quad (2.37)$$

We denote this convergence by $u_\varepsilon \xrightarrow{2Sscale} u_0$.

Remark 2.5.2. Since the $(d-1)$ -dimensional measure of the periodic surface $\partial\Omega_\varepsilon$ is of $\mathcal{O}(\varepsilon^{-1})$, a bound of the type $\sqrt{\varepsilon} \|z_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)} \leq C$ means that the sequence z_ε is bounded on the surface $\partial\Omega_\varepsilon$.

Here we state a proposition that is in the same spirit as Propositions 2.3.2 and 2.3.3 suitable for sequences on periodic surfaces.

Proposition 2.5.3. [14] Let u_ε be a sequence in $H^1(\partial\Omega_\varepsilon)$ such that

$$\varepsilon \int_{\partial\Omega_\varepsilon} \left(|u_\varepsilon(x)|^2 + |\nabla^s u_\varepsilon(x)|^2 \right) d\sigma_\varepsilon(x) \leq C.$$

Then, there exist $u_0(x) \in H^1(\Omega)$ and $u_1(x, y) \in L^2(\Omega; H_\#^1(\partial\Sigma^0))$ such that

$$u_\varepsilon \xrightarrow{2Sscale} u_0(x),$$

$$\nabla^s u_\varepsilon \xrightarrow{2Sscale} G(y) \nabla_x u_0(x) + \nabla_y^s u_1(x, y),$$

where $\nabla^s = G(y) \nabla$ is the tangential gradient with the projection operator $G(y)$ on the tangent plane of $\partial\Sigma^0$ at the point y defined as

$$G(y) = Id - n(y) \otimes n(y)$$

where $n(y)$ is the outward unit normal to Y^0 .

With the above defined notion of two-scale convergence on periodic surfaces, we will be able to pass to the limit in the third term of the variational formulation of the model problem (2.36). As this approach is very well illustrated in [14], we refrain from repeating the arguments on obtaining the homogenized limit for (2.36). The homogenized model for (2.36) turns out to be

$$\begin{cases} -\operatorname{div}(\mathcal{D}\nabla u_0) + (1+a)u_0 = f & \text{in } \Omega, \\ u_0 = 0 & \text{on } \partial\Omega, \end{cases} \quad (2.38)$$

where the diffusion matrix \mathcal{D} is given in terms of solutions of a certain cell problem and the constant a in (2.38) is given by

$$a = \frac{1}{|Y^0|} \int_{\partial\Sigma^0} \alpha(y) d\sigma(y).$$

2.6 Two-scale convergence with drift

The diffusion system (2.36) that we considered in the previous section models the diffusion of a solute in a porous medium in presence of bulk and surface reactions. In (2.36), we didn't consider the influence of the convective velocity field on the transport of the dissolved solute. Ignoring the bulk and surface reactions, just for simplicity, the convection-diffusion equation that governs the transport of a dissolved single solute is given by

$$\begin{cases} \frac{\partial u}{\partial \tau} + b(y) \cdot \nabla_y u - \operatorname{div}_y (D(y) \nabla_y u) = 0 & \text{in } (0, \zeta) \times \Omega_f, \\ D(y) \nabla_y u \cdot n = 0 & \text{on } (0, \zeta) \times \partial\Omega_s, \end{cases} \quad (2.39)$$

where the velocity field $b(y)$ is assumed to be given, periodic in space and independent of time. We also assume that the velocity field is divergence free i.e., $\operatorname{div}_y b(y) = 0$ in Ω_f , and non penetrating on the pore boundaries i.e., $b \cdot n = 0$ on $\partial\Omega_s$. The regularity that we assume on the velocity field is $b(y) \in L^\infty_{\#}(\Omega_f; \mathbb{R}^d)$. The diffusion matrix $D(y) \in L^\infty_{\#}(\Omega_f; \mathbb{R}^{d \times d})$ is assumed to be symmetric positive definite. In the Stokes systems (2.4) and (2.23) that we studied in the previous sections, the coefficients in the partial differential equations were just constants. The underlying microstructure, the porous medium, was ε -periodic. The model of interest (2.39) in this section, along with the underlying microstructure, has periodic coefficients $b(y)$ and $D(y)$. So, the process of homogenization determines the interplay between the periodicity in the microstructure and that of the partial differential equation. The equation (2.39) is posed at the level of the fluid part in an unit cell, $Y^0 = Y/\Sigma^0$. We wish to study the transport phenomena in the ε -periodic porous medium. So, we scale the equation (2.39) in space and also in time. We consider the ‘‘parabolic scaling’’ of the model (2.39). The scaled model that we wish to homogenize is

$$\begin{cases} \frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b\left(\frac{x}{\varepsilon}\right) \cdot \nabla u_\varepsilon - \operatorname{div}\left(D\left(\frac{x}{\varepsilon}\right) \nabla u_\varepsilon\right) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ D\left(\frac{x}{\varepsilon}\right) \nabla u_\varepsilon \cdot n = 0 & \text{on } (0, T) \times \partial\Omega_\varepsilon. \end{cases} \quad (2.40)$$

One can apply the method of two-scale asymptotics from Section 2.2 to find the homogenized equation for the above equation. Consider the following ansatz for the solute concentration:

$$u_\varepsilon(t, x) = u_0\left(t, x, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(t, x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(t, x, \frac{x}{\varepsilon}\right) + \dots \quad (2.41)$$

Plug the above ansatz for u_ε in (2.40). The system that we arrive at the order ε^{-2} :

$$\begin{cases} b(y) \nabla_y u_0 - \operatorname{div}_y (D(y) \nabla_y u_0) = 0 & \text{in } Y^0, \\ D(y) \nabla_y u_0 \cdot n = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow u_0 & Y\text{-periodic.} \end{cases} \quad (2.42)$$

At the order ε^{-1} :

$$\begin{cases} b(y) \left(\nabla_y u_1 + \nabla_x u_0 \right) - \operatorname{div}_y \left(D(y) \left(\nabla_y u_1 + \nabla_x u_0 \right) \right) = 0 & \text{in } Y^0, \\ D(y) \left(\nabla_y u_1 + \nabla_x u_0 \right) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow u_1 & Y\text{-periodic.} \end{cases} \quad (2.43)$$

The above system is solvable if and only if we assume that the velocity field $b(y)$ is of zero average. This is nothing but the Fredholm alternative:

$$\int_{Y^0} b(y) dy = 0.$$

Under the assumption of zero mean velocity, the homogenization of (2.40) is very classical [41, 101, 123]. To include more general velocity fields, a slight variant of the ansatz for u_ε is proposed [137, 76, 25]:

$$u_\varepsilon(t, x) = u_0 \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) + \varepsilon u_1 \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) + \varepsilon^2 u_2 \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) + \dots \quad (2.44)$$

for some constant $b^* \in \mathbb{R}^d$. The above asymptotic, with a drift in the concentration profile, is called two-scale asymptotic expansion with drift. The case $b^* = 0$ falls back to the classical two-scale asymptotic method of Section 2.2. As before, we shall plug this variant ansatz (2.44) into the convection diffusion equation (2.40). We shall use the following chain rule for the derivation with respect to time and space:

$$\begin{cases} \frac{\partial}{\partial t} \left[\phi \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) \right] = \left[\frac{\partial \phi}{\partial t} - \frac{b^*}{\varepsilon} \cdot \nabla_x \phi \right] \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right), \\ \nabla \left[\phi \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) \right] = \left[\nabla_x \phi + \frac{1}{\varepsilon} \nabla_y \phi \right] \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right). \end{cases} \quad (2.45)$$

Even with this new ansatz, the system at order ε^{-2} turns out to be the same as (2.42) which implies that the first term of the ansatz is independent of the fast variable y . That is $u_0(t, x) \equiv u_0(t, x, y)$.

At the next order of ε^{-1} , we have the following system:

$$\begin{cases} b(y) \cdot \nabla_y u_1 - \operatorname{div}_y \left(D(y) \left(\nabla_y u_1 + \nabla_x u_0 \right) \right) = \left(b^* - b(y) \right) \cdot \nabla_x u_0 & \text{in } Y^0, \\ D(y) \left(\nabla_y u_1 + \nabla_x u_0 \right) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow u_1 & Y\text{-periodic.} \end{cases} \quad (2.46)$$

We shall apply Fredholm alternative to find the compatibility condition that guarantees the existence and uniqueness of the solution u_1 . (2.46) is a steady state problem. Thus the solvability is guaranteed if the source terms are in equilibrium i.e.,

$$\int_{Y^0} \left(b^* - b(y) \right) dy = 0,$$

thus giving the value of the drift velocity which was unknown to begin with in (2.44):

$$b^* = \frac{1}{|Y^0|} \int_{Y^0} b(y) dy. \quad (2.47)$$

The linearity of (2.46) helps us deduce that

$$u_1(t, x, y) = \omega(y) \cdot \nabla_x u_0(t, x), \quad (2.48)$$

where $w_i(y)$ satisfy the following cell problem for each $1 \leq i \leq d$:

$$\begin{cases} b(y) \cdot \nabla_y \omega_i - \operatorname{div}_y \left(D(y) (\nabla_y \omega_i + e_i) \right) = (b^* - b(y)) \cdot e_i & \text{in } Y^0, \\ D(y) (\nabla_y \omega_i + e_i) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \omega_i & Y\text{-periodic.} \end{cases} \quad (2.49)$$

At the next order, we have the following system:

$$\begin{cases} \frac{\partial u_0}{\partial t} - b^* \cdot \nabla_x u_1 + b(y) \cdot (\nabla_x u_1 + \nabla_y u_2) - \operatorname{div}_x (D(y) (\nabla_x u_0 + \nabla_y u_1)) \\ - \operatorname{div}_y (D(y) (\nabla_x u_1 + \nabla_y u_2)) = 0 & \text{in } Y^0, \\ D(y) (\nabla_y u_2 + \nabla_x u_1) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow u_2 & Y\text{-periodic.} \end{cases}$$

Invoking Fredholm alternative for the solvability of the above model for u_2 leads to the following compatibility condition:

$$- \int_{Y^0} \frac{\partial u_0}{\partial t} dy + \int_{Y^0} (b^* - b(y)) \cdot \nabla_x u_1 dy + \operatorname{div}_x \int_{Y^0} D(y) (\nabla_x u_0 + \nabla_y u_1) dy = 0.$$

Using the information that u_0 is independent of y and the particular form of u_1 from (2.48), the above equation is equivalent to

$$|Y^0| \frac{\partial u_0}{\partial t} = \operatorname{div}(\mathcal{D} \nabla u_0) \quad \text{in } (0, T) \times \mathbb{R}^d, \quad (2.50)$$

where the elements of the dispersion tensor \mathcal{D} is given by the following expression:

$$\mathcal{D}_{ij} = \int_{Y^0} D(y) e_i \cdot e_j dy + \int_{Y^0} D(y) \nabla_y \omega_j \cdot e_i dy + \int_{Y^0} (b_i^* - b_i(y)) \omega_j dy.$$

For any symmetric matrix A and any other matrix B , we have the following observation regarding the inner product between matrices:

$$B : A = B^t : A = \frac{1}{2} (B + B^t) : A. \quad (2.51)$$

We know that the Hessian matrix $\nabla \nabla u_0$ is symmetric. So, in (2.50) only the symmetric part of \mathcal{D} plays a role. Thus, symmetrizing the above expression for \mathcal{D} :

$$\begin{aligned} \mathcal{D}_{ij} = & \int_{Y^0} D(y) e_i \cdot e_j dy + \frac{1}{2} \left[\int_{Y^0} D(y) \nabla_y \omega_j \cdot e_i dy + \int_{Y^0} D(y) \nabla_y \omega_i \cdot e_j dy \right] \\ & + \frac{1}{2} \left[\int_{Y^0} (b_i^* - b_i(y)) \omega_j dy + \int_{Y^0} (b_j^* - b_j(y)) \omega_i dy \right]. \end{aligned} \quad (2.52)$$

To further simplify the expression for the dispersion tensor, we shall use the information from the cell problem (2.49). Let us multiply the first line in (2.49) for ω_i by the cell solution ω_j and vice versa. Adding the thus obtained expressions lead to

$$\begin{aligned} & \int_{Y^0} D(y) \nabla_y \omega_i \cdot \nabla_y \omega_j \, dy + \frac{1}{2} \left[\int_{Y^0} D(y) \nabla_y \omega_j \cdot e_i \, dy + \int_{Y^0} D(y) \nabla_y \omega_i \cdot e_j \, dy \right] \\ &= \frac{1}{2} \left[\int_{Y^0} (b_i^* - b_i(y)) \omega_j \, dy + \int_{Y^0} (b_j^* - b_j(y)) \omega_i \, dy \right]. \end{aligned}$$

The convective term vanishes in the above equation as the velocity field $b(y)$ is periodic and assumed to be divergence free with non-penetrating boundary condition on the solid obstacle $\partial\Sigma^0$:

$$\int_{Y^0} (b(y) \cdot \nabla_y \omega_i) \omega_j \, dy + \int_{Y^0} (b(y) \cdot \nabla_y \omega_j) \omega_i \, dy = 0.$$

Hence the dispersion tensor is given by

$$D_{ij} = \int_{Y^0} D(y) (\nabla_y \omega_i + e_i) \cdot (\nabla_y \omega_j + e_j) \, dy.$$

We obtained a homogenized problem for our convection diffusion model (2.40) via the method of two-scale asymptotic expansion with drift. The next step is to justify the upscaling by a rigorous mathematical analysis. To begin with, let us derive a priori estimates for the solution u_ε of the model (2.40).

Lemma 2.6.1. *Let u_ε be a weak solution for (2.40). There exists a constant C , independent of ε , such that we have the following a priori estimates:*

$$\|u_\varepsilon\|_{L^\infty((0,T);L^2(\Omega_\varepsilon))} + \|\nabla u_\varepsilon\|_{L^2((0,T)\times\Omega_\varepsilon)} \leq C. \quad (2.53)$$

The proof of the above lemma goes via energy estimates. This is a very standard approach where we multiply the first line in (2.40) by u_ε followed by integration over the porous domain Ω_ε and then integrating over the time domain $(0, T)$.

Let us test if the approach of two-scale convergence that we used in the previous section can be used to upscale the convection-diffusion equation (2.40) with strong convection. The a priori estimates (2.53) along with Proposition 2.3.3 guarantees the existence of two-scale limits. Then, following the approach of Section 2.3, we need to pass to the limit in the variational formulation of (2.40) with properly chosen test functions. Let us consider the variational formulation of (2.40):

$$\int_0^T \int_{\Omega_\varepsilon} \frac{\partial u_\varepsilon}{\partial t} \phi \, dx \, dt + \frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi \, dx \, dt + \int_0^T \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla \phi \, dx \, dt = 0. \quad (2.54)$$

By choosing $\phi(t, x) = \phi(t, x, x/\varepsilon)$, we can try to use the method of two-scale convergence. But we face the difficulty with the singular term (second term) in the variational formulation (2.54). We have already noticed in the beginning of this section that we had to modify the usual asymptotic expansion (2.41) by the two-scale asymptotic expansion with drift (2.44) to homogenize the convection-diffusion equation (2.40).

The method of two-scale convergence takes cues from the two-scale asymptotic expansion. The asymptotic expansion has coefficients of the type $u_i(x, x/\varepsilon)$. In the Definition 2.3.1 of the two-scale convergence, the test functions are chosen to be of similar structure: $\phi(x, x/\varepsilon)$. Now, let us consider the modified two-scale asymptotic expansion with drift that helped us formally obtain the upscaled model for (2.40):

$$u_\varepsilon(t, x) = u_0\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) + \dots$$

Thus, the possibility of defining a new notion of two-scale convergence called ‘‘Two-scale convergence with drift’’. Here we shall take the test functions in moving coordinates: $\phi(t, x - b^*t/\varepsilon, x/\varepsilon)$.

Definition 2.6.2. [121] *Let $b^* \in \mathbb{R}^d$ be a constant. A sequence of functions $u_\varepsilon(t, x)$ in $L^2((0, T) \times \mathbb{R}^d)$ is said to two-scale converge with drift b^* , or equivalently in moving coordinates $(t, x) \rightarrow (t, x - \frac{b^*t}{\varepsilon})$, to a limit $u_0(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times Y)$ if, for any function $\phi(t, x, y) \in C_c^\infty((0, T) \times \mathbb{R}^d; C_\#^\infty(Y))$, we have*

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\mathbb{R}^d} u_\varepsilon(t, x) \phi\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) dx dt = \int_0^T \int_{\mathbb{R}^d} \int_Y u_0(t, x, y) \phi(t, x, y) dy dx dt. \quad (2.55)$$

We denote this convergence by $u_\varepsilon \xrightarrow{2\text{-drift}} u_0$.

Remark 2.6.3. *Definition 2.6.2 gives the compactness phenomena with test functions in moving coordinates. To demonstrate the dependence of the two-scale limit on the chosen drift velocity, we shall consider the following sequence of functions in $C_c^\infty((0, T) \times \mathbb{R}^d)$:*

$$u_\varepsilon(t, x) = u_1\left(t, x - \frac{b_1^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) + u_2\left(t, x - \frac{b_2^*t}{\varepsilon}, \frac{x}{\varepsilon}\right), \quad (2.56)$$

where $b_1^* \neq b_2^*$. By density arguments, the below calculations carry on to bounded sequences in $L^2((0, T) \times \mathbb{R}^d)$. The two-scale drift limit of u_1^ε defined as

$$u_1^\varepsilon = u_1\left(t, x - \frac{b_1^*t}{\varepsilon}, \frac{x}{\varepsilon}\right)$$

is indeed $u_1(t, x, y)$ by choosing b_1^* as the drift velocity in the Definition 2.6.2. Similarly $u_2(t, x, y)$ is the two-scale drift limit for the below sequence with b_2^* chosen as drift velocity:

$$u_2^\varepsilon = u_2\left(t, x - \frac{b_2^*t}{\varepsilon}, \frac{x}{\varepsilon}\right).$$

For the sequence u_ε as in (2.56), let us try to find the two-scale drift limit:

$$\begin{aligned} & \int_0^T \int_{\mathbb{R}^d} u_\varepsilon(t, x) \phi\left(t, x - \frac{\mathcal{V}t}{\varepsilon}, \frac{x}{\varepsilon}\right) dx dt \\ &= \int_0^T \int_{\mathbb{R}^d} u_1\left(t, x - \frac{b_1^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) \phi\left(t, x - \frac{\mathcal{V}t}{\varepsilon}, \frac{x}{\varepsilon}\right) dx dt \\ &+ \int_0^T \int_{\mathbb{R}^d} u_2\left(t, x - \frac{b_2^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) \phi\left(t, x - \frac{\mathcal{V}t}{\varepsilon}, \frac{x}{\varepsilon}\right) dx dt. \end{aligned} \quad (2.57)$$

Let us take $\mathcal{V} = b_1^*$ in (2.57), we get

$$\begin{aligned} & \int_0^T \int_{\mathbb{R}^d} u_1\left(t, x - \frac{b_1^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) \phi\left(t, x - \frac{b_1^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) dx dt \\ & + \int_0^T \int_{\mathbb{R}^d} u_2\left(t, x - \frac{b_1^* t}{\varepsilon} + \frac{(b_1^* - b_2^*)t}{\varepsilon}, \frac{x}{\varepsilon}\right) \phi\left(t, x - \frac{b_1^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) dx dt. \end{aligned} \quad (2.58)$$

When we pass to the limit in (2.58) as $\varepsilon \rightarrow 0$, thanks to the chosen drift velocity, we get $u_1(t, x, y)$ as the two-scale drift limit for u_ε because the second term goes to zero as $b_1^* \neq b_2^*$. On the other hand if we choose $\mathcal{V} = b_2^*$ in (2.57), we get $u_2(t, x, y)$ as a two-scale drift limit for u_ε . Also we remark that the only possible choices for the drift velocities is either b_1^* or b_2^* . Thus the dependence of the two-scale drift limits on the choice we make on the drift velocity. This observation will come in handy when we consider the homogenization of convection diffusion equation in the regime of compressible fluid flows in Section 3.12.

Our next task is to prove that Definition 2.6.2 does make sense i.e., the goal is to prove that there does exist some sequences, of which we can extract converging subsequences and the associated two-scale limits with drift. The following proposition is in the same spirit as the Proposition 2.3.2.

Proposition 2.6.4. [121] *Let b^* be a constant vector in \mathbb{R}^d . For any bounded sequence of functions $u_\varepsilon(t, x) \in L^2((0, T) \times \mathbb{R}^d)$ i.e., satisfying*

$$\|u_\varepsilon\|_{L^2((0, T) \times \mathbb{R}^d)} \leq C,$$

there exists a limit $u_0(t, x, y) \in L^2((0, T) \times \mathbb{R}^d; L^2_\#(Y))$ and one can extract a subsequence, still denoted by ε , such that

$$u_\varepsilon \xrightarrow{2\text{-drift}} u_0.$$

The proof of the above proposition is similar to the proof of the compactness Theorem 1.2 of [5]. The result on the oscillating test functions (Lemma 1.3 of [5]) plays a crucial role in the proof of the Theorem 1.2 in [5]. We shall prove a lemma related to the oscillating test functions in moving coordinates that plays a major role in the proof of Proposition 2.6.4.

Lemma 2.6.5. [7] *For $\phi(t, x, y) \in L^2(0, T \times \mathbb{R}^d; C_\#(Y))$, we have*

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\mathbb{R}^d} \left| \phi\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) \right|^2 dx dt = \int_0^T \int_{\mathbb{R}^d} \int_Y \left| \phi(t, x, y) \right|^2 dy dx dt. \quad (2.59)$$

Proof. The idea is to approximate ϕ by step functions. Let us introduce a paving of the unit cell Y made of n^d small cells Y_i of size $1/n$. Let χ_i be the characteristic function of Y_i extended by Y -periodicity to \mathbb{R}^d . Taking y_i to be a point in Y_i , we approximate $\phi(t, x, y)$ by

$$\phi_n(t, x, y) = \sum_{i=1}^{n^d} \phi(t, x, y_i) \chi_i(y). \quad (2.60)$$

We show that (2.59) holds true for (2.60). Consider

$$\int_0^T \int_{\mathbb{R}^d} \left| \phi\left(t, x - \frac{b^* t}{\varepsilon}, y_i\right) \chi_i\left(\frac{x}{\varepsilon}\right) \right|^2 dx dt,$$

which upon the change of variable $x' = x - \frac{b^*}{\varepsilon}t$ yields

$$\int_0^T \int_{\mathbb{R}^d} \left| \phi\left(t, x', y_i\right) \chi_i\left(\frac{x'}{\varepsilon} + \frac{b^*}{\varepsilon^2}t\right) \right|^2 dx dt.$$

For a fixed time t , the sequence $\chi_i^2\left(\frac{x'}{\varepsilon} + \frac{b^*}{\varepsilon^2}t\right)$ is a periodically oscillating function. It follows from a well known result [39] that the periodically oscillating functions converge weakly to their average in Y , thus leading to

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\mathbb{R}^d} \left| \phi\left(t, x', y_i\right) \chi_i\left(\frac{x'}{\varepsilon} + \frac{b^*}{\varepsilon^2}t\right) \right|^2 dx dt = \int_0^T \int_{\mathbb{R}^d} \int_{Y_i} \left| \phi\left(t, x', y_i\right) \chi_i(y) \right|^2 dy dx dt.$$

Summing the above expression over $1 \leq i \leq n^d$ shows that (2.59) holds true for the approximation ϕ_n by (2.60). Passing to the limit as $n \rightarrow \infty$ yields (2.59) for all $\phi(t, x, y) \in L^2(0, T \times \mathbb{R}^d; C_{\#}(Y))$. The details on this limit can be found in Section 5 of [5]. \square

The proof of Proposition 2.6.4 is similar to that of Theorem 1.2 in [5] where Lemma 2.6.5 plays an important role. In Section 2.3, we gave a result on relative compactness of sequences when we have additional bounds on the sequences. We state a result that is similar in spirit as Proposition 2.3.3. We avoid giving the proof as the arguments can be adapted to the case of two-scale convergence with drift by that of Proposition 1.14 in [5].

Proposition 2.6.6. [121, 7] *Let b^* be a constant vector in \mathbb{R}^d and let the sequence u_ε be uniformly bounded in $L^2((0, T); H^1(\mathbb{R}^d))$. Then, there exists a subsequence, still denoted by ε , and functions $u_0(t, x) \in L^2((0, T); H^1(\mathbb{R}^d))$ and $u_1(t, x, y) \in L^2((0, T) \times \mathbb{R}^d; H_{\#}^1(Y))$ such that*

$$u_\varepsilon \xrightarrow{2\text{-drift}} u_0$$

and

$$\nabla u_\varepsilon \xrightarrow{2\text{-drift}} \nabla_x u_0 + \nabla_y u_1.$$

As remarked in [5], the two-scale limit of a sequence contains more information than its weak L^2 limit. Here we give a corrector result, a kind of strong convergence, when we have some supplementary knowledge on the two-scale limit in moving coordinates. This extension to the two-scale convergence with drift case from the two-scale convergence is borrowed from [7].

Proposition 2.6.7. [7] *Let $(u_\varepsilon)_{\varepsilon > 0}$ be a sequence in $L^2((0, T) \times \mathbb{R}^d)$ which two-scale converges with drift to a limit $u_0(t, x, y) \in L^2((0, T) \times \mathbb{R}^d; L_{\#}^2(Y))$. It satisfies*

$$\lim_{\varepsilon \rightarrow 0} \|u_\varepsilon\|_{L^2((0, T) \times \mathbb{R}^d)} \geq \|u_0\|_{L^2((0, T) \times \mathbb{R}^d \times Y)}.$$

Assume further that

$$\lim_{\varepsilon \rightarrow 0} \|u_\varepsilon\|_{L^2((0, T) \times \mathbb{R}^d)} = \|u_0\|_{L^2((0, T) \times \mathbb{R}^d \times Y)}. \quad (2.61)$$

Then, it is said to two-scale converges with drift strongly and it satisfies

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\mathbb{R}^d} \left| u_\varepsilon(t, x) - u_0\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) \right|^2 dx dt = 0, \quad (2.62)$$

if $u_0(t, x, y)$ is smooth, say $u_0(t, x, y) \in L^2((0, T) \times \mathbb{R}^d; C_{\#}(Y))$.

Now we get to the point where prove, with rigor, the upscaling of (2.40) to (2.50). Let us choose the drift velocity b^* to be given by (2.47) i.e.,

$$b^* = \frac{1}{|Y^0|} \int_{Y^0} b(y) dy.$$

The above choice of the drift velocity, as we will remark during the proof of the next Theorem, guarantees the solvability of the cell problem (2.49).

Remark 2.6.8. *The Definition 2.6.2 of the two-scale convergence with drift is given in the full domain \mathbb{R}^d . All through this thesis, we will be working with perforated domains. So, Remark 2.3.4 on the trivial extension by zero of the function sequences defined in porous media extend to the notion of two-scale convergence with drift too. That is, defining an extended function $U_\varepsilon(t, x) = u_\varepsilon(t, x)$ in Ω_ε and $U_\varepsilon(t, x) = 0$ in $\mathbb{R}^d \setminus \Omega_\varepsilon$, we obtain that*

$$\int_0^T \int_{\Omega_\varepsilon} u_\varepsilon(t, x) \phi\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) dx dt = \int_0^T \int_{\mathbb{R}^d} U_\varepsilon(t, x) \phi\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) dx dt$$

and the two-scale limit $U_0(t, x, y)$ of U_ε vanishes in Σ^0 so that

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon(t, x) \phi\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) dx dt = \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} U_0(t, x, y) \phi(t, x, y) dy dx dt.$$

From now on, in all the compactness results that we state, we shall avoid explicitly stating that u_ε is extended trivially by zero on to \mathbb{R}^d .

Theorem 2.6.9. *The sequence of concentrations $\{u_\varepsilon\}$, solutions of (2.40), two-scale converges with drift b^* , as $\varepsilon \rightarrow 0$, in the following sense*

$$\begin{cases} u_\varepsilon \xrightarrow{2\text{-drift}} u_0(t, x), \\ \nabla u_\varepsilon \xrightarrow{2\text{-drift}} \nabla_x u_0(t, x) + \nabla_y \left(\sum_{i=1}^d \omega_i(y) \frac{\partial u_0}{\partial x_i}(t, x) \right), \end{cases} \quad (2.63)$$

where $u_0(t, x)$ is the unique solution of the following homogenized equation:

$$\begin{cases} |Y^0| \frac{\partial u_0}{\partial t} = \operatorname{div}(\mathcal{D} \nabla u_0) & \text{in } (0, T) \times \mathbb{R}^d, \\ u_0(0, x) = u^{in}(x) & \text{in } \mathbb{R}^d, \end{cases} \quad (2.64)$$

where the elements of the dispersion tensor is given in terms of the cell solutions ω_i by

$$\mathcal{D}_{ij} = \int_{Y^0} D(y) (\nabla_y \omega_i + e_i) \cdot (\nabla_y \omega_j + e_j) dy, \quad (2.65)$$

and the associated cell problem is (2.49).

Proof. We know from the a priori estimates (2.53) that the solutions u_ε are bounded L^2 in time and H^1 in space. Invoking Proposition 2.6.6, we have the existence of $u_0 \in L^2((0, T); H^1(\mathbb{R}^d))$ and $u_1 \in L^2((0, T) \times \mathbb{R}^d; H_{\#}^1(Y^0))$ such that

$$u_\varepsilon \xrightarrow{2\text{-drift}} u_0 \quad \text{and} \quad \nabla u_\varepsilon \xrightarrow{2\text{-drift}} \nabla_x u_0 + \nabla_y u_1.$$

Next, we wish to pass to the limit in the variational formulation (2.54) for the convection-diffusion equation (2.40). The above obtained two-scale limits with drift help us choose the proper test functions:

$$\phi_\varepsilon(t, x) = \phi\left(t, x - \frac{b^*}{\varepsilon}t\right) + \varepsilon\phi_1\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right). \quad (2.66)$$

The variational for (2.40) with ϕ_ε as test function:

$$\int_0^T \int_{\Omega_\varepsilon} \frac{\partial u_\varepsilon}{\partial t} \phi_\varepsilon dx dt + \frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi_\varepsilon dx dt + \int_0^T \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla \phi_\varepsilon dx dt = 0.$$

Upon integrating by parts, we have

$$\begin{aligned} & - \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon \frac{\partial \phi}{\partial t} \left(t, x - \frac{b^*t}{\varepsilon}\right) dx dt + \frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon b^* \cdot \nabla_x \phi \left(t, x - \frac{b^*t}{\varepsilon}\right) dx dt \\ & + \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon b^* \cdot \nabla_x \phi_1 \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) dx dt - \int_{\Omega_\varepsilon} u^{in}(x) \phi(0, x) dx \\ & - \frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon b_\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^*t}{\varepsilon}\right) dx dt + \int_0^T \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi_1 \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) dx dt \\ & + \int_0^T \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^*t}{\varepsilon}\right) dx dt + \int_0^T \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla_y \phi_1 \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) dx dt + \mathcal{O}(\varepsilon) = 0. \end{aligned} \quad (2.67)$$

Using the two-scale limits obtained, we can pass to the limit in the above expression as $\varepsilon \rightarrow 0$, except for some singular terms. Let us gather the singular terms:

$$\int_0^T \int_{\Omega_\varepsilon} u_\varepsilon \frac{b^* - b_\varepsilon}{\varepsilon} \cdot \nabla_x \phi \left(t, x - \frac{b^*t}{\varepsilon}\right) dx dt. \quad (2.68)$$

To handle (2.68), we introduce the following auxiliary problem:

$$\begin{cases} -\Delta_{yy} \alpha_i(y) = b_i^* - b_i(y) & \text{in } Y^0, \\ \nabla \alpha_i \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \alpha_i(y) & \text{is } Y\text{-periodic.} \end{cases} \quad (2.69)$$

The scaled auxiliary problem, with $y = x/\varepsilon$, for $\alpha_i^\varepsilon(x) = \alpha_i(x/\varepsilon)$ is

$$\begin{cases} -\varepsilon^2 \Delta_{xx} \alpha_i^\varepsilon(x) = b_i^* - b_i^\varepsilon(x) & \text{in } \Omega_\varepsilon, \\ \nabla \alpha_i^\varepsilon \cdot n = 0 & \text{on } \partial \Omega_\varepsilon, \\ x \rightarrow \alpha_i^\varepsilon & \text{is } \varepsilon\text{-periodic.} \end{cases} \quad (2.70)$$

Using (2.70) in the singular term (2.68), we have

$$\int_0^T \int_{\Omega_\varepsilon} \varepsilon \sum_{i=1}^d \nabla \alpha_i^\varepsilon \cdot \nabla \left(\partial_{x_i} \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) u_\varepsilon \right) dx dt. \quad (2.71)$$

Taking $\phi \equiv 0$ in the variational formulation (2.67), we arrive at the following variational formulation just with ϕ_1 as the test function:

$$\begin{aligned} & \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon b^* \cdot \nabla_x \phi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt + \int_0^T \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt \\ & + \int_0^T \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla_y \phi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt = 0. \end{aligned}$$

Passing to the limit in the above expression leads to

$$\begin{aligned} & - \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} b^* \cdot \nabla_x u_0(t, x) \phi_1(t, x, y) dy dx dt \\ & + \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} b(y) \cdot \left(\nabla_x u_0(t, x) + \nabla_y u_1(t, x, y) \right) \phi_1(t, x, y) dy dx dt \\ & + \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} D(y) \left(\nabla_x u_0(t, x) + \nabla_y u_1(t, x, y) \right) \cdot \nabla_y \phi_1(t, x, y) dy dx dt = 0. \end{aligned} \quad (2.72)$$

The partial differential equation corresponding to the variational formulation (2.72) is nothing but the system (2.46) that we had obtained in our formal approach at order ε^{-1} . The solvability of (2.46) is guaranteed for the particularly chosen drift velocity (2.47). The linearity of (2.46) helps us deduce that we can separate the slow and fast variables in $u_1(t, x, y)$ as

$$u_1(t, x, y) = \sum_{i=1}^d \omega_i(y) \frac{\partial u_0}{\partial x_i}(t, x),$$

where ω_i solves the cell problem (2.49).

Taking $\phi_1 \equiv 0$ in the variational formulation (2.67), we arrive at the following variational formulation just with ϕ as the test function:

$$\begin{aligned} & - \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon \frac{\partial \phi}{\partial t} \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt + \int_0^T \int_{\Omega_\varepsilon} \varepsilon \sum_{i=1}^d \nabla \alpha_i^\varepsilon \cdot \nabla \left(\partial_{x_i} \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) u_\varepsilon \right) dx dt \\ & + \int_0^T \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt - \int_{\Omega_\varepsilon} u^{in}(x) \phi(0, x) dx = 0. \end{aligned}$$

Making note that $\varepsilon \nabla \alpha_i^\varepsilon(x) = (\nabla_y \alpha_i)(x/\varepsilon)$, we pass to the limit in the above expression to arrive at

$$|Y^0| \int_0^T \int_{\mathbb{R}^d} \frac{\partial u_0}{\partial t} \phi dx dt - |Y^0| \int_{\mathbb{R}^d} u^{in}(x) \phi(0, x) dx + \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} \sum_{i,j=1}^d \sum_{l=1}^d \frac{\partial \alpha_i(y)}{\partial y_l} \frac{\partial \omega_j(y)}{\partial y_l} \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} dy dx dt$$

$$+ \sum_{i,j=1}^d \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} D_{ij}(y) \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} dy dx dt + \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} \sum_{i,j=1}^d \sum_{l=1}^d D_{il}(y) \frac{\partial \omega_j(y)}{\partial y_l} \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} dy dx dt = 0.$$

The above expression is a variational formulation for the diffusion equation (2.64) with the entries of the diffusion matrix given by

$$\begin{aligned} \mathcal{D}_{ij} = & \int_{Y^0} D(y) e_i \cdot e_j dy + \frac{1}{2} \left[\int_{Y^0} D \nabla_y \omega_i \cdot e_j dy + \int_{Y^0} D \nabla_y \omega_j \cdot e_i dy \right] \\ & + \frac{1}{2} \left[\int_{Y^0} \nabla_y \alpha_i \cdot \nabla_y \omega_j dy + \int_{Y^0} \nabla_y \alpha_j \cdot \nabla_y \omega_i dy \right]. \end{aligned} \quad (2.73)$$

The diffusion matrix is symmetrized as was done before because the Hessian matrix $\nabla \nabla u_0$ is symmetric. Now to arrive at the expression (2.65) for the dispersion matrix, we shall use the auxiliary problem (2.69). Let us test the auxiliary problem (2.69) for α_i by ω_j and vice versa leading to

$$\int_{Y^0} \nabla_y \alpha_i \cdot \nabla_y \omega_j dy + \int_{Y^0} \nabla_y \alpha_j \cdot \nabla_y \omega_i dy = \int_{Y^0} (b_i^* - b_i(y)) \omega_j dy + \int_{Y^0} (b_j^* - b_j(y)) \omega_i dy. \quad (2.74)$$

Using (2.74) in (2.73), we arrive at (2.52). This was the intermediate expression for the dispersion matrix that we had obtained in our formal analysis using the two-scale asymptotic expansion with drift. We had used information from the cell problem (2.49) to further simplify the expression for the dispersion matrix. As the calculations were presented before, we avoid repeating the same calculations here. Even though Proposition 2.6.6 that we used to deduce the existence of two-scale limits such that the sequences are relatively compact, we need to show that the entire sequence converges to the limit. The dispersion tensor \mathcal{D} is positive definite. So, the homogenized equation (2.64) is wellposed. That is, there exists a unique solution to the homogenized problem. So the entire sequence converges. \square

2.7 Two-scale convergence with drift on periodic surfaces

Section 2.5 was devoted to adapt the notion of two-scale convergence defined in Section 2.3 for function sequences defined on periodic surfaces. Having defined a variant of two-scale convergence called two-scale convergence with drift in Definition 2.6.2, the objective of this section is to introduce a new notion of convergence on the sequences defined on periodic surfaces. This notion of convergence appears for the first time in this thesis.

Definition 2.7.1. *Let $b^* \in \mathbb{R}^d$ be a constant. A sequence of functions $u_\varepsilon(t, x)$ in $L^2((0, T) \times \partial\Omega_\varepsilon)$ is said to two-scale converge with drift b^* , or equivalently in moving coordinates $(t, x) \rightarrow \left(t, x - \frac{b^* t}{\varepsilon}\right)$, to a limit $u_0(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times \partial\Sigma^0)$ if, for any function $\phi(t, x, y) \in C_c^\infty((0, T) \times \mathbb{R}^d; C_\#^\infty(Y))$, we have*

$$\lim_{\varepsilon \rightarrow 0} \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} u_\varepsilon(t, x) \phi\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) dx dt = \int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} u_0(t, x, y) \phi(t, x, y) dy dx dt. \quad (2.75)$$

We denote this convergence by $u_\varepsilon \xrightarrow{2s\text{-drift}} u_0$.

The above definition comes in handy to treat, for example, the convection-diffusion equation posed on porous skeleton,

$$\begin{cases} \frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s u_\varepsilon - \operatorname{div}^s (D_\varepsilon^s \nabla^s u_\varepsilon) = 0 & \text{in } (0, T) \times \partial\Omega_\varepsilon, \\ u_\varepsilon(0, x) = u^{in}(x) & \text{in } \partial\Omega_\varepsilon, \end{cases} \quad (2.76)$$

where the velocity field on the porous skeleton $b^s(y) \in L^\infty_{\#}(\partial\Sigma^0; \mathbb{R}^d)$ and is of null divergence. The diffusion matrix $D^s(y) \in L^\infty_{\#}(\partial\Sigma^0; \mathbb{R}^{d \times d})$ represents the diffusion process on the solid fluid interface of the porous medium. By definition, $b^s = G(y)b^s$ and $D^s = G(y)D^sG(y)$ where $G(y)$ is the projection matrix on the tangent hyperplane of Σ^0 . The diffusion matrix is assumed to be symmetric and coercive. The initial data $u^{in}(x) \in H^1(\mathbb{R}^d)$ (chosen such that the trace exists on the skeleton $\partial\Omega_\varepsilon$). ∇^s and div^s represent the surface gradient and surface divergence respectively.

The a priori estimates on the solution u_ε for (2.76) is given by

$$\sqrt{\varepsilon} \|u_\varepsilon\|_{L^\infty((0, T); L^2(\partial\Omega_\varepsilon))} + \sqrt{\varepsilon} \|\nabla u_\varepsilon\|_{L^2((0, T) \times \partial\Omega_\varepsilon)} \leq C. \quad (2.77)$$

Next compactness result will show that the Definition 2.7.1 does make sense.

Proposition 2.7.2. *Let b^* be a constant vector in \mathbb{R}^d and let u_ε be a sequence in $L^2((0, T) \times \partial\Omega_\varepsilon)$ such that*

$$\varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} |u_\varepsilon(t, x)|^2 d\sigma_\varepsilon(x) dt \leq C.$$

Then, there exists a subsequence, still denoted by ε , and a function $u_0(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times \partial\Sigma^0)$ such that

$$u_\varepsilon(t, x) \xrightarrow{2s\text{-drift}} u_0(t, x, y).$$

We wish to use the notion of two-scale convergence with drift on surfaces to upscale the model (2.76). The a priori estimates (2.77) on the solution u_ε has H^1 bounds. So, we state the following generalization of Proposition 2.7.2.

Proposition 2.7.3. *Let $u_\varepsilon(t, x) \in L^2((0, T); H^1(\partial\Omega_\varepsilon))$ be such that*

$$\varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} (|u_\varepsilon(t, x)|^2 + |\nabla^s u_\varepsilon(t, x)|^2) d\sigma_\varepsilon(x) dt \leq C.$$

There exist $u_0(t, x) \in L^2((0, T); H^1(\mathbb{R}^d))$ and $u_1(t, x, y) \in L^2((0, T) \times \mathbb{R}^d; H^1_{\#}(\partial\Sigma^0))$ such that

$$\begin{aligned} u_\varepsilon &\xrightarrow{2s\text{-drift}} u_0(t, x), \\ \nabla^s u_\varepsilon &\xrightarrow{2s\text{-drift}} G(y) \nabla_x u_0(t, x) + \nabla_y^s u_1(t, x, y). \end{aligned}$$

Proposition 2.6.7 gave a strong convergence (corrector type) result for sequences with respect to the notion of two-scale convergence with drift. On similar lines, we can blend the notion of strong two-scale convergence with drift to sequences defined on surfaces.

Proposition 2.7.4. *Let $(u_\varepsilon)_{\varepsilon>0}$ be a sequence in $L^2((0, T) \times \partial\Omega_\varepsilon)$ which two-scale converges with drift to a limit $u_0(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times \partial\Sigma^0)$. It satisfies*

$$\lim_{\varepsilon \rightarrow 0} \sqrt{\varepsilon} \|u_\varepsilon\|_{L^2((0, T) \times \partial\Omega_\varepsilon)} \geq \|u_0\|_{L^2((0, T) \times \mathbb{R}^d \times \partial\Sigma^0)}. \quad (2.78)$$

Assume further that the inequality in (2.78) is an equality. Then, u_ε is said to two-scale converges with drift strongly and, if $u_0(t, x, y)$ is smooth enough, say $u_0(t, x, y) \in L^2((0, T) \times \mathbb{R}^d; C_\#(\partial\Sigma^0))$, it satisfies

$$\lim_{\varepsilon \rightarrow 0} \varepsilon \int_0^T \int_{\mathbb{R}^d} \left| u_\varepsilon(t, x) - u_0\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) \right|^2 dx dt = 0.$$

Consider the a priori estimates (2.77) and invoking the above compactness result, we have the existence of u_0 and u_1 as in Proposition 2.7.3. Having known the two-scale limits, our goal is to pass to the limit in the variational formulation for (2.76):

$$\varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \frac{\partial u_\varepsilon}{\partial t} \phi_\varepsilon dx dt + \int_0^T \int_{\partial\Omega_\varepsilon} b_\varepsilon^s \cdot \nabla^s u_\varepsilon \phi_\varepsilon dx dt + \varepsilon \int_0^T \int_{\Omega_\varepsilon} D_\varepsilon^s \nabla^s u_\varepsilon \cdot \nabla^s \phi_\varepsilon dx dt = 0, \quad (2.79)$$

where the test function ϕ_ε is chosen as in (2.66) and pass to the two-scale limit as $\varepsilon \rightarrow 0$. The homogenized equation for (2.76) turns out to be the similar to (2.64) only that, in this case, the diffusion matrix \mathcal{D} depends on the solutions of a cell problem posed on the solid surface $\partial\Sigma^0$ and also it depends on the geometry of $\partial\Sigma^0$.

2.8 Factorization principle

In Sections 2.2 and 2.3, while working with the upscaling of the Stokes systems (2.4) and (2.23), we arrived at two-scale homogenized systems (2.8) and (2.30). The two-scale limit of the velocity field, $u_0(x, y)$, had both the slow and fast variables. To eliminate the fast variable y , we averaged $u_0(x, y)$ over the unit cell. Thus obtained average, $u(x)$, had just the slow variable x . In order to represent the effective behaviour of a given physical system, it is of paramount importance to eliminate the fast variable from the effective limit and to find the upscaled equation with no fast variable. Averaging over the unit cell is one such technique to eliminate the fast variable. Another well known approach to eliminate the fast variable is the ‘‘Method of Factorization’’. This approach was introduced by Vanninathan in [161]. We present the essence of this approach through an application to an example, asymptotics of the Dirichlet eigenvalue problem, the one studied in [161]. Let us consider the following spectral problem:

$$\left\{ \begin{array}{l} \text{Find } (u_\varepsilon, \lambda_\varepsilon) \in H^1(\Omega_\varepsilon) \times \mathbb{R} \text{ such that} \\ -\Delta u_\varepsilon = \lambda_\varepsilon u_\varepsilon \quad \text{in } \Omega_\varepsilon, \\ u_\varepsilon = 0 \quad \text{on } \partial\Omega_\varepsilon, \\ \int_{\Omega_\varepsilon} |u_\varepsilon(x)|^2 dx = 1. \end{array} \right. \quad (2.80)$$

From the standard Spectral theory, there exist a sequence of eigenvalues $\{\lambda_\varepsilon^i\}_{i \in \mathbb{N}}$ and a sequence of corresponding eigenvectors $\{u_\varepsilon^i\}_{i \in \mathbb{N}}$ such that

$$\left\{ \begin{array}{l} 0 < \lambda_\varepsilon^1 < \lambda_\varepsilon^2 \leq \lambda_\varepsilon^3 \cdots \rightarrow \infty, \\ \lambda_\varepsilon^i \text{ is of finite multiplicity for each } i \in \mathbb{N}, \\ \{u_\varepsilon^i\}_{i \in \mathbb{N}} \text{ form an orthonormal basis in } L^2(\Omega_\varepsilon). \end{array} \right. \quad (2.81)$$

Let us introduce a spectral problem in the unit cell:

$$\left\{ \begin{array}{l} \text{Find } (\phi, \lambda) \in H^1(Y^0) \times \mathbb{R} \text{ such that} \\ -\Delta_y \phi = \lambda \phi \quad \text{in } Y^0, \\ \phi = 0 \quad \text{on } \partial\Sigma^0, \\ \int_{Y^0} |\phi(y)|^2 dx = 1. \end{array} \right. \quad (2.82)$$

We consider only the first eigenpair (λ, ϕ) associated with (2.82). The objective of this study is to learn the behaviour of $(\lambda_\varepsilon^i, u_\varepsilon^i)_{i \in \mathbb{N}}$, eigenpairs associated with (2.80), as $\varepsilon \rightarrow 0$.

Here we apply the method of two-scale asymptotics to upscale the spectral problem (2.80). We propose the following ansatz for $(\lambda_\varepsilon, u_\varepsilon)$:

$$u_\varepsilon(x) = u_0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(x, \frac{x}{\varepsilon}\right) + \dots \quad (2.83)$$

$$\lambda_\varepsilon = \varepsilon^{-2} \lambda_{-2} + \varepsilon^{-1} \lambda_{-1} + \lambda_0 + \dots \quad (2.84)$$

The above particular form for λ_ε follows from [161]. As usual, we plug (2.83) and (2.84) into (2.80), identify the powers of ε . We give a formal result on the homogenization of our spectral problem (2.80).

Proposition 2.8.1. [161] *Under the assumption (2.83) and (2.84), the eigenpairs for (2.80) satisfy*

$$u_\varepsilon^k(x) \approx \phi\left(\frac{x}{\varepsilon}\right) u^k(x) + \varepsilon \sum_{i=1}^d \psi_i\left(\frac{x}{\varepsilon}\right) \frac{\partial u^k}{\partial x_i}(x) \quad (2.85)$$

and

$$\lambda_\varepsilon^k \approx \varepsilon^{-2} \lambda + \lambda^k + \dots \quad (2.86)$$

where (λ, ϕ) is the first eigenpair of (2.82) and $(\psi_i)_{1 \leq i \leq d}$ are the solutions to the following cell problem, for each $1 \leq i \leq d$,

$$\left\{ \begin{array}{ll} -\Delta_{yy} \psi_i(y) = \lambda \psi_i(y) + 2 \nabla \phi(y) \cdot e_i & \text{in } Y^0, \\ \psi_i(y) = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow \psi_i & Y\text{-periodic,} \end{array} \right. \quad (2.87)$$

and $u^k(x)$ is the k th eigenvector associated with the following homogenized spectral problem

$$\left\{ \begin{array}{l} \text{Find } (u, \lambda_0) \in H^1(\Omega) \times \mathbb{R} \text{ such that} \\ -\operatorname{div}(A \nabla u) = \lambda_0 u \quad \text{in } \Omega, \\ u = 0 \quad \text{on } \partial\Omega, \end{array} \right. \quad (2.88)$$

where the homogenized coefficients are given by

$$A_{ij} = \delta_{ij} + 2 \int_{Y^0} \nabla_y \psi_j \cdot e_i dy \quad (2.89)$$

with Kronecker delta symbol, δ_{ij} .

The above formal result, obtained using the two-scale asymptotics, can be made rigorous using the energy method by Tartar [153] or the two-scale convergence method by Nguetseng [132] and Allaire [5]. Both the formal method and the energy method are employed in [161] to upscale spectral problems with different kinds of boundary data.

In (2.85), we remark that the first term can be written as a product of an oscillating function and an other function depending only on the slow variable x . So, there is a possibility of factoring out the fast oscillations off $u_0(x, y)$. The idea is to redefine the unknown as

$$v_\varepsilon(x) = \frac{u_\varepsilon(x)}{\phi(x/\varepsilon)}, \quad (2.90)$$

where ϕ is the first eigenvector associated with the spectral cell problem (2.82). Then, the spectral problem for $v_\varepsilon(x)$ becomes

$$\left\{ \begin{array}{l} \text{Find } (v_\varepsilon, \mu_\varepsilon) \text{ such that} \\ -\operatorname{div}(\phi_\varepsilon^2(x) \nabla v_\varepsilon(x)) = \mu_\varepsilon \phi_\varepsilon^2(x) v_\varepsilon(x) \quad \text{in } \Omega_\varepsilon, \\ \int_{\Omega_\varepsilon} \phi_\varepsilon^2(x) v_\varepsilon^2 dx = 1, \end{array} \right. \quad (2.91)$$

where the k th eigenvalue μ_ε^k in (2.91) is related to the k th eigenvalue λ_ε^k of (2.80) as

$$\lambda_\varepsilon^k = \varepsilon^{-2} \lambda + \mu_\varepsilon^k \quad \text{for } k \geq 1. \quad (2.92)$$

Once we have obtained the spectral problem for v_ε , we shall employ the method of two-scale asymptotics with the following ansatz:

$$v_\varepsilon(x) = v_0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon v_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 v_2\left(x, \frac{x}{\varepsilon}\right) + \dots \quad (2.93)$$

$$\mu_\varepsilon = \mu_0 + \varepsilon \mu_1 + \varepsilon^2 \mu_2 + \dots \quad (2.94)$$

Upon some calculations, we deduce that $v_0(x, y) = v(x)$ i.e., independent of any oscillations in the first term. Then, we derive the homogenized spectral problem for $(\mu_0, v(x))$. This approach is called ‘‘The method of Factorization’’ because in the very beginning we factor out the possible oscillations from u_ε by (2.90), thus simplifying the analysis. The details can be found in [161] where the energy method is used to rigorously justify the upscaling. This Factorization principle is used in the homogenization of neutron diffusion models in steady state regimes [51, 11, 53].

It is interesting to study how the Factorization principle adapts itself in unsteady regimes. This is demonstrated in the homogenization of a parabolic equation, convection-diffusion-reaction equation, scaled in the parabolic regime as was done with the convection-diffusion equation in Section 2.6. The results are documented in [23, 76]. We shall illustrate the Factorization principle in case of the following convection-diffusion-reaction equation:

$$\left\{ \begin{array}{ll} \frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b\left(\frac{x}{\varepsilon}\right) - \operatorname{div}\left(D\left(\frac{x}{\varepsilon}\right) \nabla u_\varepsilon\right) + \frac{1}{\varepsilon^2} r\left(\frac{x}{\varepsilon}\right) u_\varepsilon = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ D\left(\frac{x}{\varepsilon}\right) \nabla u_\varepsilon \cdot n = 0 & \text{on } (0, T) \times \partial\Omega_\varepsilon, \\ u_\varepsilon(0, x) = u^{in}(x) & \text{in } \Omega_\varepsilon. \end{array} \right. \quad (2.95)$$

As in Section 2.6, b_ε and D_ε denote the convective velocity field and the diffusion matrix respectively. The new term r_ε represents the reaction that might take place in the bulk of the porous

medium. We assume it to be periodic. A generalization of (2.95) is studied in [25] along with an added complexity of surface reaction. As in the steady state regime, we pass through eigenvalue problems. The eigenvalue problem associated with the parabolic equation (2.95) is given by

$$\begin{cases} b(y) \cdot \nabla_y \phi - \operatorname{div}_y (D(y) \nabla_y \phi) + r(y) \phi = r^* \phi & \text{in } Y^0, \\ D(y) \nabla_y \phi \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \phi(y) & Y\text{-periodic,} \end{cases} \quad (2.96)$$

where $(r^*, \phi(y))$ is the first eigenpair associated with (2.96). The adjoint of the above spectral problem is given by

$$\begin{cases} -\operatorname{div}_y (b(y) \phi^*) - \operatorname{div}_y (D(y) \nabla_y \phi^*) + r(y) \phi^* = r^* \phi^* & \text{in } Y^0, \\ D(y) \nabla_y \phi^* \cdot n + b(y) \cdot n \phi^* = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \phi^*(y) & Y\text{-periodic,} \end{cases} \quad (2.97)$$

where $(r^*, \phi^*(y))$ is the first eigenpair associated with (2.97). The existence of the first eigenpairs for both the spectral problems follows from the Krein-Rutman theorem [108, 152]. The common first eigenvalue happens to be real and simple. The corresponding eigenvectors are chosen positive.

Because of the presence of strong convection in (2.95), taking ideas from Section 2.6, we need to postulate an ansatz for u_ε as a two-scale asymptotic expansion with drift. Because of the large lower order term in (2.95), we have to modify the ansatz with respect to the time parameter. Taking cues from [76, 25], we shall postulate the following ansatz for u_ε :

$$u_\varepsilon(t, x) = \exp(-r^* t / \varepsilon^2) \sum_{i \geq 0} \varepsilon^i u_i \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right). \quad (2.98)$$

We can formally show that u_ε is approximated as

$$u_\varepsilon(t, x) \approx \exp(-r^* t / \varepsilon^2) \phi \left(\frac{x}{\varepsilon} \right) \left(u_0 \left(t, x - \frac{b^*}{\varepsilon} t \right) + \varepsilon \sum_{i=1}^d \omega_i \left(\frac{x}{\varepsilon} \right) \frac{\partial u_0}{\partial x_i} \left(t, x - \frac{b^*}{\varepsilon} t \right) \right), \quad (2.99)$$

where u_0 satisfies a homogenized equation and ω_i are solutions to a cell problem.

To rigorously justify the upscaling process, we need to pass via a priori estimates. If we start with the given convection-diffusion-reaction equation (2.95), it is impossible to derive estimates on u_ε with bounds independent of ε because of the large lower order term. Here we employ the Factorization principle via the change the unknown:

$$v_\varepsilon(t, x) = \exp(r^* t / \varepsilon^2) \frac{u_\varepsilon(t, x)}{\phi(x/\varepsilon)}. \quad (2.100)$$

Then the partial differential equation satisfied by v_ε is

$$\begin{cases} \phi_\varepsilon \phi_\varepsilon^* \frac{\partial v_\varepsilon}{\partial t} + \frac{1}{\varepsilon} \tilde{b}_\varepsilon \cdot \nabla v_\varepsilon - \operatorname{div} (\tilde{D}_\varepsilon \nabla v_\varepsilon) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ \tilde{D}_\varepsilon \nabla v_\varepsilon \cdot n = 0 & \text{on } (0, T) \times \partial \Omega_\varepsilon, \\ v_\varepsilon(0, x) = u^{in}(x) \int_{Y^0} \phi^*(y) dy & \text{in } \Omega_\varepsilon, \end{cases} \quad (2.101)$$

where the velocity field $\tilde{b}(y)$ and the diffusion matrix $\tilde{D}(y)$ are given in terms of the original velocity field $b(y)$, diffusion matrix $D(y)$ and the eigenvectors $\phi(y)$ and $\phi^*(y)$:

$$\begin{aligned}\tilde{b}(y) &= \phi\phi^*b(y) + \phi D\nabla_y\phi^* - \phi^*D\nabla_y\phi, \\ \tilde{D}(y) &= \phi\phi^*D(y).\end{aligned}\tag{2.102}$$

The a priori estimates for the solution v_ε of (2.101) is given by

$$\|v_\varepsilon\|_{L^\infty((0,T);L^2(\Omega_\varepsilon))} + \|\nabla v_\varepsilon\|_{L^2((0,T)\times\Omega_\varepsilon)} \leq C.\tag{2.103}$$

Using the above a priori estimates and invoking the compactness results of two-scale convergence with drift, we extract a convergent subsequence and a two-scale limit u_0 such that the subsequence converges to u_0 . This two-scale limit matches with the u_0 in the formal approximation (2.99). This approach by Factorization principle will be employed in Chapter 5 where we homogenize a system of convection-diffusion-reaction equations modelling the transport of multiple dissolved solutes in a fluid filling the porous medium.

2.9 Comments

All the averaging (homogenization) methods presented in this chapter are devoted to periodic structures. In case there aren't any restrictions on the structure of the heterogeneities, there are more general approaches: Γ -convergence [74, 75]; H -convergence [153, 131]; G -convergence [151]. In case of probabilistic and stochastic heterogeneities there have been proposed approaches to upscaling [105], Chapter 3 of [41]. The theory of periodic homogenization gets interesting as explicit expressions for the effective coefficients are obtained in terms of the microscale parameters as is demonstrated in the expression (2.10) for the permeability tensor, (2.65) for the dispersion tensor.

Under parabolic scaling the convection diffusion equation (2.39) that we studied in Section 2.6 is

$$\frac{\partial u}{\partial \tau} + b \cdot \nabla u - \operatorname{div}(D\nabla u) = 0.$$

As mentioned in the introduction G.I. Taylor in [157] derived explicit expression for the dispersion. This was an attempt to study the interplay between the fluid mechanics and the transport experimentally studied. An aspect of paramount interest regarding the effective dispersion has been to study its dependence on the molecular diffusion and the Péclet number. Some interesting experimental results regarding this are documented in [150]. There have been immense amount of work to study the small D -asymptotics (study of effective dispersion with respect to the molecular diffusion when molecular diffusion gets smaller and smaller). For a divergence-free velocity field $b(y)$ with mean zero i.e.,

$$\int_{\mathbb{T}^d} b(y) dy = 0,$$

the effective diffusivity satisfies the upper and lower bounds:

$$D|\xi|^2 \leq \mathcal{D}\xi \cdot \xi \leq \left(D + \frac{C}{D}\right)|\xi|^2,\tag{2.104}$$

where $C > 0$ is a constant. The lower bound becomes an equality for all ξ only when $b(y) \equiv 0$ i.e., effective dispersion is enhanced for mean zero divergence free flows.

However, when the fluid velocity is a potential flow i.e., $b = \nabla V$, where V is called the potential, the effective diffusivity satisfies

$$\frac{D}{Z\hat{Z}} \leq \mathcal{D}\xi \cdot \xi \leq D|\xi|^2 \quad \text{where } \hat{Z} = \int_{\mathbb{T}^d} \exp(V/D) dy \quad (2.105)$$

i.e., effective diffusion is always depleted when compared to molecular diffusion. The proofs of the above two results in case of periodic velocity fields are documented in [138]. Other good references are [85, 54]. In case of non zero drift b^* , the quantitative results similar to (2.104) and (2.105) are very interesting depending on whether b^* is rational or not [93, 119, 42]. Similar study related to compressible flows are found in [162].

Constant drift velocity b^*

In the Definition 2.6.2 of two-scale convergence with drift, we chose the drift velocity b^* to be a constant. It should be noted that in [121], where the concept of two-scale convergence with drift was introduced, the drift velocity can be time dependent. However, the two-scale convergence with drift tools don't work if we choose the drift velocity to be dependent on the slow variable x . Even the formal two-scale asymptotic analysis with drift doesn't work when the drift velocity depends on x . Let us consider a function:

$$\phi^\varepsilon = \phi\left(t, x - \frac{b^*(x)t}{\varepsilon}, \frac{x}{\varepsilon}\right).$$

Then the chain rule for differentiation given in (2.45) doesn't hold true anymore and the formal calculations get more complicated and involved. Two-scale asymptotic analysis with drift was introduced in Section 2.6 to handle the convection diffusion equation in the strong convection regime which couldn't be handled by the usual two-scale asymptotics without zero mean condition being imposed on the convective velocity field. This above observation of the drift velocity not being dependent on x highlights the handicap of the two-scale convergence with drift method. This will be apparent in Chapter 4 where we will try to homogenize a nonlinear convection-diffusion-reaction model. There, for the drift velocity to be independent of x we shall be making some assumptions on the velocity fields. This shows the need for the development of new tools in the theory of homogenization.

Numerical Homogenization

Consider a partial differential equation with highly oscillating coefficients:

$$L_\varepsilon u_\varepsilon = f \quad \text{in } \Omega, \quad (2.106)$$

where $\varepsilon > 0$ stands for small scales. When this scale parameter is too small i.e., $\varepsilon \ll 1$, the classical finite element methods [57] can result in a good approximation only if the mesh size h is smaller than the fine scale i.e., $h \ll \varepsilon$. As the CPU time and the memory storage grow polynomially with h^{-1} , the numerical computation of the fine scale solution to the microscopic problem gets costly and in some scenarios even impossible. The theoretical aspects of homogenization methods have been incorporated in the numerical methods that have come to be known as "Multiscale finite element methods". Some of the notable references being [99, 82, 9]. The crux of these approaches is the construction of adapted finite element basis which incorporates the fine scales of (2.106). A very good pedagogical review of these numerical methods are found in [83]. In this chapter, we have realized that the classical two-scale asymptotic method has to be modified in the regime of strong convection. There have been some very recent works to coalesce the method of "two-scale asymptotic expansions with drift" into the numerical methods to handle transport problems [15, 136].

Chapter 3

Linear isotherm in porous media

Allaire G, Hutridurga H. *Homogenization of reactive flows in porous media and competition between bulk and surface diffusion*, IMA J Appl Math., Vol 77, Issue 6, pp.788-815, (2012).

3.1 Introduction

Our objective with this chapter is to study the transport of a single solute dissolved in a fluid filling an ε -periodic porous domain. The physical phenomena at the pore scale is modelled by a convection-diffusion-reaction equation (3.11)-(3.13). We work with adsorption, surface reactions of mass exchange between the fluid and the porous skeleton. As far as this chapter is concerned we work with non-equilibrium reactions with linear isotherms (3.2). The coupled system is scaled by “parabolic scaling”. This model is a generalization of that studied in [10, 20]: the novelty of this work is the presence of convection and diffusion on the pores surfaces too (not only in the bulk). In particular we study the possible competition between surface and bulk molecular diffusion. Higher values of the surface diffusion may favor a solute transport along the pore boundaries rather than in the bulk of the fluid. The goal is to derive the effective equation for our pore scale model. Our main result says that the homogenized or upscaled limit of both surface and bulk concentrations is given by the solution $\tilde{u}_0^\varepsilon(t, x)$ of the following macroscopic convection-diffusion equation:

$$K_d \frac{\partial \tilde{u}_0^\varepsilon}{\partial t} + \frac{1}{\varepsilon} b^* \cdot \nabla \tilde{u}_0^\varepsilon - \operatorname{div}(\mathcal{D} \nabla \tilde{u}_0^\varepsilon) = 0,$$

where K_d is the effective porosity, \mathcal{D} is the effective diffusion (or dispersion) tensor and b^*/ε is the effective velocity. Note that, as usual, ε is the small positive parameter which is the ratio between the heterogeneities length scale and a characteristic macroscopic length scale. The expression for b^* is given by

$$K_d b^* = \int_{Y^0} b(y) dy + K \int_{\partial \Sigma^0} b^s(y) d\sigma(y),$$

where K is a reaction parameter and b, b^s are the bulk and surface velocity fields respectively.

The results are obtained formally by a method of two-scale asymptotic expansion with drift in Proposition 3.7.2. The drift being equal to b^* . The same results are obtained rigorously in Theorem 3.9.1 using two-scale convergence with drift. The relative compactness of solution sequences are proved in Theorem 3.8.2. We improve the result regarding compactness by proving that the convergence is actually strong in Theorem 3.10.1. The same approach has also been

employed to upscale convection-diffusion equations in [10, 20, 25, 76, 121].

A modified model is also considered with rescaled reaction rate ($\kappa \rightarrow \varepsilon^2 \kappa$). In this new scaling, the effective equation turns out to be a coupled convection-diffusion equation for u_0 , the two-scale limit of bulk concentration u_ε , and v_0 , the two-scale limit of surface concentration v_ε . Different effective equations are derived depending on the mean value of the bulk velocity field b and that of the surface velocity field b^s . Also, we study the effect of having divergent flows on the upscaled equation. This is achieved by the method of Factorization where we factor out the possible oscillations from the solution sequences as is done in [25].

The contents of this Chapter is the following. Section 3.2 describes the chemistry of adsorption via a linear isotherm. Section 3.3 is devoted to the mathematical modelling of the transport phenomenon. Section 3.4 aims at proving that the model (3.11)-(3.13) is wellposed. Section 3.5 is concerned with deriving maximum principles in the sense that the solutions remain positive and bounded for a positive and bounded initial data. Section 3.6 derives a priori estimates on the solutions of (3.11)-(3.13). The formal approach of obtaining effective equation is presented in Section 3.7. The rigorous justification of the formal Proposition 3.7.2 is done through Theorems 3.8.2, 3.9.1 in Sections 3.8 and 3.9 respectively. An improved convergence theorem (in the strong norm) is proved in Section 3.10. A slightly modified model (with rescaled reaction rate) is studied in Section 3.11. The divergence free condition is lifted in Section 3.12 where we employ the method of factorization in arriving at the effective equation. Eventually, Section 3.13 is concerned with some numerical tests done in two dimensions using the FreeFem++ package [141]. In particular we study the behavior of the cell solutions and of the homogenized dispersion tensor with respect to variations of various microscopic parameters like the local Péclet number, the reaction rate and the surface molecular diffusion. Finally, in Section 3.14 we comment on the results obtained in the present chapter with emphasis on the perspectives and other directions of study related to the reactive flows in a linear setting.

Most of the results presented in this chapter have appeared in a publication [17] mentioned in the very beginning of this chapter. However, there are some additional results and remarks that have been added in this chapter to those that appeared in [17]. The Sections 3.11 and 3.12 are almost entirely new even though a remark was made in [17] about the possibility of homogenizing the mesoscale model in presence of compressible fluid fields.

3.2 Henry's Adsorption Isotherm

In 1803, William Henry formulated one of the gas laws: "At a constant temperature, the amount of a given gas that dissolves in a given type and volume of liquid is directly proportional to the partial pressure of that gas in equilibrium with that liquid." In resemblance to Henry's law, we have Henry's adsorption isotherm in surface chemistry. It is stated as "The amount of surface adsorbate is proportional to the partial pressure of the adsorbative gas" [118]. In case of liquid-solid interface, we shall replace the partial pressure by concentration of the solute dissolved in the liquid phase. Let u be the concentration of the dissolved solute and v be the concentration of that adsorbed on the solid-liquid interface. We have, via linear adsorption isotherm:

$$v = K u, \tag{3.1}$$

where K is the proportionality constant (positive) called "Henry's Adsorption Constant" which can be determined experimentally. Isotherms give a relation between the two concentrations at equilibrium (i.e., when $dv/dt = 0$). Our goal is to study non-equilibrium reaction kinetics. Thus

the rate of change of the adsorbed concentration at a time t is proportional to the difference between the concentration v at time t and the concentration v at equilibrium (3.1):

$$\frac{dv}{dt} = \kappa \left(u - \frac{v}{K} \right), \quad (3.2)$$

where the proportionality constant κ is the reaction rate of the chemical kinetics. The above linear kinetics is the simplest form of adsorption phenomenon. There are more complicated adsorption isotherms. Among them, are the Langmuir isotherm:

$$v = \frac{\alpha u}{1 + \beta u} \quad \text{with } \alpha, \beta > 0 \quad (3.3)$$

and the Freundlich isotherm:

$$v = \gamma u^\delta \quad \text{with } \gamma > 0 \text{ and } 0 < \delta < 1. \quad (3.4)$$

The analysis of the above two nonlinear isotherms will be the objective of Chapter 4. It should be noted that the expression (3.1), (3.3) and (3.4) describe adsorption of a single phase component. When more than one component are dissolved in the fluid and in presence of bulk chemical reactions, the functional form of Henry's adsorption no longer holds true. In all these latter cases, the expressions for the isotherms get more complicated. Also, these expressions aren't generally extensible to describe arbitrarily complex surface chemical reaction mechanisms. The expressions representing reaction phenomena, if they exist, are often very case specific, thus making the study of reactive flows more and more involved.

3.3 Mathematical Model

Transport of any dissolved solutes in fluid filling a porous domain are subjected to convection, diffusion and possible reactions, in bulk or on surface, among solutes. Convection is via velocity field of the fluid in which the solutes are dissolved in. In this chapter, except for the Section 3.11, we shall assume that the porous medium is saturated with an incompressible fluid. The velocity of the incompressible fluid is assumed to be independent of time, periodic in space and given. We also suppose that the fluid cannot penetrate the solid obstacles but can slip on their surface. Therefore, we consider two periodic vector fields: $b(y)$, defined in the bulk Ω_f , and $b^s(y)$, defined on the surface $\partial\Omega_s$ and belonging at each point of $\partial\Omega_s$ to its tangent hyperplane. As we wish to work in the regime of periodic coefficients, we assume that both the velocity fields $b(y)$ and $b^s(y)$ are Y -periodic. Assuming that the fluid is incompressible and does not penetrate the obstacles means that

$$\begin{aligned} \operatorname{div}_y b(y) &= 0 \quad \text{in } \Omega_f, \quad b(y) \cdot n(y) = 0 \quad \text{on } \partial\Omega_s, \\ \operatorname{div}_y^s b^s(y) &= 0 \quad \text{on } \partial\Omega_s, \end{aligned}$$

where $n(y)$ is the exterior unit normal to Ω_f . In truth, $b^s(y)$ should be the trace of $b(y)$ on $\partial\Omega_s$ but, since this property is not necessary for our analysis, we shall not make such an assumption. Of course, some regularity is required for these vector fields and we assume that $b(y) \in L_{\#}^\infty(\Omega_f; \mathbb{R}^d)$, $b^s(y) \in L_{\#}^\infty(\partial\Omega_s; \mathbb{R}^d)$ and $b^s = Gb$ is always tangential to the surface where $G(y)$ is the projection matrix on the tangent hyperplane to the surface $\partial\Omega_f = \partial\Omega_s$ defined as

$$G(y) = \operatorname{Id} - n(y) \otimes n(y). \quad (3.5)$$

The tangential gradient is defined as

$$\nabla^s = G(y) \nabla \quad (3.6)$$

and the tangential divergence for any vector field $\Psi(y) : \Omega_f \rightarrow \mathbb{R}^d$ is defined as

$$\operatorname{div}^s \Psi = \operatorname{div}(G(y)\Psi). \quad (3.7)$$

We assume that the molecular diffusion is periodic, possibly anisotropic, varying in space and different in the bulk and on the surface. In other words, we introduce two periodic symmetric tensors $D(y) \in L^\infty_{\#}(\Omega_f)^{d \times d}$ and $D^s(y) \in L^\infty_{\#}(\partial\Omega_s)^{d \times d}$ which are assumed to be uniformly coercive, namely there exists a constant $C > 0$ such that, for any $\xi \in \mathbb{R}^d$,

$$D(y)\xi \cdot \xi \geq C|\xi|^2 \text{ a.e. in } \Omega_f, \quad D^s(y)\xi \cdot \xi \geq C|\xi|^2 \text{ a.e. on } \partial\Omega_s.$$

Without loss of generality, we also assume that D^s acts only on the tangent hyperplane of Ω_s , i.e., $D^s = GD^sG$.

After having introduced the velocity fields and the diffusion matrices, we write down a convection-diffusion equation for the solute concentration in the fluid bulk:

$$\frac{\partial u}{\partial \tau} + b \cdot \nabla u - \operatorname{div}(D\nabla u) = 0 \text{ in } (0, \zeta) \times \Omega_f. \quad (3.8)$$

The above partial differential equation in the bulk has to be supplemented by the boundary conditions on the fluid-solid interface and by an initial datum. We plan to study the surface reaction of exchange type taking place at the interface. The expression for the non-equilibrium adsorption given by (3.2) is used to model the reaction process. Thus, we introduce an unknown v that represents the solute concentration on the porous skeleton. Having assumed the presence of surface convection and the surface diffusion, we shall replace the ordinary differential equation (3.2) for v by the following partial differential equation on the porous skeleton:

$$\frac{\partial v}{\partial \tau} + b^s \cdot \nabla^s v - \operatorname{div}^s(D^s \nabla^s v) = \kappa \left(u - \frac{v}{K} \right) \text{ on } (0, \zeta) \times \partial\Omega_s. \quad (3.9)$$

We are still to impose the boundary conditions for (3.8). Taking into consideration the surface phenomenon modelled by (3.9), to balance the mass, we impose the right hand side of (3.9) as the Neumann boundary condition for the solute concentration u :

$$-D\nabla u \cdot n = \kappa \left(u - \frac{v}{K} \right) \text{ on } (0, \zeta) \times \partial\Omega_s. \quad (3.10)$$

We wish to study the transport of the given solute in an ε -periodic porous medium. So we shall have to scale the coupled equation in space. In order to study the long time behavior of our physical system, taking cues from Section 1.6, we shall employ parabolic scaling $(\tau, y) \rightarrow (\varepsilon^{-2}t, \varepsilon^{-1}x)$. The resulting adimensionalized coupled convection-diffusion-reaction equations for the solute concentrations $(u_\varepsilon, v_\varepsilon)$ is

$$\frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) = 0 \text{ in } (0, T) \times \Omega_\varepsilon, \quad (3.11)$$

$$-\frac{D_\varepsilon}{\varepsilon} \nabla u_\varepsilon \cdot n = \frac{\partial v_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon - \operatorname{div}^s(D_\varepsilon^s \nabla^s v_\varepsilon) = \frac{\kappa}{\varepsilon^2} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right) \text{ on } (0, T) \times \partial\Omega_\varepsilon, \quad (3.12)$$

$$u_\varepsilon(0, x) = u^{in}(x) \text{ in } \Omega_\varepsilon, \quad v_\varepsilon(0, x) = v^{in}(x) \text{ on } \partial\Omega_\varepsilon, \quad (3.13)$$

for some final time $T = \varepsilon^2 \zeta$. As $\zeta = \mathcal{O}(\varepsilon^{-2})$, the final time T is indeed of $\mathcal{O}(1)$. The initial data are chosen such that $u^{in}(x) \in L^2(\mathbb{R}^d)$ and $v^{in}(x) \in H^1(\mathbb{R}^d)$ (so that its trace is well-defined on $\partial\Omega_\varepsilon$). Remark that the coefficients in (3.11)-(3.12) are all ε -periodic with the following notations: $D_\varepsilon(x) = D(x/\varepsilon)$, $D_\varepsilon^s(x) = D^s(x/\varepsilon)$, $b_\varepsilon(x) = b(x/\varepsilon)$ and $b_\varepsilon^s(x) = b^s(x/\varepsilon)$.

Remark 3.3.1. We notice also the presence of ε^{-1} next to the velocity and ε^{-2} next to reaction term. This means that the convection, diffusion and reaction are of same order of magnitude at the mesoscale. This regime is also referred to as that of strong convection or that of Taylor Dispersion mediated mixing (refer to the general introduction to this thesis (Chapter 1)) in the literature. Homogenization of the convection-diffusion models in this regime of strong convection has been successfully achieved quite recently (To name a few references: [121, 76, 10, 20, 17]).

3.4 Existence and Uniqueness

Proving the existence and uniqueness of the coupled parabolic equations (3.11)-(3.13) is quite classical. One can either use the argument of Galerkin approximation followed by the a priori estimates as in [84] or use a variant of the Lax-Milgram lemma due to Lions-Magenes. We shall employ the latter. For easy reference, we shall state the lemma due to Lions-Magenes. The proof of which can be found in [116].

Lemma 3.4.1. [116, 50] Let V and H be two Hilbert spaces such that $V \subset H \subset V'$. Their respective norms be $\|\cdot\|_V$ and $\|\cdot\|_H$. For a fixed time $T > 0$, let us consider a bilinear form $a(t; u, v) : V \times V \rightarrow \mathbb{R}$ defined for almost every $t \in [0, T]$ verifying the following properties:

$$\begin{aligned} t \mapsto a(t; u, v) \text{ is measurable } \forall u, v \in V, \\ |a(t; u, v)| \leq C \|u\|_V \|v\|_V, \\ a(t; u, u) \geq \alpha \|u\|_V^2 - \beta \|u\|_H^2. \end{aligned} \quad (3.14)$$

Given a source term $f \in L^2(0, T; V')$ and an initial data $u^{in} \in H$, there exists a unique function u such that

$$\begin{aligned} u \in L^2(0, T; V) \cap C([0, T]; H), \quad \frac{du}{dt} \in L^2(0, T; V'), \\ \langle \frac{du}{dt}, v \rangle + a(t; u(t), v) = \langle f(t), v \rangle \quad \text{a.e } t \in [0, T], \forall v \in V, \\ u(0) = u^{in}. \end{aligned} \quad (3.15)$$

An application of the above lemma is demonstrated in [50]. We state the wellposedness result.

Proposition 3.4.2. Suppose the initial data $(u^{in}, v^{in}) \in L^2(\mathbb{R}^d) \times H^1(\mathbb{R}^d)$. For a fixed ε in the scaled coupled parabolic system (3.11)-(3.13), there exists a unique solution $(u_\varepsilon, v_\varepsilon)$ in the following energy space:

$$u_\varepsilon \in L^2((0, T); H^1(\Omega_\varepsilon)) \cap C([0, T]; L^2(\Omega_\varepsilon))$$

and

$$v_\varepsilon \in L^2((0, T); H^1(\partial\Omega_\varepsilon)) \cap C([0, T]; L^2(\partial\Omega_\varepsilon)).$$

Remark 3.4.3. In Proposition 3.4.2, ε is fixed. While applying Lemma 3.4.1, the constants in (3.14) may depend on ε . We are not looking for bounds independent of ε .

Proof of Proposition 3.4.2: Let us consider the variational formulation for (3.11)-(3.13) by taking $(\phi_\varepsilon, \varepsilon\psi_\varepsilon)$ as test function with $\phi_\varepsilon \in H^1(\Omega_\varepsilon)$ and $\psi_\varepsilon \in H^1(\partial\Omega_\varepsilon)$:

$$\int_{\Omega_\varepsilon} \left(\frac{\partial u_\varepsilon}{\partial t} \phi_\varepsilon + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi_\varepsilon + D_\varepsilon \nabla u_\varepsilon \cdot \nabla \phi_\varepsilon \right) dx + \frac{\varepsilon}{K} \int_{\partial\Omega_\varepsilon} \left(\frac{\partial v_\varepsilon}{\partial t} \psi_\varepsilon + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon \psi_\varepsilon + D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s \psi_\varepsilon \right) d\sigma_\varepsilon(x)$$

$$+\frac{\kappa}{\varepsilon} \int_{\partial\Omega_\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K}\right) \left(\phi_\varepsilon - \frac{\psi_\varepsilon}{K}\right) d\sigma_\varepsilon(x) = 0. \quad (3.16)$$

Consider $V = H^1(\Omega_\varepsilon) \times H^1(\partial\Omega_\varepsilon)$ and $H = L^2(\Omega_\varepsilon) \times L^2(\partial\Omega_\varepsilon)$ in the Lemma 3.4.1. The norms associated with V and H are

$$\|(u, v)\|_V = \|u\|_{H^1(\Omega_\varepsilon)} + \sqrt{\varepsilon}\|v\|_{H^1(\partial\Omega_\varepsilon)}$$

and

$$\|(u, v)\|_H = \|u\|_{L^2(\Omega_\varepsilon)} + \sqrt{\varepsilon}\|v\|_{L^2(\partial\Omega_\varepsilon)}.$$

Identifying (3.16) with (3.15), we shall recognize the bilinear form $a(t; (u_\varepsilon, v_\varepsilon), (\phi_\varepsilon, \psi_\varepsilon))$ as

$$\begin{aligned} & \frac{1}{\varepsilon} \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi_\varepsilon + \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla \phi_\varepsilon dx + \int_{\partial\Omega_\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon \psi_\varepsilon \\ & + \varepsilon \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s \psi_\varepsilon d\sigma_\varepsilon(x) + \int_{\partial\Omega_\varepsilon} \left[\frac{\kappa}{\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K}\right) \left(\phi_\varepsilon - \frac{\psi_\varepsilon}{K}\right) \right] d\sigma_\varepsilon(x). \end{aligned} \quad (3.17)$$

Next task is to verify that the above expression for the bilinear form does satisfy the three conditions in (3.14). The measurability is straightforward. The third condition in (3.14) can be shown as follows:

$$a(t; (u_\varepsilon, v_\varepsilon), (u_\varepsilon, v_\varepsilon)) = \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon dx + \varepsilon \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s v_\varepsilon d\sigma_\varepsilon(x) + \frac{\kappa}{\varepsilon} \int_{\partial\Omega_\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K}\right)^2 d\sigma_\varepsilon(x).$$

The convection terms in the bilinear form disappear as the velocity field is considered to be divergence free. By the coercivity of D and D^s , we can bound the above expression from below as

$$\begin{aligned} a(t; (u_\varepsilon, v_\varepsilon), (u_\varepsilon, v_\varepsilon)) & \geq \alpha \|\nabla u_\varepsilon\|_{L^2(\Omega_\varepsilon)}^2 + C\varepsilon \|\nabla v_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)}^2 \\ & = C \|(u_\varepsilon, v_\varepsilon)\|_V^2 - \|(u_\varepsilon, v_\varepsilon)\|_H^2. \end{aligned}$$

Now, we need to show boundedness of the bilinear form a with respect to $\|\cdot\|_V$. For the convective terms in (3.17):

$$\begin{aligned} & \frac{1}{\varepsilon} \left| \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi_\varepsilon dx \right| + \left| \int_{\partial\Omega_\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon \psi_\varepsilon d\sigma(x) \right| \leq \frac{1}{\varepsilon} \|b\|_{L^\infty} \|\nabla u_\varepsilon\|_{L^2(\Omega_\varepsilon)} \|\phi_\varepsilon\|_{L^2(\Omega_\varepsilon)} \\ & + \frac{1}{\varepsilon} \|b^s\|_{L^\infty} \sqrt{\varepsilon} \|\nabla^s v_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)} \sqrt{\varepsilon} \|\psi_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)} \end{aligned}$$

Using the boundedness property of the diffusion matrices D and D^s , for the diffusive terms in (3.17), we have:

$$\begin{aligned} & \left| \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla \phi_\varepsilon dx \right| + \left| \varepsilon \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s \psi_\varepsilon d\sigma_\varepsilon(x) \right| \\ & \leq \|\nabla u_\varepsilon\|_{L^2(\Omega_\varepsilon)} \|\nabla \phi_\varepsilon\|_{L^2(\Omega_\varepsilon)} + \sqrt{\varepsilon} \|\nabla^s v_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)} \sqrt{\varepsilon} \|\nabla^s \psi_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)}. \end{aligned}$$

Except for the reaction term, the bounds regroup as:

$$\begin{aligned} & \leq C_\varepsilon \|\nabla u_\varepsilon\|_{L^2(\Omega_\varepsilon)} \left(\|\phi_\varepsilon\|_{L^2(\Omega_\varepsilon)} + \|\nabla \phi_\varepsilon\|_{L^2(\Omega_\varepsilon)} \right) \\ & + C_\varepsilon \sqrt{\varepsilon} \|\nabla^s v_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)} \left(\sqrt{\varepsilon} \|\psi_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)} + \sqrt{\varepsilon} \|\nabla^s \psi_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)} \right) \end{aligned}$$

$$= C_\varepsilon \|\nabla u_\varepsilon\|_{L^2(\Omega_\varepsilon)} \|\phi_\varepsilon\|_{H^1(\Omega_\varepsilon)} + C_\varepsilon \sqrt{\varepsilon} \|\nabla^s v_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)} \sqrt{\varepsilon} \|\psi_\varepsilon\|_{H^1(\partial\Omega_\varepsilon)}$$

Using Cauchy-Schwartz inequality for the reaction term, we have

$$\begin{aligned} \left| \frac{\kappa}{\varepsilon} \int_{\partial\Omega_\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right) \left(\phi_\varepsilon - \frac{\psi_\varepsilon}{K} \right) d\sigma_\varepsilon(x) \right| &\leq C_\varepsilon \sqrt{\varepsilon} \left\| u_\varepsilon - \frac{v_\varepsilon}{K} \right\|_{L^2(\partial\Omega_\varepsilon)} \sqrt{\varepsilon} \left\| \phi_\varepsilon - \frac{\psi_\varepsilon}{K} \right\|_{L^2(\partial\Omega_\varepsilon)} \\ &\leq C_\varepsilon \left(\sqrt{\varepsilon} \|u_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)} + \sqrt{\varepsilon} \|v_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)} \right) \left(\sqrt{\varepsilon} \|\phi_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)} + \sqrt{\varepsilon} \|\psi_\varepsilon\|_{L^2(\partial\Omega_\varepsilon)} \right) \\ &\leq C_\varepsilon \left(\|u_\varepsilon\|_{H^1(\Omega_\varepsilon)} + \sqrt{\varepsilon} \|v_\varepsilon\|_{H^1(\partial\Omega_\varepsilon)} \right) \left(\|\phi_\varepsilon\|_{H^1(\Omega_\varepsilon)} + \sqrt{\varepsilon} \|\psi_\varepsilon\|_{H^1(\partial\Omega_\varepsilon)} \right) \\ &= C_\varepsilon \left\| (u_\varepsilon, v_\varepsilon) \right\|_V \left\| (\phi_\varepsilon, \psi_\varepsilon) \right\|_V, \end{aligned}$$

thus the boundedness property of the bilinear form. Then, we invoke the Lemma 3.4.1 resulting in the existence and uniqueness of solutions in the given energy space. \square

3.5 Maximum Principles

This section concerns itself with proving maximum principles for (3.11)-(3.13) in the sense that starting with a non-negative bounded initial data (u^{in}, v^{in}) , the coupled system always results in non-negative bounded solute concentrations $(u_\varepsilon, v_\varepsilon)$ at any positive time. We use the standard notations $h^+ = \max(0, h)$ and $h^- = \min(0, h)$.

Proposition 3.5.1. *Let $(u_\varepsilon, v_\varepsilon)$ be the weak solution of (3.11)-(3.13) in the space defined by Proposition 3.4.2. Assume that the initial data (u^{in}, v^{in}) satisfy $0 \leq u^{in} \leq M$, $0 \leq v^{in} \leq M$ for some positive constant M . Then,*

$$\begin{cases} 0 \leq u_\varepsilon(t, x) \leq M & \text{for } (t, x) \in (0, T) \times \Omega_\varepsilon, \\ 0 \leq v_\varepsilon(t, x) \leq M & \text{for } (t, x) \in (0, T) \times \partial\Omega_\varepsilon. \end{cases}$$

Proof. We use the standard variational approach. To begin with, we prove that the solutions remain non-negative for non-negative initial data. Let us consider $(u_\varepsilon^-, v_\varepsilon^-)$ as test functions in the variational formulation of (3.11)-(3.13):

$$\begin{aligned} &\frac{1}{2} \int_0^T \frac{d}{dt} \int_{\Omega_\varepsilon} |u_\varepsilon^-|^2 dx dt + \frac{1}{2} \frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla |u_\varepsilon^-|^2 dx dt - \int_0^T \int_{\Omega_\varepsilon} \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) u_\varepsilon^- dx dt \\ &\quad + \frac{\varepsilon}{2} \int_0^T \frac{d}{dt} \int_{\partial\Omega_\varepsilon} |v_\varepsilon^-|^2 d\sigma(x) dt + \frac{\varepsilon}{2} \int_0^T \int_{\partial\Omega_\varepsilon} b_\varepsilon^s \cdot \nabla^s |v_\varepsilon^-|^2 d\sigma(x) dt \\ &\quad - \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \operatorname{div}^s(D_\varepsilon^S \nabla^s v_\varepsilon) v_\varepsilon^- d\sigma(x) dt - \frac{\kappa}{\varepsilon} \int_0^T \int_{\partial\Omega_\varepsilon} (u_\varepsilon - v_\varepsilon) v_\varepsilon^- d\sigma(x) dt = 0. \end{aligned}$$

The convective terms in the above expression vanish due to the divergence free property of b, b^s and the boundary condition $b \cdot n = 0$ on $\partial\Omega_\varepsilon$. Thus, we get

$$\frac{1}{2} \int_{\Omega_\varepsilon} |u_\varepsilon^-(T)|^2 dx + \frac{\varepsilon}{2} \int_{\partial\Omega_\varepsilon} |v_\varepsilon^-(T)|^2 d\sigma(x) + \int_0^T \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon^- \cdot \nabla u_\varepsilon^- dx dt$$

$$\begin{aligned}
& +\varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon^- \cdot \nabla^s v_\varepsilon^- d\sigma(x) dt + \frac{\kappa}{\varepsilon} \int_0^T \int_{\partial\Omega_\varepsilon} (u_\varepsilon - v_\varepsilon) (u_\varepsilon^- - v_\varepsilon^-) d\sigma(x) dt \\
& = \frac{1}{2} \int_{\Omega_\varepsilon} |u_\varepsilon^-(0)|^2 dx + \frac{\varepsilon}{2} \int_{\partial\Omega_\varepsilon} |v_\varepsilon^-(0)|^2 d\sigma(x).
\end{aligned}$$

Since the function $h \rightarrow h^-$ is monotone, all terms in the above left hand side are non-negative. The assumption on the non-negative initial data implies that the right hand side vanishes, therefore proving that $u_\varepsilon^-(t, x) = 0$, $v_\varepsilon^-(t, x) = 0$. Thus the solutions u_ε and v_ε stay non negative at all times.

Next, we show that the solutions stay bounded from above if we start with a bounded initial data. We choose $((u_\varepsilon - M)^+, \varepsilon(v_\varepsilon - M)^+)$ as test functions in the variational formulation of (3.11)-(3.13):

$$\begin{aligned}
& \int_{\Omega_\varepsilon} |(u_\varepsilon(T) - M)^+|^2 dx + \frac{\varepsilon}{2} \int_{\partial\Omega_\varepsilon} |(v_\varepsilon(T) - M)^+|^2 d\sigma(x) + \int_0^T \int_{\Omega_\varepsilon} D_\varepsilon \nabla (u_\varepsilon(T) - M)^+ \cdot \nabla (u_\varepsilon(T) - M)^+ dx dt \\
& + \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s (v_\varepsilon(T) - M)^+ \cdot \nabla^s (v_\varepsilon - M)^+ d\sigma(x) dt \\
& + \frac{\kappa}{\varepsilon} \int_0^T \int_{\partial\Omega_\varepsilon} ((u_\varepsilon - M) - (v_\varepsilon - M)) ((u_\varepsilon - M)^+ - (v_\varepsilon - M)^+) d\sigma(x) dt \\
& = \int_{\Omega_\varepsilon} ((u^{in} - M)^+)^2 dx + \frac{\varepsilon}{2} \int_{\partial\Omega_\varepsilon} ((v^{in} - M_v)^+)^2 d\sigma(x).
\end{aligned}$$

The upper bound on the initial data implies that the right hand side vanishes. The left hand side is non-negative because $h \rightarrow h^+$ is monotone. Hence, we deduce that $u_\varepsilon(t, x) \leq M$ and $v_\varepsilon(t, x) \leq M$. \square

3.6 A priori estimates

Here, we derive a priori estimates for the solute concentrations $(u_\varepsilon, v_\varepsilon)$ based on energy equalities. These estimates will come in handy to apply the compactness result of the two-scale convergence in Section 3.8. The following lemma summarizes the result on the estimates.

Lemma 3.6.1. *There exists a constant C , which is independent of ε , such that the solution of (3.11)-(3.13) satisfies*

$$\begin{aligned}
& \|u_\varepsilon\|_{L^\infty((0,T);L^2(\Omega_\varepsilon))} + \sqrt{\varepsilon} \|v_\varepsilon\|_{L^\infty((0,T);L^2(\partial\Omega_\varepsilon))} \\
& + \|\nabla u_\varepsilon\|_{L^2((0,T)\times\Omega_\varepsilon)} + \sqrt{\varepsilon} \|\nabla^s v_\varepsilon\|_{L^2((0,T)\times\partial\Omega_\varepsilon)} \\
& + \sqrt{\varepsilon} \|w_\varepsilon\|_{L^\infty((0,T);L^2(\partial\Omega_\varepsilon))} \leq C \left(\|u^{in}\|_{L^2(\mathbb{R}^d)} + \|v^{in}\|_{H^1(\mathbb{R}^d)} \right)
\end{aligned} \tag{3.18}$$

where $w_\varepsilon = \varepsilon^{-1}(u_\varepsilon - K^{-1}v_\varepsilon)$.

Proof. We first derive an energy equality for (3.11)-(3.13). We multiply (3.11) by u_ε and then integrate over Ω_ε :

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega_\varepsilon} |u_\varepsilon|^2 dx + \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon dx + \frac{\kappa \varepsilon}{\varepsilon^2} \int_{\partial \Omega_\varepsilon} \left(u_\varepsilon^2 - \frac{u_\varepsilon v_\varepsilon}{K} \right) d\sigma_\varepsilon(x) = 0, \quad (3.19)$$

where the integral of the convective term has disappeared since

$$\int_{\Omega_\varepsilon} \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon u_\varepsilon dx = \frac{1}{2\varepsilon} \int_{\Omega_\varepsilon} \operatorname{div}(b_\varepsilon |u_\varepsilon|^2) dx = \frac{1}{2\varepsilon} \int_{\partial \Omega_\varepsilon} |u_\varepsilon|^2 b_\varepsilon \cdot n d\sigma_\varepsilon(x) = 0.$$

Multiply the second equality in (3.12) by $K^{-1} \varepsilon v_\varepsilon$ and integrate over $\partial \Omega_\varepsilon$ to get

$$\frac{\varepsilon}{2K} \frac{d}{dt} \int_{\partial \Omega_\varepsilon} |v_\varepsilon|^2 d\sigma_\varepsilon(x) + \frac{\varepsilon}{K} \int_{\partial \Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s v_\varepsilon d\sigma_\varepsilon(x) + \frac{\varepsilon \kappa}{\varepsilon^2} \int_{\partial \Omega_\varepsilon} \left(\frac{v_\varepsilon^2}{K^2} - \frac{u_\varepsilon v_\varepsilon}{K} \right) d\sigma_\varepsilon(x) = 0, \quad (3.20)$$

where the integral of the convective term has also disappeared since b_ε^s is divergence free. Adding (3.19) and (3.20) results in the following energy equality:

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_{\Omega_\varepsilon} |u_\varepsilon|^2 dx + \frac{\varepsilon}{2K} \frac{d}{dt} \int_{\partial \Omega_\varepsilon} |v_\varepsilon|^2 d\sigma_\varepsilon(x) + \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon dx \\ & + \frac{\varepsilon}{K} \int_{\partial \Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s v_\varepsilon d\sigma_\varepsilon(x) + \frac{\varepsilon \kappa}{\varepsilon^2} \int_{\partial \Omega_\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right)^2 d\sigma_\varepsilon(x) = 0. \end{aligned} \quad (3.21)$$

Integrating (3.21) over the time interval $(0, T)$ leads to the desired estimate (3.18). \square

3.7 Formal asymptotics

This section and the sections to follow concentrate on the process of homogenizing our scaled coupled equations (3.11)-(3.13). As the title of this section suggests, we shall be employing the formal method of two-scale asymptotics with drift in arriving at the homogenized model. The induction of drift in the concentration profiles is due the presence of strong convection. This method has already been employed in [10, 25, 76, 137], to name a few. This approach helps us guess the effective behavior of the scaled equations. As explained in Chapter 2, this formal method can be rigorously justified using the method of two-scale convergence with drift. This shall be the object of Sections 3.8 and 3.9. As per the method outlined in Section 2.6 of Chapter 2, we will be assuming an asymptotic expansion for the unknowns. Upon substituting the assumed series expansion into the given model, we identify the cascade of equations at various powers of ε , the scaling parameter. We formulate a Fredholm type result that guarantees the existence of solutions to the thus obtained cascade of equations under some constraints.

Let us assume that the solute concentrations u_ε and v_ε of (3.11)-(3.12) can be written in terms of an infinite series as

$$u_\varepsilon(t, x) = \sum_{i=0}^{\infty} \varepsilon^i u_i \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \quad (3.22)$$

and

$$v_\varepsilon(t, x) = \sum_{i=0}^{\infty} \varepsilon^i v_i \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \quad (3.23)$$

where $u_i(t, x, y)$ and $v_i(t, x, y)$ are functions of macroscopic variable x and the microscopic variable $y = \frac{x}{\varepsilon} \in]0, 1[^d$. The drift $b^* \in \mathbb{R}^d$ is unknown to start with. It shall be determined along the process of homogenization. The idea is to plug (3.22) and (3.23) in (3.11)-(3.12) keeping in mind the following chain rule differentiation:

$$\begin{aligned} \frac{\partial}{\partial t} \left[\phi \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \right] &= \left[\frac{\partial \phi}{\partial t} - \sum_{j=1}^d \frac{b_j^*}{\varepsilon} \frac{\partial \phi}{\partial x_j} \right] \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right), \\ \frac{\partial}{\partial x_j} \left[\phi \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \right] &= \left[\frac{\partial \phi}{\partial x_j} + \frac{1}{\varepsilon} \frac{\partial \phi}{\partial y_j} \right] \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right). \end{aligned} \quad (3.24)$$

As the equations are coupled, it shall be interesting to look for any interactions between the bulk and surface velocity fields and the underlying reaction via the induced drift. Now, we shall present a lemma of Fredholm type that is very crucial in solving the cascade of equations posed in the unit cell Y that we are going to obtain upon substitution of (3.22) and (3.23) in (3.11)-(3.12).

Lemma 3.7.1. *For $f \in L^2(Y^0)$, $g \in L^2(\partial\Sigma^0)$ and $h \in L^2(\partial\Sigma^0)$, the following system of equations*

$$\begin{cases} b(y) \cdot \nabla_y u - \operatorname{div}_y (D(y) \nabla_y u) = f & \text{in } Y^0, \\ -D(y) \nabla_y u \cdot n + g = \kappa \left(u - \frac{v}{K} \right) & \text{on } \partial\Sigma^0, \\ b^s(y) \cdot \nabla_y^s v - \operatorname{div}_y^s (D^s(y) \nabla_y^s v) - h = \kappa \left(u - \frac{v}{K} \right) & \text{on } \partial\Sigma^0, \\ y \rightarrow (u(y), v(y)) & Y - \text{periodic}, \end{cases} \quad (3.25)$$

admits a solution $(u, v) \in H_{\#}^1(Y^0) \times H_{\#}^1(\partial\Sigma^0)$, unique up to the addition of a constant multiple of $(1, K)$, if and only if

$$\int_{Y^0} f \, dy + \int_{\partial\Sigma^0} (g + h) \, d\sigma(y) = 0. \quad (3.26)$$

Proof. The variational formulation of (3.25) is

$$\begin{aligned} \int_{Y^0} (b \cdot \nabla_y u) \phi \, dy + \int_{Y^0} D(y) \nabla_y u \cdot \nabla_y \phi \, dy + \frac{1}{K} \int_{\partial\Sigma^0} (b^s \cdot \nabla_y^s v) \psi \, dy + \frac{1}{K} \int_{\partial\Sigma^0} D^s(y) \nabla_y^s v \cdot \nabla_y^s \psi \, d\sigma(y) \\ + \kappa \int_{\partial\Sigma^0} \left(u - \frac{v}{K} \right) \left(\phi - \frac{\psi}{K} \right) \, d\sigma(y) = \int_{Y^0} f \phi \, dy + \int_{\partial\Sigma^0} \left(g \phi + \frac{h}{K} \psi \right) \, d\sigma(y). \end{aligned}$$

Taking $(\phi, \psi) = (1, K)$ we find the necessary condition (3.26). Let us define the quotient space $[H_{\#}^1(Y^0) \times H_{\#}^1(\partial\Sigma^0)]/\mathbb{R}(1, K)$ of functions defined in $H_{\#}^1(Y^0) \times H_{\#}^1(\partial\Sigma^0)$ up to an additive constant (C, KC) when C takes values in \mathbb{R} . It is easily seen that $\|\nabla u\|_{L^2(Y^0)^d} + \|\nabla v\|_{L^2(\partial\Sigma^0)^d}$ is a norm for this quotient space. To show existence, we shall have to check the assumptions of the Lax-Milgram Lemma. The left hand side of the variational formulation is coercive on the quotient space. The right hand side of the variational formulation is a continuous linear form on the quotient space under the assumption (3.26). \square

Now, we state our formal result.

Proposition 3.7.2. *Under the assumption (3.22)-(3.23), the solution $(u_\varepsilon, v_\varepsilon)$ of (3.11)-(3.13) formally satisfy*

$$\begin{aligned} u_\varepsilon(t, x) &\approx u_0\left(t, x - \frac{b^*t}{\varepsilon}\right) + \varepsilon u_1\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right), \\ v_\varepsilon(t, x) &\approx K u_0\left(t, x - \frac{b^*t}{\varepsilon}\right) + \varepsilon v_1\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right), \end{aligned}$$

with the effective drift

$$b^* = \frac{\int_{Y^0} b(y) dy + K \int_{\partial\Sigma^0} b^s(y) d\sigma(y)}{|Y^0| + K|\partial\Sigma^0|_{d-1}} \quad (3.27)$$

and, u_0 , the solution of the homogenized problem:

$$\begin{cases} K_d \frac{\partial u_0}{\partial t} - \operatorname{div}_x (\mathcal{D} \nabla_x u_0) = 0 & \text{in } (0, T) \times \mathbb{R}^d, \\ K_d u_0(0, x) = |Y^0| u^{in}(x) + |\partial\Sigma^0|_{d-1} v^{in}(x), & x \in \mathbb{R}^d, \end{cases} \quad (3.28)$$

where $K_d = |Y^0| + K|\partial\Sigma^0|_{d-1}$ and the dispersion tensor \mathcal{D} is given by

$$\begin{aligned} \mathcal{D}_{ij} &= \int_{Y^0} D(y) (\nabla_y \chi_i + e_i) \cdot (\nabla_y \chi_j + e_j) dy + \kappa \int_{\partial\Sigma^0} \left(\chi_i - \frac{\omega_i}{K}\right) \left(\chi_j - \frac{\omega_j}{K}\right) d\sigma(y) \\ &\quad + K^{-1} \int_{\partial\Sigma^0} D^s(y) (K e_i + \nabla_y^s \omega_i) \cdot (K e_j + \nabla_y^s \omega_j) d\sigma(y), \end{aligned} \quad (3.29)$$

with $(\chi, \omega) = (\chi_i, \omega_i)_{1 \leq i \leq d}$ being the solution of the cell problem such that

$$u_1(t, x, y) = \sum_{i=1}^d \chi_i(y) \frac{\partial u_0}{\partial x_i}(t, x), \quad v_1(t, x, y) = \sum_{i=1}^d \omega_i(y) \frac{\partial u_0}{\partial x_i}(t, x) \quad (3.30)$$

and the cell problem is

$$\begin{cases} b(y) \cdot \nabla_y \chi_i - \operatorname{div}_y (D(\nabla_y \chi_i + e_i)) = (b^* - b) \cdot e_i & \text{in } Y^0, \\ b^s(y) \cdot \nabla_y^s \omega_i - \operatorname{div}_y^s (D^s(\nabla_y^s \omega_i + K e_i)) = K(b^* - b^s) \cdot e_i + \kappa (\chi_i - K^{-1} \omega_i) & \text{on } \partial\Sigma^0, \\ -D(\nabla_y \chi_i + e_i) \cdot n = \kappa (\chi_i - K^{-1} \omega_i) & \text{on } \partial\Sigma^0, \\ y \rightarrow (\chi_i, \omega_i) & Y - \text{periodic.} \end{cases} \quad (3.31)$$

Proof. Inserting the ansatz (3.22) and (3.23) in the equations (3.11) and (3.12) yields the following cascade of equations:

At order ε^{-2} :

$$\begin{cases} b(y) \cdot \nabla_y u_0 - \operatorname{div}_y (D(y) \nabla_y u_0) = 0 & \text{in } Y^0, \\ -D \nabla_y u_0 \cdot n = b^s(y) \cdot \nabla_y^s v_0 - \operatorname{div}_y^s (D^s(y) \nabla_y^s v_0) = \kappa (u_0 - K^{-1} v_0) & \text{on } \partial\Sigma^0, \\ y \rightarrow (u_0(y), v_0(y)) & Y - \text{periodic.} \end{cases} \quad (3.32)$$

From Lemma 3.7.1 we deduce that the solution of (3.32) does not depend on y and satisfy $v_0(t, x) = K u_0(t, x)$.

At order ε^{-1} :

$$\left\{ \begin{array}{l} -b^* \cdot \nabla_x u_0 + b(y) \cdot (\nabla_x u_0 + \nabla_y u_1) - \operatorname{div}_y(D(y)(\nabla_x u_0 + \nabla_y u_1)) = 0 \quad \text{in } Y^0, \\ -b^* \cdot \nabla_x v_0 + b^s(y) \cdot (\nabla_x v_0 + \nabla_y^s v_1) - \operatorname{div}_y^s(D^s(y)(\nabla_x v_0 + \nabla_y^s v_1)) \\ \quad = -D(y)(\nabla_x u_0 + \nabla_y u_1) \cdot n = \kappa(u_1 - K^{-1}v_1) \quad \text{on } \partial\Sigma^0, \\ y \rightarrow (u_1(y), v_1(y)) \quad \quad \quad Y - \text{periodic.} \end{array} \right. \quad (3.33)$$

The compatibility condition (3.26) of Lemma 3.7.1 yields the desired value (3.27) of the drift velocity b^* in order to solve (3.33). By linearity of (3.33) we deduce that its solution is given by

$$u_1(t, x, y) = \chi(y) \cdot \nabla_x u_0 \quad \text{and} \quad v_1(t, x, y) = \omega(y) \cdot \nabla_x u_0,$$

where (χ, ω) is the solution of the cell problem (3.31).

At order ε^0 :

$$\left\{ \begin{array}{l} \frac{\partial u_0}{\partial t} - b^* \cdot \nabla_x u_1 + b(y) \cdot (\nabla_x u_1 + \nabla_y u_2) \\ - \operatorname{div}_x(D(y)(\nabla_x u_0 + \nabla_y u_1)) - \operatorname{div}_y(D(y)(\nabla_x u_1 + \nabla_y u_2)) = 0 \quad \text{in } Y^0, \\ \frac{\partial v_0}{\partial t} - b^* \cdot \nabla_x v_1 + b^s(y) \cdot (\nabla_x u_1 + \nabla_y^s u_2) \\ - \operatorname{div}_x(D^s(y)(\nabla_x v_0 + \nabla_y^s v_1)) - \operatorname{div}_y^s(D^s(y)(\nabla_x v_1 + \nabla_y^s v_2)) \\ = -D(y)(\nabla_y u_2 + \nabla_x u_1) \cdot n = \kappa(u_2 - K^{-1}v_2) \quad \text{on } \partial\Sigma^0, \\ y \rightarrow (u_2(y), v_2(y)) \quad \quad \quad Y - \text{periodic.} \end{array} \right. \quad (3.34)$$

On identifying (3.34) with (3.25) we get the following right hand sides:

$$\left\{ \begin{array}{l} f = (b^* - b) \cdot \nabla_x u_1 + \operatorname{div}_x(D(\nabla_x u_0 + \nabla_y u_1)) - \frac{\partial u_0}{\partial t} + \operatorname{div}_y(D(\nabla_x u_1)) \quad \text{in } Y^0, \\ g = -D \nabla_x u_1 \cdot n \quad \text{on } \partial\Sigma^0, \\ h = -\frac{\partial v_0}{\partial t} + b^* \cdot \nabla_x v_1 - b^s \cdot (\nabla_x u_1) + \operatorname{div}_x(D^s(\nabla_x v_0 + \nabla_y^s v_1)) + \operatorname{div}_y^s(D^s \nabla_x v_1) \quad \text{on } \partial\Sigma^0. \end{array} \right. \quad (3.35)$$

According to Lemma 3.7.1, there exists a solution (u_2, v_2) provided (3.26) holds true. This compatibility condition leads to the homogenized problem:

$$K_d \partial_t u_0 = \operatorname{div}_x(\mathcal{D} \nabla_x u_0) \quad \text{in } (0, T) \times \mathbb{R}^d,$$

where $K_d = |Y^0| + K|\partial\Sigma^0|_{d-1}$ and the entries of the dispersion tensor \mathcal{D} are given by

$$\begin{aligned} \mathcal{D}_{ij} &= \int_{Y^0} D e_i \cdot e_j \, dy + \frac{1}{2} \left[\int_{Y^0} D \nabla_y \chi_j \cdot e_i \, dy + \int_{Y^0} D \nabla_y \chi_i \cdot e_j \, dy \right] \\ &+ K \int_{\partial\Sigma^0} D^s e_i \cdot e_j \, d\sigma(y) + \frac{1}{2} \left[\int_{\partial\Sigma^0} D^s \nabla_y^s \omega_j \cdot e_i \, d\sigma(y) + \int_{\partial\Sigma^0} D^s \nabla_y^s \omega_i \cdot e_j \, d\sigma(y) \right] \\ &+ \frac{1}{2} \left[\int_{Y^0} (b_i^* - b_i(y)) \chi_j(y) \, dy + \int_{Y^0} (b_j^* - b_j(y)) \chi_i(y) \, dy \right] \end{aligned}$$

$$+\frac{1}{2} \left[\int_{\partial\Sigma^0} (b_i^* - b_i^s(y)) \omega_j(y) d\sigma(y) + \int_{\partial\Sigma^0} (b_j^* - b_j^s(y)) \omega_i(y) d\sigma(y) \right].$$

Remark that we have symmetrized the dispersion tensor \mathcal{D} since only its contraction with the (symmetric) Hessian matrix $\nabla^2 u_0$ plays a role in the homogenized equation. In other words its antisymmetric part (if any) cannot be deduced from the above method of obtaining the homogenized equation. Testing the cell problem (3.31) for (χ_i, ω_i) by (χ_j, ω_j) and vice-versa leads to the following relationship:

$$\begin{aligned} & \int_{Y^0} D\nabla_y \chi_i \cdot \nabla_y \chi_j dy + \frac{1}{K} \int_{\partial\Sigma^0} D^s \nabla_y^s \omega_i \cdot \nabla_y^s \omega_j d\sigma(y) + \kappa \int_{\partial\Sigma^0} \left[\chi_i - \frac{\omega_i}{K} \right] \left[\chi_j - \frac{\omega_j}{K} \right] d\sigma(y) \\ & + \frac{1}{2} \left[\int_{Y^0} D\nabla_y \chi_j \cdot e_i dy + \int_{Y^0} D\nabla_y \chi_i \cdot e_j dy \right] + \frac{1}{2} \left[\int_{\partial\Sigma^0} D^s \nabla_y^s \omega_j \cdot e_i d\sigma(y) + \int_{\partial\Sigma^0} D^s \nabla_y^s \omega_i \cdot e_j d\sigma(y) \right] \\ & = \frac{1}{2} \left[\int_{Y^0} (b_i^* - b_i(y)) \chi_j(y) dy + \int_{Y^0} (b_j^* - b_j(y)) \chi_i(y) dy \right] \\ & + \frac{1}{2} \left[\int_{\partial\Sigma^0} (b_i^* - b_i^s(y)) \omega_j(y) d\sigma(y) + \int_{\partial\Sigma^0} (b_j^* - b_j^s(y)) \omega_i(y) d\sigma(y) \right]. \end{aligned}$$

Adding the above equality to the previous expression for \mathcal{D} yields the desired formula (3.29). To obtain the initial condition of the homogenized equation we use a conservation property in the unit cell which says that

$$\int_{Y^0} u_0(0, x) dy + \int_{\partial\Sigma^0} v_0(0, x) dy = \int_{Y^0} u^{in}(x) dy + \int_{\partial\Sigma^0} v^{in}(x) dy,$$

which leads to the desired initial condition upon recalling that $v_0 = K u_0$. \square

3.8 Two-scale compactness

Previous section is about formally deriving the the effective equation for our coupled convection-diffusion-reaction model. This formal method can be justified mathematically using the notion of “Two-scale convergence with drift”, a variant of “Two-scale convergence”. This justification shall be the objective of the next section. In order to be able to pass to the limit in the variational formulation, we need to have some compactness results for the solution sequences $\{u_\varepsilon\}$ and $\{v_\varepsilon\}$. The a priori estimates (3.18) along with the compactness theorems from Chapter 2 shall aid us in proving the existence of limits for the sequences $\{u_\varepsilon\}$, $\{v_\varepsilon\}$ and for the sequence $\{w_\varepsilon\}$ with $w_\varepsilon = \frac{1}{\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right)$.

Eventually we state a technical lemma which will play a key role in the convergence analysis.

Lemma 3.8.1. *Let $\phi(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times \partial\Sigma^0)$ be such that*

$$\int_{\partial\Sigma^0} \phi(t, x, y) d\sigma(y) = 0 \quad \forall (t, x) \in (0, T) \times \mathbb{R}^d. \quad (3.36)$$

There exist two vector fields $\theta(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times \mathbb{T}^d)^d$ and $\Theta(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times \partial\Sigma^0)^d$ such that

$$\begin{aligned} \operatorname{div}_y \theta &= 0 & \text{in } Y^0, \\ \theta \cdot n &= \phi & \text{on } \partial\Sigma^0, \\ \operatorname{div}_y^s \Theta &= \phi & \text{on } \partial\Sigma^0. \end{aligned} \tag{3.37}$$

Proof. We choose $\theta = \nabla_y \xi$ with $\xi \in H_{\#}^1(Y^0)$ a solution to

$$\begin{cases} \Delta_y \xi = 0 & \text{in } Y^0, \\ \nabla_y \xi \cdot n = \phi & \text{on } \partial\Sigma^0, \end{cases} \tag{3.38}$$

which admits a unique solution, up to an additive constant, since the compatibility condition of (3.38) is satisfied. On similar lines, we choose $\Theta = \nabla_y^s \psi$ where ψ is the unique solution in $H_{\#}^1(\partial\Sigma^0)/\mathbb{R}$ of $\Delta_y^s \psi = \phi$ on $\partial\Sigma^0$, the solvability of which is guaranteed by (3.36). \square

Theorem 3.8.2. *Let $\{u_\varepsilon\}$ and $\{v_\varepsilon\}$ be the sequence of bulk and surface concentrations, solutions of system (3.11)-(3.13). There exist limit functions $u_0 \in L^2((0, T); H^1(\mathbb{R}^d))$, $u_1 \in L^2((0, T) \times \mathbb{R}^d; H_{\#}^1(Y^0))$ and $v_1 \in L^2((0, T) \times \mathbb{R}^d; H_{\#}^1(\partial\Sigma^0))$ such that the sequences two-scale converge with drift b^* , as $\varepsilon \rightarrow 0$, in the following sense:*

$$\begin{cases} u_\varepsilon \xrightarrow{2\text{-drift}} u_0(t, x) \\ v_\varepsilon \xrightarrow{2s\text{-drift}} K u_0(t, x) \\ \nabla u_\varepsilon \xrightarrow{2\text{-drift}} \nabla_x u_0(t, x) + \nabla_y u_1(t, x, y) \\ \nabla^s v_\varepsilon \xrightarrow{2s\text{-drift}} K G(y) \nabla_x u_0(t, x) + \nabla_y^s v_1(t, x, y) \\ \frac{1}{\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right) \xrightarrow{2s\text{-drift}} u_1(t, x, y) - v_1(t, x, y) \end{cases} \tag{3.39}$$

Proof. Consider the a priori bound on u_ε from Lemma 3.6.1. Invoking the compactness result of two-scale convergence with drift, Proposition 2.6.6, we have the existence of $u_0(t, x) \in L^2((0, T); H^1(\mathbb{R}^d))$ and $u_1(t, x, y) \in L^2((0, T) \times \mathbb{R}^d; H^1(\mathbb{T}^d))$ such that

$$u_\varepsilon \xrightarrow{2\text{-drift}} u_0$$

and

$$\nabla u_\varepsilon \xrightarrow{2\text{-drift}} \nabla_x u_0 + \nabla_y u_1,$$

up to a subsequence. Now for the second and fourth lines in (3.39). We have from the a priori estimate (3.18):

$$\varepsilon \int_{\partial\Omega_\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right)^2 \leq C\varepsilon^2,$$

implying that the two-scale limits of $\{u_\varepsilon\}$ and $\{v_\varepsilon/K\}$ match. For the fourth line, we shall use the a priori bound for v_ε from Lemma 3.6.1, thus we have the existence of $v_1(t, x, y) \in L^2((0, T) \times \mathbb{R}^d; H_{\#}^1(\partial\Sigma^0))$ such that

$$v_\varepsilon \xrightarrow{2s\text{-drift}} K u_0$$

and

$$\nabla^s v_\varepsilon \xrightarrow{2s\text{-drift}} K G(y) \nabla_x u_0 + \nabla_y^s v_1.$$

The only limit that deserves some attention is that for $w_\varepsilon = \frac{1}{\varepsilon}(u_\varepsilon - K^{-1}v_\varepsilon)$. From Lemma 3.6.1, we know that it satisfies the uniform estimate:

$$\varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} |w_\varepsilon(t, x)|^2 d\sigma_\varepsilon(x) dt \leq C,$$

from which, by virtue of Proposition 2.7.2, we deduce, for a subsequence, that $w_\varepsilon \xrightarrow{2s\text{-drift}} q(t, x, y)$ for some $q(t, x, y) \in L^2((0, T) \times \mathbb{R}^d; L^2_{\#}(\partial\Sigma^0))$. Let us choose a test function ϕ as in Lemma 3.8.1 i.e., $\int_{\partial\Sigma^0} \phi(t, x, y) d\sigma(y) = 0$. To pass to the limit in

$$\lim_{\varepsilon \rightarrow 0} \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} w_\varepsilon(t, x) \phi\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) d\sigma_\varepsilon(x) dt,$$

we separate w_ε in a difference of two terms. In view of (3.37), the first one is

$$\begin{aligned} \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \frac{1}{\varepsilon} u_\varepsilon \phi\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) d\sigma_\varepsilon(x) dt &= \int_0^T \int_{\Omega_\varepsilon} \operatorname{div}\left(u_\varepsilon \theta\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right)\right) dx dt \\ &= \int_0^T \int_{\Omega_\varepsilon} \left[\nabla u_\varepsilon \cdot \theta\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) + u_\varepsilon (\operatorname{div}_x \theta)\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right)\right] dx dt \\ &\xrightarrow{2\text{-drift}} \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} \left[(\nabla_x u + \nabla_y u_1) \cdot \theta + u \operatorname{div}_x \theta\right] dy dx dt \\ &= \int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} u_1 \theta \cdot n d\sigma(y) dx dt = \int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} u_1 \phi d\sigma(y) dx dt. \end{aligned}$$

Now, the second term is

$$\begin{aligned} \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \frac{1}{K\varepsilon} v_\varepsilon \phi\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) d\sigma_\varepsilon(x) dt &= \frac{1}{K} \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon (\operatorname{div}_y^s \Theta)\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) d\sigma_\varepsilon(x) dt \\ &= \frac{\varepsilon}{K} \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon \left[\operatorname{div}^s\left(\Theta\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right)\right) - \operatorname{div}_x(G\Theta)\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right)\right] d\sigma_\varepsilon(x) dt \\ &= \frac{\varepsilon}{K} \int_0^T \int_{\partial\Omega_\varepsilon} \left[-\Theta\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) \cdot \nabla^s v_\varepsilon - \operatorname{div}_x(G\Theta)\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) v_\varepsilon\right] d\sigma_\varepsilon(x) dt \\ &\xrightarrow{2s\text{-drift}} \frac{1}{K} \int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} \left[-\Theta \cdot (KG(y)\nabla_x u_0 + \nabla_y^s v_1) - \operatorname{div}_x(G(y)\Theta) K u_0\right] d\sigma(y) dx dt \end{aligned}$$

$$= \frac{1}{K} \int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} v_1 \operatorname{div}_y^s \Theta \, d\sigma(y) \, dx \, dt = \frac{1}{K} \int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} v_1 \phi \, d\sigma(y) \, dx \, dt.$$

Subtracting the two terms, we have shown that

$$\int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} q \phi \, d\sigma(y) \, dx \, dt = \int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} \left(u_1 - \frac{v_1}{K} \right) \phi \, d\sigma(y) \, dx \, dt,$$

for all ϕ such that $\int_{\partial\Sigma^0} \phi \, dy = 0$. Hence,

$$q(t, x, y) = u_1(t, x, y) - \frac{v_1(t, x, y)}{K} + l(t, x)$$

for some function $l(t, x)$ which does not depend on y . Since, u_1 and v_1 are also defined up to the addition of a function solely dependent on (t, x) , we can get rid of $l(t, x)$ and we recover indeed the last line of (3.39). \square

3.9 Proof of the homogenization result

Now, the moment to characterize the two-scale limits obtained in Theorem 3.8.2. This result shall be the rigorous justification of the formal result obtained in Proposition 3.7.2.

Theorem 3.9.1. *The two-scale limit u_0 of Theorem 3.8.2 satisfies the homogenized equation (3.28) and the limits u_1 and v_1 satisfy*

$$u_1(t, x, y) = \sum_{i=1}^d \chi_i(y) \frac{\partial u_0}{\partial x_i}(t, x) \quad \text{and} \quad v_1(t, x, y) = \sum_{i=1}^d \omega_i(y) \frac{\partial u_0}{\partial x_i}(t, x).$$

The functions $(\chi_i, \omega_i)_{1 \leq i \leq d}$ satisfy the cell problem (3.31).

Proof. The idea of the proof is to pass to the limit in the coupled variational formulation of (3.11)-(3.13):

$$\begin{aligned} & \int_0^T \int_{\Omega_\varepsilon} \left[\frac{\partial u_\varepsilon}{\partial t} \phi_\varepsilon + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi_\varepsilon + D_\varepsilon \nabla u_\varepsilon \cdot \nabla \phi_\varepsilon \right] dx \, dt \\ & + \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \frac{1}{K} \left[\frac{\partial v_\varepsilon}{\partial t} \psi_\varepsilon + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon \psi_\varepsilon + D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s \psi_\varepsilon \right] d\sigma_\varepsilon(x) \, dt \\ & + \frac{\kappa}{\varepsilon} \int_0^T \int_{\partial\Omega_\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right) \left(\phi_\varepsilon - \frac{\psi_\varepsilon}{K} \right) d\sigma_\varepsilon(x) \, dt = 0, \end{aligned} \tag{3.40}$$

with the test functions

$$\begin{aligned} \phi_\varepsilon &= \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon \phi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right), \\ \psi_\varepsilon &= K \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon \psi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right). \end{aligned}$$

Here $\phi(t, x)$, $\phi_1(t, x, y)$ and $\psi_1(t, x, y)$ are smooth compactly supported functions which vanish at $t = T$. Let us consider the convective terms in (3.40) and perform integrations by parts:

$$\begin{aligned}
& \int_0^T \int_{\Omega_\varepsilon} \left(\frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \right) \phi_\varepsilon dx dt + \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \frac{1}{K} \left(\frac{\partial v_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon \right) \psi_\varepsilon d\sigma_\varepsilon(x) dt \\
&= - \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon \frac{\partial \phi}{\partial t} \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt + \frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon b^* \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt \\
&\quad + \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon b^* \cdot \nabla_x \phi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt - \int_{\Omega_\varepsilon} u^{in}(x) \phi(0, x) dx + \mathcal{O}(\varepsilon) \\
&\quad - \frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon b_\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt + \int_0^T \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt \\
&\quad - \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon \frac{\partial \phi}{\partial t} \left(t, x - \frac{b^* t}{\varepsilon} \right) d\sigma_\varepsilon(x) dt + \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon b^* \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) d\sigma_\varepsilon(x) dt \\
&\quad + \frac{\varepsilon}{K} \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon b^* \cdot \nabla_x \psi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) d\sigma_\varepsilon(x) dt - \varepsilon \int_{\partial\Omega_\varepsilon} v^{in}(x) \phi(0, x) d\sigma_\varepsilon(x) + \mathcal{O}(\varepsilon) \\
&\quad - \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon b_\varepsilon^s \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) d\sigma_\varepsilon(x) dt + \frac{\varepsilon}{K} \int_0^T \int_{\partial\Omega_\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon \psi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) d\sigma_\varepsilon(x) dt.
\end{aligned}$$

We cannot directly pass to the two-scale limit since there are terms which apparently are of order ε^{-1} . We, thus regroup them:

$$\begin{aligned}
& \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon \frac{b^* - b_\varepsilon}{\varepsilon} \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt + \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon (b^* - b_\varepsilon^s) \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) d\sigma_\varepsilon(x) dt \quad (3.41) \\
&= \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon \frac{b^* - b_\varepsilon}{\varepsilon} \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt + K \int_0^T \int_{\partial\Omega_\varepsilon} u_\varepsilon (b^* - b_\varepsilon^s) \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) d\sigma_\varepsilon(x) dt \\
&\quad + K\varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \frac{1}{\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right) (b_\varepsilon^s - b^*) \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) d\sigma_\varepsilon(x) dt.
\end{aligned}$$

We introduce an auxiliary problem:

$$\begin{cases} \Delta \alpha_i(y) = b_i(y) - b_i^* & \text{in } Y^0, \\ \nabla \alpha_i \cdot n = K(b_i^* - b_i^s(y)) & \text{on } \partial\Sigma^0, \\ \alpha_i & \text{is } Y\text{-periodic,} \end{cases} \quad (3.42)$$

which admits a unique solution (up to an additive constant) since, by definition of b^* , the source terms in (3.42) are in equilibrium. Defining $\alpha^\varepsilon(x) = \alpha(x/\varepsilon)$, thanks to (3.42), the ε^{-1} -order term (3.41) is equal to

$$\begin{aligned} & \int_0^T \int_{\Omega_\varepsilon} \varepsilon \sum_{i=1}^d \nabla \alpha_i^\varepsilon \cdot \nabla \left(\partial_{x_i} \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) u_\varepsilon \right) dx dt \\ & + K \varepsilon \int_0^T \int_{\partial \Omega_\varepsilon} \frac{1}{\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right) (b_\varepsilon^s - b^*) \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) d\sigma_\varepsilon(x) dt, \end{aligned}$$

for which we can pass to the two-scale limit.

In a first step, we choose $\phi \equiv 0$ i.e., we consider only the terms involving ϕ_1 and ψ_1 in the variational formulation (3.40):

$$\begin{aligned} & \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon b^* \cdot \nabla_x \phi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt + \int_0^T \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt \\ & + \int_0^T \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla_y \phi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt + \frac{\varepsilon}{K} \int_0^T \int_{\partial \Omega_\varepsilon} v_\varepsilon b^* \cdot \nabla_x \psi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) d\sigma_\varepsilon(x) dt \\ & + \frac{\varepsilon}{K} \int_0^T \int_{\partial \Omega_\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon \psi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) d\sigma_\varepsilon(x) dt + \frac{\varepsilon}{K} \int_0^T \int_{\partial \Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla_y^s \psi_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) d\sigma_\varepsilon(x) dt \\ & + \varepsilon \int_0^T \int_{\partial \Omega_\varepsilon} \frac{\kappa}{\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right) \left(\phi_1 - \frac{\psi_1}{K} \right) d\sigma_\varepsilon(x) dt = 0. \end{aligned}$$

Passing to the two-scale limit with drift, we obtain

$$\begin{aligned} & - \int_{\mathbb{R}^d} \int_{Y^0} b^* \cdot \nabla_x u_0(t, x) \phi_1(t, x, y) dy dx dt + \int_{\mathbb{R}^d} \int_{Y^0} b(y) \cdot (\nabla_x u_0(t, x) + \nabla_y u_1(t, x, y)) \phi_1(t, x, y) dy dx dt \\ & - \int_{\mathbb{R}^d} \int_{Y^0} \operatorname{div}_y (D(y) (\nabla_x u_0(t, x) + \nabla_y u_1(t, x, y))) \phi_1(t, x, y) dy dx dt \\ & - \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} b^* \cdot \nabla_x u_0(t, x) \psi_1(t, x, y) d\sigma(y) dx dt \\ & + \frac{1}{K} \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} b^s(y) \cdot (KG \nabla_x u_0(t, x) + \nabla^s v_1(t, x, y)) \psi_1(t, x, y) d\sigma(y) dx dt \\ & - \frac{1}{K} \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} \operatorname{div}_y^s (D^s(y) (KG \nabla_x u_0(t, x) + \nabla^s v_1(t, x, y))) \psi_1(t, x, y) d\sigma(y) dx dt \\ & + \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} \kappa \left(u_1 - \frac{v_1}{K} \right) \left(\phi_1 - \frac{\psi_1}{K} \right) d\sigma(y) dx dt = 0 \end{aligned}$$

The above expression is precisely the variational formulation of (3.33). For easy reference, let us state the coupled partial differential equation for (u_1, v_1) .

$$\left\{ \begin{array}{l} -b^* \cdot \nabla_x u_0 + b(y) \cdot (\nabla_x u_0 + \nabla_y u_1) - \operatorname{div}_y(D(y)(\nabla_x u_0 + \nabla_y u_1)) = 0 \quad \text{in } Y^0, \\ -b^* \cdot \nabla_x v_0 + b^s(y) \cdot (\nabla_x v_0 + \nabla_y^s v_1) - \operatorname{div}_y^s(D^s(y)(\nabla_x v_0 + \nabla_y^s v_1)) \\ \quad \quad \quad = -D(y)(\nabla_x u_0 + \nabla_y u_1) \cdot n = \kappa(u_1 - K^{-1}v_1) \quad \text{on } \partial\Sigma^0, \\ y \rightarrow (u_1(y), v_1(y)) \quad \quad \quad Y - \text{periodic.} \end{array} \right.$$

The linearity of the above coupled system helps us deduce that

$$u_1(t, x, y) = \sum_{i=1}^d \chi_i(y) \frac{\partial u_0}{\partial x_i}(t, x) \quad \text{and} \quad v_1(t, x, y) = \sum_{i=1}^d \omega_i(y) \frac{\partial u_0}{\partial x_i}(t, x).$$

which leads to the cell problem (3.31).

In a second step we choose $\phi_1 \equiv 0$ and $\psi_1 \equiv 0$ in (3.40), i.e., we consider only the terms involving ϕ

$$\begin{aligned} & - \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon \frac{\partial \phi}{\partial t} \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt + \int_0^T \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt \\ & - \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon \frac{\partial \phi}{\partial t} \left(t, x - \frac{b^* t}{\varepsilon} \right) d\sigma_\varepsilon(x) dt + \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) d\sigma_\varepsilon(x) dt \\ & + \int_0^T \int_{\Omega_\varepsilon} \varepsilon \sum_{i=1}^d \nabla \alpha_i^\varepsilon \cdot \nabla \left(\partial_{x_i} \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) u_\varepsilon \right) dx dt \\ & + K\varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \frac{1}{\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right) (b_\varepsilon^s - b^*) \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) d\sigma_\varepsilon(x) dt \\ & - \int_{\Omega_\varepsilon} u^{in}(x) \phi(0, x) dx - \varepsilon \int_{\partial\Omega_\varepsilon} v^{in}(x) \phi(0, x) d\sigma_\varepsilon(x) = 0. \end{aligned}$$

Taking into account formula (3.30) for u_1 and v_1 , passing to the two-scale limit with drift yields

$$\begin{aligned} & |Y^0| \int_{\mathbb{R}^d} \frac{\partial u_0}{\partial t} \phi dx dt + \int_{\mathbb{R}^d} \int_{Y^0} \sum_{i,j=1}^d D_{ij}(y) \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} dx dt \\ & - |Y^0| \int_{\mathbb{R}^d} u^{in}(x) \phi(0, x) dx + \int_{\mathbb{R}^d} \int_{Y^0} \sum_{i,j=1}^d \sum_{l=1}^d D_{il}(y) \frac{\partial \chi_j(y)}{\partial y_l} \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} dx dt \\ & + K |\partial\Sigma^0| \int_{\mathbb{R}^d} \frac{\partial u_0}{\partial t} \phi dx dt + K \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} \sum_{i,j=1}^d \sum_{l=1}^d D_{il}^s(y) G_{lj}(y) \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} d\sigma(y) dx dt \\ & - |\partial\Sigma^0| \int_{\mathbb{R}^d} v^{in}(x) \phi(0, x) dx + \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} \sum_{i,j=1}^d \sum_{l=1}^d D_{il}^s(y) \frac{\partial^s \omega_j(y)}{\partial y_l} \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} d\sigma(y) dx dt \end{aligned}$$

$$\begin{aligned}
& +K \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} \sum_{i,j=1}^d \left(\chi_j - \frac{\omega_j}{K} \right) (b_i^s(y) - b_i^*) \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} d\sigma(y) dx dt \\
& + \int_{\mathbb{R}^d} \int_{Y^0} \sum_{i,j=1}^d \sum_{l=1}^d \frac{\partial \alpha_i(y)}{\partial y_l} \frac{\partial \chi_j(y)}{\partial y_l} \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} dy dx dt = 0.
\end{aligned}$$

Introducing $K_d = |Y^0| + K|\partial\Sigma^0|_{d-1}$, the above equation is just the variational formulation of the homogenized problem

$$\begin{cases} K_d \partial_t u_0 = \operatorname{div}_x (\mathcal{D} \nabla_x u_0) & \text{in } (0, T) \times \mathbb{R}^d \\ K_d u_0(0, x) = |Y^0| u^0(x) + |\partial\Sigma^0|_{d-1} v^0(x), & x \in \mathbb{R}^d \end{cases}$$

with the expression for \mathcal{D} given by

$$\begin{aligned}
\mathcal{D}_{ij} &= \int_{Y^0} D e_i \cdot e_j dy + \frac{1}{2} \left[\int_{Y^0} D \nabla_y \chi_j \cdot e_i dy + \int_{Y^0} D \nabla_y \chi_i \cdot e_j dy \right] \\
&+ K \int_{\partial\Sigma^0} D^s e_i \cdot e_j d\sigma(y) + \frac{1}{2} \left[\int_{\partial\Sigma^0} D^s \nabla_y^s \omega_j \cdot e_i d\sigma(y) + \int_{\partial\Sigma^0} D^s \nabla_y^s \omega_i \cdot e_j d\sigma(y) \right] \\
&\quad + \frac{1}{2} \left[\int_{Y^0} \nabla_y \alpha_i \cdot \nabla_y \chi_j dy + \int_{Y^0} \nabla_y \alpha_j \cdot \nabla_y \chi_i dy \right] \\
&+ \frac{K}{2} \left[\int_{\partial\Sigma^0} \left(\chi_j - \frac{\omega_j}{K} \right) (b_i^s(y) - b_i^*) d\sigma(y) + \int_{\partial\Sigma^0} \left(\chi_i - \frac{\omega_i}{K} \right) (b_j^s(y) - b_j^*) d\sigma(y) \right]
\end{aligned}$$

Now we need to recognize that the above cell average for \mathcal{D} coincides with formula (3.29). To check this point, we shall make the following observation. Let us test the boundary value problem (3.42) for α_i by χ_j which yields

$$\int_{Y^0} \sum_{l=1}^d \frac{\partial \alpha_i(y)}{\partial y_l} \frac{\partial \chi_j(y)}{\partial y_l} dy = \int_{Y^0} (b_i^* - b_i(y)) \chi_j(y) dy + K \int_{\partial\Sigma^0} (b_i^* - b_i^s(y)) \chi_j(y) d\sigma(y).$$

Using the above information, the expression for \mathcal{D} is updated as

$$\begin{aligned}
\mathcal{D}_{ij} &= \int_{Y^0} D e_i \cdot e_j dy + \frac{1}{2} \left[\int_{Y^0} D \nabla_y \chi_j \cdot e_i dy + \int_{Y^0} D \nabla_y \chi_i \cdot e_j dy \right] \\
&+ K \int_{\partial\Sigma^0} D^s e_i \cdot e_j d\sigma(y) + \frac{1}{2} \left[\int_{\partial\Sigma^0} D^s \nabla_y^s \omega_j \cdot e_i d\sigma(y) + \int_{\partial\Sigma^0} D^s \nabla_y^s \omega_i \cdot e_j d\sigma(y) \right] \\
&\quad + \frac{1}{2} \left[\int_{Y^0} (b_i^* - b_i(y)) \chi_j(y) dy + \int_{Y^0} (b_j^* - b_j(y)) \chi_i(y) dy \right]
\end{aligned}$$

$$+\frac{1}{2} \left[\int_{\partial\Sigma^0} (b_i^* - b_i^s(y)) \omega_j(y) d\sigma(y) + \int_{\partial\Sigma^0} (b_j^* - b_j^s(y)) \omega_i(y) d\sigma(y) \right] \quad (3.43)$$

Testing the cell problem (3.31) for (χ_i, ω_i) by (χ_j, ω_j) and vice-versa leads to the following relationship

$$\begin{aligned} & \int_{Y^0} D\nabla_y \chi_i \cdot \nabla_y \chi_j dy + \frac{1}{K} \int_{\partial\Sigma^0} D^s \nabla_y^s \omega_i \cdot \nabla_y^s \omega_j d\sigma(y) + \kappa \int_{\partial\Sigma^0} \left(\chi_i - \frac{\omega_i}{K} \right) \left(\chi_j - \frac{\omega_j}{K} \right) d\sigma(y) \\ & + \frac{1}{2} \left[\int_{Y^0} D\nabla_y \chi_j \cdot e_i dy + \int_{Y^0} D\nabla_y \chi_i \cdot e_j dy \right] + \frac{1}{2} \left[\int_{\partial\Sigma^0} D^s \nabla_y^s \omega_j \cdot e_i d\sigma(y) + \int_{\partial\Sigma^0} D^s \nabla_y^s \omega_i \cdot e_j d\sigma(y) \right] \\ & = \frac{1}{2} \left[\int_{Y^0} (b_i^* - b_i(y)) \chi_j(y) dy + \int_{Y^0} (b_j^* - b_j(y)) \chi_i(y) dy \right] \\ & + \frac{1}{2} \left[\int_{\partial\Sigma^0} (b_i^* - b_i^s(y)) \omega_j(y) d\sigma(y) + \int_{\partial\Sigma^0} (b_j^* - b_j^s(y)) \omega_i(y) d\sigma(y) \right] \end{aligned} \quad (3.44)$$

Using (3.44) in (3.43), leads to the expression for the dispersion tensor \mathcal{D} given in (3.29). Finally, although we proved convergence only for a subsequence, the uniqueness of the homogenized solution $u_0(t, x)$ to (3.28) implies that the entire sequence $\{u_\varepsilon, v_\varepsilon\}$ converge. \square

3.10 Strong convergence

In the previous section, we proved the (weak) two-scale convergence with drift of $(u_\varepsilon, v_\varepsilon)$ to (u_0, Ku_0) . In this section, we improve Theorem 3.9.1 by proving that the convergence is actually strong, in a sense which is made precise in the following Theorem.

Theorem 3.10.1. *Let $(u_\varepsilon, v_\varepsilon)$ be the solution to (3.11)-(3.13). Then, $u_\varepsilon(t, x) \mathbb{I}_{\Omega_\varepsilon}$ strongly two-scale converges with drift towards $\mathbb{I}_{Y^0} u_0(t, x)$ and $v_\varepsilon(t, x) \mathbb{I}_{\partial\Omega_\varepsilon}$ strongly two-scale converges with drift on surfaces towards $K \mathbb{I}_{\partial\Sigma^0} u_0(t, x)$, in the sense that*

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \left\| u_\varepsilon(t, x) - u_0 \left(t, x - \frac{b^*}{\varepsilon} t \right) \right\|_{L^2((0, T) \times \Omega_\varepsilon)} &= 0, \\ \lim_{\varepsilon \rightarrow 0} \sqrt{\varepsilon} \left\| v_\varepsilon(t, x) - K u_0 \left(t, x - \frac{b^*}{\varepsilon} t \right) \right\|_{L^2((0, T) \times \partial\Omega_\varepsilon)} &= 0. \end{aligned} \quad (3.45)$$

Proof. To begin with, we treat the case of well-prepared initial data, that is, $v^0(x) = Ku^0(x) \in H^1(\mathbb{R}^d)$. Later we shall consider more general initial data. The energy equality of (3.11)-(3.13) for a time interval $(0, t)$ is

$$\begin{aligned} & \frac{1}{2} \left[\|u_\varepsilon(t)\|_{L^2(\Omega_\varepsilon)}^2 + \frac{\varepsilon}{K} \|v_\varepsilon(t)\|_{L^2(\partial\Omega_\varepsilon)}^2 \right] + \int_0^t \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon(s, x) \cdot \nabla u_\varepsilon(s, x) dx ds \\ & + \frac{\varepsilon}{K} \int_0^t \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon(s, x) \cdot \nabla^s v_\varepsilon(s, x) d\sigma_\varepsilon(x) ds \end{aligned}$$

$$+ \frac{\varepsilon \kappa}{\varepsilon^2} \int_0^t \int_{\partial \Omega_\varepsilon} \left(u_\varepsilon(s, x) - \frac{v_\varepsilon}{K}(s, x) \right)^2 d\sigma_\varepsilon(x) ds = \frac{1}{2} \left[\|u^0\|_{L^2(\Omega_\varepsilon)}^2 + \frac{\varepsilon}{K} \|v^0\|_{L^2(\partial \Omega_\varepsilon)}^2 \right]$$

Following the lead of [20] we do not expect a point wise (in time) strong convergence of the sequence $(u_\varepsilon, v_\varepsilon)$. Thus, we integrate once more with respect to time the above energy equality to obtain

$$\begin{aligned} & \frac{1}{2} \int_0^T \left[\|u_\varepsilon(t)\|_{L^2(\Omega_\varepsilon)}^2 + \frac{\varepsilon}{K} \|v_\varepsilon(t)\|_{L^2(\partial \Omega_\varepsilon)}^2 \right] dt + \int_0^T \int_0^t \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon(s, x) \cdot \nabla u_\varepsilon(s, x) dx ds dt \\ & \quad + \frac{\varepsilon}{K} \int_0^T \int_0^t \int_{\partial \Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon(s, x) \cdot \nabla^s v_\varepsilon(s, x) d\sigma_\varepsilon(x) ds dt \\ & \quad + \frac{\varepsilon \kappa}{\varepsilon^2} \int_0^T \int_0^t \int_{\partial \Omega_\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right)^2 d\sigma_\varepsilon(x) ds dt = \frac{T}{2} \left(\|u^0\|_{L^2(\Omega_\varepsilon)}^2 + \frac{\varepsilon}{K} \|v^0\|_{L^2(\partial \Omega_\varepsilon)}^2 \right) \end{aligned}$$

In the previous section, we established that all terms in the above formula have actually (weak) two-scale limits. Since the corresponding norms are lower semi-continuous with respect to the (weak) two-scale convergence, we deduce

$$\begin{aligned} \liminf_{\varepsilon \rightarrow 0} \frac{1}{2} \int_0^T \left[\|u_\varepsilon(t)\|_{L^2(\Omega_\varepsilon)}^2 + \frac{\varepsilon}{K} \|v_\varepsilon(t)\|_{L^2(\partial \Omega_\varepsilon)}^2 \right] dt & \geq \frac{1}{2} (|Y^0| + K |\partial \Sigma^0|) \|u_0\|_{L^2(\mathbb{R}^d \times (0, T))}^2, \\ \liminf_{\varepsilon \rightarrow 0} \int_0^T \int_0^t \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon(s, x) \cdot \nabla u_\varepsilon(s, x) dx ds dt \\ & \geq \int_0^T \int_0^t \int_{\mathbb{R}^d} \int_{Y^0} D(y) |\nabla_x u_0(s, x) + \nabla_y (\chi(y) \cdot \nabla_x u_0(s, x))|^2 dy dx ds dt, \\ \liminf_{\varepsilon \rightarrow 0} \frac{\varepsilon}{K} \int_0^T \int_0^t \int_{\partial \Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon(s, x) \cdot \nabla^s v_\varepsilon(s, x) d\sigma_\varepsilon(x) ds dt \\ & \geq \frac{1}{K} \int_0^T \int_0^t \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} D^s(y) |KG(y) \nabla_x u_0(s, x) + \nabla_y^s (\omega(y) \cdot \nabla_x u_0(s, x))|^2 d\sigma(y) dx ds dt, \\ \liminf_{\varepsilon \rightarrow 0} \frac{\varepsilon \kappa}{\varepsilon^2} \int_0^T \int_0^t \int_{\partial \Omega_\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right)^2 d\sigma_\varepsilon(x) ds dt \\ & \geq \kappa \int_0^T \int_0^t \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} |(\chi(y) - K^{-1} \omega(y)) \cdot \nabla_x u_0(s, x)|^2 d\sigma(y) dx ds dt. \end{aligned}$$

On the other hand we have

$$\lim_{\varepsilon \rightarrow 0} \left(\|u^0\|_{L^2(\Omega_\varepsilon)}^2 + \frac{\varepsilon}{K} \|v^0\|_{L^2(\partial \Omega_\varepsilon)}^2 \right) = |Y^0| \|u^0\|_{L^2(\mathbb{R}^d)}^2 + \frac{|\partial \Sigma^0|}{K} \|v^0\|_{L^2(\mathbb{R}^d)}^2.$$

Summing up those limits and recognizing the formula for \mathcal{D} yields the inequality

$$\begin{aligned} \frac{1}{2} (|Y^0| + K|\partial\Sigma^0|) \|u_0\|_{L^2(\mathbb{R}^d \times (0,T))}^2 + \int_0^T \int_0^t \int_{\mathbb{R}^d} \mathcal{D} \nabla_x u_0(s,x) \cdot \nabla_x u_0(s,x) dx ds dt \\ \leq \frac{T}{2} \left(|Y^0| \|u^0\|_{L^2(\mathbb{R}^d)}^2 + \frac{|\partial\Sigma^0|}{K} \|v^0\|_{L^2(\mathbb{R}^d)}^2 \right). \end{aligned} \quad (3.46)$$

However, if we write the same type of time integral of the energy equality for the homogenized equation (3.28), we get an equality with the same left hand side but a different right hand side

$$\begin{aligned} \frac{1}{2} [|Y^0| + K|\partial\Sigma^0|] \|u_0\|_{L^2(\mathbb{R}^d \times (0,T))}^2 + \int_0^T \int_0^t \int_{\mathbb{R}^d} \mathcal{D} \nabla u_0(s,x) \cdot \nabla u_0(s,x) dx ds dt \\ = \frac{T}{2(|Y^0| + K|\partial\Sigma^0|)} \| |Y^0| u^0 + |\partial\Sigma^0| v^0 \|_{L^2(\mathbb{R}^d)}^2. \end{aligned} \quad (3.47)$$

It is easy to check that the two right hand sides in (3.46) and (3.47) coincide if and only if

$$\|u^0 - K^{-1}v^0\|_{L^2(\mathbb{R}^d)}^2 = 0,$$

which is precisely our assumption of well prepared initial data. Therefore, under this assumption we deduce that (3.46) is not an inequality but rather an equality, which in turn implies that all the previous lower semi-continuity of norm sequences are actually exact convergence. We can thus apply Proposition 2.6.7 and conclude to the strong convergence (see Section 2.6 of Chapter 2 for details if necessary).

We now turn to the case of general initial data $(u^0, v^0) \in L^2(\mathbb{R}^d) \times H^1(\mathbb{R}^d)$. Let us consider a small $\delta_0 > 0$, to be chosen precisely at the end of the proof. Due to Lemma 3.6.1 on a priori estimates, by a contradiction argument, it follows that there exists a time sequence $\{\delta_\varepsilon\}$, $\delta_0/2 \leq \delta_\varepsilon \leq \delta_0$, converging to some limit $\bar{\delta}$, $\delta_0/2 \leq \bar{\delta} \leq \delta_0$, and a positive constant C , which does not depend on δ_0 or on ε (but only on the initial data), such that

$$\begin{cases} \|u_\varepsilon(\cdot, \delta_\varepsilon)\|_{H^1(\Omega_\varepsilon)}^2 \leq C/\delta_0, & \varepsilon \|v_\varepsilon(\cdot, \delta_\varepsilon)\|_{H^1(\partial\Omega_\varepsilon)}^2 \leq C/\delta_0, \\ \varepsilon \|Ku_\varepsilon(\cdot, \delta_\varepsilon) - v_\varepsilon(\cdot, \delta_\varepsilon)\|_{L^2(\partial\Omega_\varepsilon)}^2 \leq C\varepsilon^2/\delta_0. \end{cases} \quad (3.48)$$

We now follow an idea of [20] which amounts to consider system (3.11)-(3.13) on a smaller time interval (δ_ε, T) where $\delta_\varepsilon \geq \delta_0/2 > 0$ is such that the initial data at this time should be almost well-prepared because of parabolic dissipation on the earlier time interval $(0, \delta_\varepsilon)$. We decompose the solution $(u_\varepsilon, v_\varepsilon)$ of (3.11)-(3.13) as

$$u_\varepsilon(t, x) = u_{1,\varepsilon}(t, x) + u_{2,\varepsilon}(t, x) \quad \text{and} \quad v_\varepsilon(t, x) = v_{1,\varepsilon}(t, x) + v_{2,\varepsilon}(t, x),$$

in such way that the initial data are well prepared for the first problem while the solution of the second one will converge strongly to zero

$$\begin{cases} \frac{\partial u_{1,\varepsilon}}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_{1,\varepsilon} - \operatorname{div}(D_\varepsilon \nabla u_{1,\varepsilon}) = 0 & \text{in } (\delta_\varepsilon, T) \times \Omega_\varepsilon, \\ -\frac{D_\varepsilon}{\varepsilon} \nabla u_{1,\varepsilon} \cdot n = \frac{\partial v_{1,\varepsilon}}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_{1,\varepsilon} - \operatorname{div}^s(D_\varepsilon^s \nabla^s v_{1,\varepsilon}) & \text{on } (\delta_\varepsilon, T) \times \partial\Omega_\varepsilon, \\ -\frac{D_\varepsilon}{\varepsilon} \nabla u_{1,\varepsilon} \cdot n = \frac{\kappa}{\varepsilon^2} (u_{1,\varepsilon} - K^{-1}v_{1,\varepsilon}) & \text{on } (\delta_\varepsilon, T) \times \partial\Omega_\varepsilon, \\ u_{1,\varepsilon}(\delta_\varepsilon, x) = u_\varepsilon(\delta_\varepsilon, x), \quad v_{1,\varepsilon}(\delta_\varepsilon, x) = Ku_\varepsilon(\delta_\varepsilon, x), \end{cases} \quad (3.49)$$

and

$$\left\{ \begin{array}{ll} \frac{\partial u_{2,\varepsilon}}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_{2,\varepsilon} - \operatorname{div} (D_\varepsilon \nabla u_{2,\varepsilon}) = 0 & \text{in } (\delta_\varepsilon, T) \times \Omega_\varepsilon, \\ -\frac{D_\varepsilon}{\varepsilon} \nabla u_{2,\varepsilon} \cdot n = \frac{\partial v_{2,\varepsilon}}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_{2,\varepsilon} - \operatorname{div}^s (D_\varepsilon^s \nabla^s v_{2,\varepsilon}) & \text{on } (\delta_\varepsilon, T) \times \partial\Omega_\varepsilon, \\ -\frac{D_\varepsilon}{\varepsilon} \nabla u_{2,\varepsilon} \cdot n = \frac{\kappa}{\varepsilon^2} (u_{2,\varepsilon} - K^{-1} v_{2,\varepsilon}) & \text{on } (\delta_\varepsilon, T) \times \partial\Omega_\varepsilon, \\ u_{2,\varepsilon}(\delta_\varepsilon, x) = 0, \quad v_{2,\varepsilon}(\delta_\varepsilon, x) = v_\varepsilon(\delta_\varepsilon, x) - K u_\varepsilon(\delta_\varepsilon, x). \end{array} \right. \quad (3.50)$$

Since (3.50) is similar in structure to (3.11)-(3.13), the standard a priori estimate of Lemma 3.6.1, together with estimate (3.48) for the initial data at time δ_ε , yields for any $t \geq \delta_\varepsilon$

$$\|u_{2,\varepsilon}(\cdot, t)\|_{L^2(\Omega_\varepsilon)}^2 + \varepsilon \|v_{2,\varepsilon}(\cdot, t)\|_{L^2(\partial\Omega_\varepsilon)}^2 \leq C\varepsilon^2/\delta_0.$$

Thus, the sequence $(u_{2,\varepsilon}, v_{2,\varepsilon})$ strongly converges to 0. The initial data in (3.49) are well prepared but we cannot apply directly our previous results because the initial time $\delta_\varepsilon \neq 0$ is varying with ε . The new difficulty is to prove that the initial data of (3.49) strongly two-scale converge with drift to some limit.

Let us recall the existence of a uniformly bounded extension operator [1] from $H^1(\Omega_\varepsilon)$ into $H^1(\mathbb{R}^d)$. Thus, the sequence $u_\varepsilon(\delta_\varepsilon, x)$ can be thought of being defined in the whole space \mathbb{R}^d and, by virtue of (3.48) it satisfies the bound $\|u_\varepsilon(\delta_\varepsilon, x)\|_{H^1(\mathbb{R}^d)}^2 \leq C/\delta_0$. Shifting the sequence does not change its bound, so we have

$$\|u_\varepsilon(\delta_\varepsilon, x + (b^*/\varepsilon)\delta_\varepsilon)\|_{H^1(\mathbb{R}^d)}^2 \leq C/\delta_0. \quad (3.51)$$

Together with Lemma 3.10.2 which says that the L^2 -norm of $u_\varepsilon(\delta_\varepsilon, x + (b^*/\varepsilon)\delta_\varepsilon)$ does not escape at infinity, we deduce from (3.51) that this sequence is (pre-)compact in $L^2(\mathbb{R}^d)$. Therefore, up to a subsequence, $u_\varepsilon(\delta_\varepsilon, x + (b^*/\varepsilon)\delta_\varepsilon)$ converges strongly to some limit $\tilde{u}^0(x)$ in $L^2(\mathbb{R}^d)$.

Thus we can use the same arguments as in the case of well-prepared initial data to conclude that $u_{1,\varepsilon}$ and $v_{1,\varepsilon}$ strongly two-scale converge with drift to $\tilde{u}(t, x)$ and $K\tilde{u}(t, x)$ respectively where \tilde{u} satisfies the following limit equation of (3.49)

$$\left\{ \begin{array}{l} K_d \partial_t \tilde{u} = \operatorname{div}_x (\mathcal{D} \nabla_x \tilde{u}) \quad \text{in } (\bar{\delta}, T) \times \mathbb{R}^d \\ K_d \tilde{u}(\bar{\delta}, x) = |Y^0| \tilde{u}^0(x) + |\partial\Sigma^0|_{d-1} \tilde{u}^0(x), \quad x \in \mathbb{R}^d \end{array} \right. \quad (3.52)$$

where $K_d = |Y^0| + K|\partial\Sigma^0|_{d-1}$ and \mathcal{D} is given by (3.29). In particular,

$$\lim_{\varepsilon \rightarrow 0} \|u_{1,\varepsilon}\|_{L^2((\delta_\varepsilon, T) \times \Omega_\varepsilon)}^2 = |Y^0| \|\tilde{u}\|_{L^2((\bar{\delta}, T) \times \mathbb{R}^d)}^2$$

and

$$\lim_{\varepsilon \rightarrow 0} \varepsilon \|v_{1,\varepsilon}\|_{L^2((\delta_\varepsilon, T) \times \partial\Omega_\varepsilon)}^2 = K^2 |\partial\Sigma^0| \|\tilde{u}\|_{L^2((\bar{\delta}, T) \times \mathbb{R}^d)}^2.$$

Of course, since u_ε was converging weakly to u_0 , we deduce that $\tilde{u}(t, x) = u_0(t, x)$ for $t \geq \bar{\delta}$, and

$$\lim_{\varepsilon \rightarrow 0} \|u_\varepsilon\|_{L^2((\delta_\varepsilon, T) \times \Omega_\varepsilon)}^2 = |Y^0| \|u_0\|_{L^2((\bar{\delta}, T) \times \mathbb{R}^d)}^2 \quad (3.53)$$

$$\lim_{\varepsilon \rightarrow 0} \varepsilon \|v_\varepsilon\|_{L^2((\delta_\varepsilon, T) \times \partial\Omega_\varepsilon)}^2 = K^2 |\partial\Sigma^0| \|u_0\|_{L^2((\bar{\delta}, T) \times \mathbb{R}^d)}^2.$$

Now, let us assume that there is a lack of strong two-scale convergence for $(u_\varepsilon, v_\varepsilon)$, namely that the L^2 -norm of this sequence is not continuous (as required by (??) in Proposition 2.6.7). In other words, either

$$\lim_{\varepsilon \rightarrow 0} \|u_\varepsilon\|_{L^2((0, T) \times \Omega_\varepsilon)}^2 > |Y^0| \|u_0\|_{L^2(\mathbb{R}^d \times (0, T))}^2 \quad (3.54)$$

or

$$\lim_{\varepsilon \rightarrow 0} \varepsilon \|v_\varepsilon\|_{L^2((0,T) \times \partial\Omega_\varepsilon)}^2 > K^2 |\partial\Sigma^0| \|u_0\|_{L^2(\mathbb{R}^d \times (0,T))}^2. \quad (3.55)$$

Lemma 3.6.1 implies that $\|u_\varepsilon(t)\|_{L^2(\Omega_\varepsilon)}^2 + \varepsilon \|v_\varepsilon(t)\|_{L^2(\partial\Omega_\varepsilon)}^2 \leq C$ uniformly in time. So, we can find a small $\delta_0 > 0$ such that, the same strict inequalities hold true on a smaller time interval, namely, either

$$\liminf_{\varepsilon \rightarrow 0} \|u_\varepsilon\|_{L^2((\delta,T) \times \Omega_\varepsilon)}^2 > |Y^0| \|u_0\|_{L^2((0,T) \times \mathbb{R}^d)}^2 \quad \text{for any } 0 < \delta < \delta_0, \quad (3.56)$$

or

$$\liminf_{\varepsilon \rightarrow 0} \varepsilon \|v_\varepsilon\|_{L^2((\delta,T) \times \partial\Omega_\varepsilon)}^2 > K^2 |\partial\Sigma^0| \|u_0\|_{L^2((0,T) \times \mathbb{R}^d)}^2 \quad \text{for any } 0 < \delta < \delta_0. \quad (3.57)$$

Obviously, (3.56) or (3.57) contradicts (3.53). Therefore, there must be continuity of the L^2 -norm of $(u_\varepsilon, v_\varepsilon)$ and both (3.54) and (3.55) must be equalities. Thus, we have proved the strong two-scale convergence with drift in case of a general initial data. \square

Lemma 3.10.2. *Let $u_\varepsilon(t, x)$ be the solution of (3.11)-(3.13). For any $\delta > 0$ there is $R(\delta) > 0$ such that, for any $t \in [0, T]$,*

$$\left\| u_\varepsilon \left(t, x + \frac{b^* t}{\varepsilon} \right) \right\|_{L^2(\Omega_\varepsilon \cap \{x \geq R(\delta)\})} \leq \delta.$$

Proof. We again follow an idea of [20]. Let $\phi \in C^\infty(\mathbb{R})$ be a cut-off function such that $0 \leq \phi(r) \leq 1$, $\phi = 0$ for $r \leq 1$, $\phi = 1$ for $r \geq 2$. For $x \in \mathbb{R}^d$, denote $\phi_R(x) = \phi(|x|/R)$ and $\phi_R^\varepsilon(t, x) = \phi_R(x - b^* t/\varepsilon)$. In the variational formulation (3.40) of system (3.11)-(3.12) we take the test function $\{u_\varepsilon(t, x)\phi_R^\varepsilon(t, x), v_\varepsilon(t, x)\phi_R^\varepsilon(t, x)\}$ and we integrate by parts the time and convective derivatives (calculations are shown one term at a time)

$$\begin{aligned} 2 \int_0^t \int_{\Omega_\varepsilon} \frac{\partial u_\varepsilon}{\partial t}(s, x) u_\varepsilon(s, x) \phi_R^\varepsilon(s, x) ds dx &= \int_0^t \int_{\Omega_\varepsilon} \frac{b^*}{\varepsilon} \cdot \nabla \phi_R^\varepsilon(s, x) (u_\varepsilon(s, x))^2 ds dx \\ &\quad + \int_{\Omega_\varepsilon} \phi_R^\varepsilon(t, x) (u_\varepsilon(t, x))^2 dx - \int_{\Omega_\varepsilon} \phi_R(x) (u^0(x))^2 dx, \\ 2 \int_0^t \int_{\Omega_\varepsilon} \frac{b_\varepsilon}{\varepsilon} \cdot \nabla u_\varepsilon(s, x) u_\varepsilon(s, x) \phi_R^\varepsilon(s, x) ds dx &= - \int_0^t \int_{\Omega_\varepsilon} \frac{b_\varepsilon}{\varepsilon} \cdot \nabla \phi_R^\varepsilon(s, x) (u_\varepsilon(s, x))^2 ds dx, \\ \frac{2\varepsilon}{K} \int_0^t \int_{\partial\Omega_\varepsilon} \frac{\partial v_\varepsilon}{\partial t} \phi_R^\varepsilon v_\varepsilon ds d\sigma(x) &= \int_0^t \int_{\partial\Omega_\varepsilon} \frac{b^*}{K} \cdot \nabla \phi_R^\varepsilon (v_\varepsilon)^2 ds d\sigma(x) \\ &\quad + \frac{\varepsilon}{K} \int_{\partial\Omega_\varepsilon} \phi_R^\varepsilon (v_\varepsilon)^2 d\sigma(x) - \frac{\varepsilon}{K} \int_{\partial\Omega_\varepsilon} \phi_R(x) (v^0(x))^2 d\sigma(x), \\ \frac{2}{K} \int_0^t \int_{\partial\Omega_\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon \phi_R^\varepsilon ds d\sigma(x) &= - \frac{1}{K} \int_0^t \int_{\partial\Omega_\varepsilon} (v_\varepsilon)^2 b_\varepsilon^s \cdot \nabla^s \phi_R^\varepsilon ds d\sigma(x). \end{aligned}$$

This yields

$$\frac{1}{2} \int_{\Omega_\varepsilon} \phi_R^\varepsilon(t, x) (u_\varepsilon(t, x))^2 dx + \int_0^t \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon \phi_R^\varepsilon ds dx$$

$$\begin{aligned}
& + \frac{\varepsilon}{2K} \int_{\partial\Omega_\varepsilon} \phi_R^\varepsilon(t, x) (v_\varepsilon(t, x))^2 d\sigma(x) + \frac{\varepsilon}{K} \int_0^t \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s v_\varepsilon \phi_R^\varepsilon ds d\sigma(x) \\
& \quad + \frac{\kappa\varepsilon}{\varepsilon^2} \int_0^t \int_{\partial\Omega_\varepsilon} \phi_R^\varepsilon (u_\varepsilon - K^{-1}v_\varepsilon)^2 ds d\sigma(x) \\
& = - \int_0^t \int_{\Omega_\varepsilon} u_\varepsilon D_\varepsilon \nabla u_\varepsilon \cdot \nabla \phi_R^\varepsilon ds dx - \frac{\varepsilon}{K} \int_0^t \int_{\partial\Omega_\varepsilon} v_\varepsilon D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s \phi_R^\varepsilon ds d\sigma(x) \\
& \quad + \int_0^t \int_{\Omega_\varepsilon} \frac{1}{\varepsilon} (b_\varepsilon - b^*) \cdot \nabla \phi_R^\varepsilon (u_\varepsilon)^2 ds dx + \frac{1}{2} \int_{\Omega_\varepsilon} \phi_R(x) (u^0(x))^2 dx \\
& \quad + \int_0^t \int_{\partial\Omega_\varepsilon} \frac{1}{K} (b_\varepsilon^s - b^*) \cdot \nabla^s \phi_R^\varepsilon (v_\varepsilon)^2 ds d\sigma(x) + \frac{\varepsilon}{2K} \int_{\partial\Omega_\varepsilon} \phi_R(x) (v^0(x))^2 d\sigma(x) \tag{3.58}
\end{aligned}$$

Due to the a priori estimate of Lemma 3.6.1 and the definition of ϕ_R , the first and second integrals on the right hand side of (3.58) are uniformly bounded by C/R . The terms involving the initial data $(u^0(x), v^0(x))$ do not depend on ε and tend to zero as R tends to ∞ . To get a bound on the remaining (convective) terms on the right hand side of (3.58), we rely again on the auxiliary problem (3.42) which allows us to remove the ε^{-1} singularity of the convective terms

$$\begin{aligned}
& \int_0^t \int_{\Omega_\varepsilon} \frac{1}{\varepsilon} (b_\varepsilon - b^*) \cdot \nabla \phi_R^\varepsilon (u_\varepsilon)^2 ds dx + \int_0^t \int_{\partial\Omega_\varepsilon} \frac{1}{K} (b_\varepsilon^s - b^*) \cdot \nabla^s \phi_R^\varepsilon (v_\varepsilon)^2 ds d\sigma(x) \tag{3.59} \\
& = \varepsilon \sum_{i=1}^d \int_0^t \int_{\Omega_\varepsilon} \nabla \alpha_i^\varepsilon \cdot \nabla \left((u_\varepsilon)^2 \partial_{x_i} \phi_R^\varepsilon \right) ds dx + K \int_0^t \int_{\partial\Omega_\varepsilon} \nabla \phi_R^\varepsilon \cdot (b^* - b_\varepsilon^s) \left((u_\varepsilon)^2 - K^{-2} (v_\varepsilon)^2 \right) ds d\sigma(x).
\end{aligned}$$

Since $(u_\varepsilon^2 - K^{-2}v_\varepsilon^2) = (u_\varepsilon + K^{-1}v_\varepsilon)(u_\varepsilon - K^{-1}v_\varepsilon)$ and $\varepsilon \nabla \alpha_i^\varepsilon(x) = (\nabla_y \alpha_i)(x/\varepsilon)$, the a priori estimates of Lemma 3.6.1 imply that (3.59) is uniformly bounded by C/R too, which yields the desired statement. \square

3.11 Slow reaction

We shall consider a different scaling for the reaction as is done in [81], [109]. It should be noted, however, that the scaling considered in [81] and [109] isn't in the strong convection regime. We shall only be scaling the reaction parameter by $\kappa \rightarrow \varepsilon^2 \kappa$ in (3.11)-(3.13). In other words, the reaction is considered to be small. As far as this section is considered, we shall be working with the following coupled parabolic equations in the ε -periodic porous domain.

$$\frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div} (D_\varepsilon \nabla u_\varepsilon) = 0 \text{ in } (0, T) \times \Omega_\varepsilon, \tag{3.60}$$

$$-\frac{D_\varepsilon}{\varepsilon} \nabla u_\varepsilon \cdot n = \frac{\partial v_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon - \operatorname{div}^s (D_\varepsilon^s \nabla^s v_\varepsilon) = \kappa \left(u_\varepsilon - \frac{v_\varepsilon}{K} \right) \text{ on } (0, T) \times \partial\Omega_\varepsilon, \tag{3.61}$$

$$u_\varepsilon(0, x) = u^{in}(x) \text{ in } \Omega_\varepsilon, \quad v_\varepsilon(0, x) = v^{in}(x) \text{ on } \partial\Omega_\varepsilon. \tag{3.62}$$

Under this scaling, the homogenization result is very different from the one obtained in the previous sections.

Lemma 3.11.1. *There exists a constant C , independent of ε , such that*

$$\begin{aligned} & \|u_\varepsilon\|_{L^\infty((0,T);L^2(\Omega_\varepsilon))} + \sqrt{\varepsilon}\|v_\varepsilon\|_{L^\infty((0,T);L^2(\partial\Omega_\varepsilon))} \\ & + \|\nabla u_\varepsilon\|_{L^2((0,T)\times\Omega_\varepsilon)} + \sqrt{\varepsilon}\|\nabla^s v_\varepsilon\|_{L^2((0,T)\times\partial\Omega_\varepsilon)} \\ & + \sqrt{\varepsilon}\left\|u_\varepsilon - \frac{v_\varepsilon}{K}\right\|_{L^\infty((0,T);L^2(\partial\Omega_\varepsilon))} \leq C \left(\|u^{in}\|_{L^2(\mathbb{R}^d)} + \|v^{in}\|_{H^1(\mathbb{R}^d)} \right), \end{aligned} \quad (3.63)$$

Proof. As usual, the approach we shall take to derive the a priori estimates is via energy estimates. Let us multiply (3.60) by u_ε and integrate over Ω_ε

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega_\varepsilon} |u_\varepsilon|^2 dx + \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon dx + \kappa \varepsilon \int_{\partial\Omega_\varepsilon} (u_\varepsilon - v_\varepsilon) u_\varepsilon d\sigma(x) = 0.$$

Then, let us multiply the second part of (3.61) by $\varepsilon v_\varepsilon$ and integrate over $\partial\Omega_\varepsilon$

$$\frac{\varepsilon}{2} \frac{d}{dt} \int_{\partial\Omega_\varepsilon} |v_\varepsilon|^2 d\sigma(x) + \varepsilon \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s v_\varepsilon d\sigma(x) - \kappa \varepsilon \int_{\partial\Omega_\varepsilon} (u_\varepsilon - v_\varepsilon) v_\varepsilon d\sigma(x) = 0.$$

Adding the above two equations results in the energy equality

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_{\Omega_\varepsilon} |u_\varepsilon|^2 dx + \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon dx + \frac{\varepsilon}{2} \frac{d}{dt} \int_{\partial\Omega_\varepsilon} |v_\varepsilon|^2 d\sigma(x) \\ & + \varepsilon \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s v_\varepsilon d\sigma(x) + \kappa \varepsilon \int_{\partial\Omega_\varepsilon} (u_\varepsilon - v_\varepsilon)^2 d\sigma(x) = 0 \end{aligned}$$

Integrating the above energy equality with respect to time on the time interval $(0, T)$ yields the a priori estimates as in (3.63). \square

In the homogenization result regarding (3.11)-(3.13) given by the Proposition 3.7.2, the induced drift b^* in the concentration profiles was given by (3.27). Both the bulk velocity field b and the surface velocity field b^s contributed to the drift b^* as suggested by the expression (3.27). Also, the drift velocity happened to be the same for both the bulk and surface concentrations. The two-scale limits for both $\{u_\varepsilon\}$ and $\{v_\varepsilon\}$ were given by u_0 which is characterized by the single effective diffusion equation (3.28). Here the situations is different. We consider different drift velocities for the two concentrations.

$$u_\varepsilon(t, x) = \sum_{i=0}^{\infty} \varepsilon^i u_i \left(t, x - \frac{b_1^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \quad (3.64)$$

and

$$v_\varepsilon(t, x) = \sum_{i=0}^{\infty} \varepsilon^i v_i \left(t, x - \frac{b_2^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \quad (3.65)$$

Proposition 3.11.2. *Define two constants $b_1^*, b_2^* \in \mathbb{R}^d$ by*

$$b_1^* = \frac{1}{|Y^0|} \int_{Y^0} b(y) dy \quad \text{and} \quad b_2^* = \frac{1}{|\partial\Sigma^0|} \int_{\partial\Sigma^0} b^s(y) d\sigma(y). \quad (3.66)$$

Then the solution $(u_\varepsilon, v_\varepsilon)$ for (3.60)-(3.62), under the assumption (3.64)-(3.65), formally satisfy

$$u_\varepsilon(t, x) \approx u_0 \left(t, x - \frac{b_1^* t}{\varepsilon} \right) + \varepsilon u_1 \left(t, x - \frac{b_1^* t}{\varepsilon}, \frac{x}{\varepsilon} \right)$$

$$v_\varepsilon(t, x) \approx v_0 \left(t, x - \frac{b_2^* t}{\varepsilon} \right) + \varepsilon v_1 \left(t, x - \frac{b_2^* t}{\varepsilon}, \frac{x}{\varepsilon} \right).$$

In case the drift velocities $b_1^* = b_2^* = b^*$ (say), the zero order approximations u_0, v_0 satisfy the following coupled effective equations

$$\begin{cases} |Y^0| \frac{\partial u_0}{\partial t} + \kappa |\partial \Sigma^0| \left(u_0 - \frac{v_0}{K} \right) = \operatorname{div}(A^* \nabla_x u_0) & \text{in } \mathbb{R}^d \times (0, T), \\ |\partial \Sigma^0| \frac{\partial v_0}{\partial t} - \kappa |\partial \Sigma^0| \left(u_0 - \frac{v_0}{K} \right) = \operatorname{div}(B^* \nabla_x v_0) & \text{in } \mathbb{R}^d \times (0, T) \end{cases} \quad (3.67)$$

with the dispersion tensors A^* and B^* given by

$$A_{ij}^* = \int_{Y^0} D(y) (\nabla_y \chi_i + e_i) \cdot (\nabla_y \chi_j + e_j) dy \quad (3.68)$$

$$B_{ij}^* = \int_{\partial \Sigma^0} D^s(y) (\nabla_y^s \omega_i + e_i) \cdot (\nabla_y^s \omega_j + e_j) d\sigma(y) \quad (3.69)$$

with $(\chi, \omega) = (\chi_i, \omega_i)_{1 \leq i \leq d}$ being the solution of the cell problem such that

$$u_1(t, x, y) = \sum_{i=1}^d \chi_i(y) \frac{\partial u_0}{\partial x_i}(t, x) \quad v_1(t, x, y) = \sum_{i=1}^d \omega_i(y) \frac{\partial v_0}{\partial x_i}(t, x). \quad (3.70)$$

and the cell problem satisfied by (χ_i, ω_i) , for every $1 \leq i \leq d$, is

$$\begin{cases} b(y) \cdot \nabla_y \chi_i - \operatorname{div}_y(D(\nabla_y \chi_i + e_i)) = (b^* - b) \cdot e_i & \text{in } Y^0, \\ -D(\nabla_y \chi_i + e_i) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \chi_i(y) & Y\text{-periodic.} \end{cases} \quad (3.71)$$

and the surface cell problem satisfied by ω_i is

$$\begin{cases} b^s(y) \cdot \nabla_y^s \omega_i - \operatorname{div}_y^s(D^s(\nabla_y^s \omega_i + K e_i)) = (b^* - b^s) \cdot e_i & \text{on } \partial \Sigma^0, \\ y \rightarrow \omega_i(y) & Y\text{-periodic.} \end{cases} \quad (3.72)$$

In case the drift velocities $b_1^* \neq b_2^*$, the zero order approximations u_0 and v_0 satisfy the following homogenized equations.

$$\begin{cases} |Y^0| \frac{\partial u_0}{\partial t} + \kappa |\partial \Sigma^0| u_0 = \operatorname{div}(A^* \nabla_x u_0) & \text{in } \mathbb{R}^d \times (0, T) \end{cases} \quad (3.73)$$

$$\begin{cases} |\partial \Sigma^0| \frac{\partial v_0}{\partial t} + \frac{\kappa}{K} |\partial \Sigma^0| v_0 = \operatorname{div}(B^* \nabla_x v_0) & \text{in } \mathbb{R}^d \times (0, T) \end{cases} \quad (3.74)$$

The dispersion tensors A^* and B^* are given by (3.68) and (3.69) respectively which are in terms of the solutions (χ_i, ω_i) for the cell problems

$$\begin{cases} b(y) \cdot \nabla_y \chi_i - \operatorname{div}_y(D(\nabla_y \chi_i + e_i)) = (b_1^* - b) \cdot e_i & \text{in } Y^0, \\ -D(\nabla_y \chi_i + e_i) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \chi_i(y) & Y\text{-periodic.} \end{cases} \quad (3.75)$$

$$\begin{cases} b^s(y) \cdot \nabla_y^s \omega_i - \operatorname{div}_y^s(D^s(\nabla_y^s \omega_i + K e_i)) = (b_2^* - b^s) \cdot e_i & \text{on } \partial \Sigma^0, \\ y \rightarrow \omega_i(y) & Y\text{-periodic.} \end{cases} \quad (3.76)$$

Proof. Case I: $b_1^* = b_2^* = b^*$

Plugging the expressions for u_ε and v_ε from (3.64)-(3.65) into the coupled equations (3.60)-(3.62), we identify the cascade of equations as the coefficients of various powers of ε .

At order ε^{-2} :

$$\begin{cases} b(y) \cdot \nabla_y u_0 - \operatorname{div}_y(D(y)\nabla_y u_0) = 0 & \text{in } Y^0, \\ -D\nabla_y u_0 \cdot n = 0 & \text{on } \partial\Sigma^0, \\ b^s(y) \cdot \nabla_y^s v_0 - \operatorname{div}_y^s(D^s(y)\nabla_y^s v_0) = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow (u_0(y), v_0(y)) & Y - \text{periodic.} \end{cases} \quad (3.77)$$

From (3.78), it follows that (u_0, v_0) are independent of the fast variable y . Note that there is no contribution from the reaction in (3.77) because of the chosen scaling for the reaction rate.

At order ε^{-1} :

$$\begin{cases} -b^* \cdot \nabla_x u_0 + b(y) \cdot (\nabla_x u_0 + \nabla_y u_1) - \operatorname{div}_y(D(y)(\nabla_x u_0 + \nabla_y u_1)) = 0 & \text{in } Y^0, \\ -D(y)(\nabla_x u_0 + \nabla_y u_1) \cdot n = 0 & \text{on } \partial\Sigma^0, \\ -b^* \cdot \nabla_x v_0 + b^s(y) \cdot (\nabla_x v_0 + \nabla_y^s v_1) - \operatorname{div}_y^s(D^s(y)(\nabla_x v_0 + \nabla_y^s v_1)) = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow (u_1(y), v_1(y)) & Y - \text{periodic.} \end{cases} \quad (3.78)$$

By linearity of (3.78) we deduce that

$$u_1(t, x, y) = \chi(y) \cdot \nabla_x u_0 \quad \text{and} \quad v_1(t, x, y) = \omega(y) \cdot \nabla_x v_0$$

where χ_i and ω_i are the solutions of the cell problems (3.71) and (3.72) respectively. The compatibility condition for the well-posedness of the cell problems give the expressions for the common drift velocity b^* given by (3.66).

At order ε^0 :

$$\begin{cases} \frac{\partial u_0}{\partial t} - b^* \cdot \nabla_x u_1 + b(y) \cdot (\nabla_x u_1 + \nabla_y u_2) \\ -\operatorname{div}_x(D(y)(\nabla_x u_0 + \nabla_y u_1)) - \operatorname{div}_y(D(y)(\nabla_x u_1 + \nabla_y u_2)) = 0 & \text{in } Y^0, \\ -D(y)(\nabla_y u_2 + \nabla_x u_1) \cdot n = \kappa \left(u_0 - \frac{v_0}{K} \right) & \text{on } \partial\Sigma^0, \\ \frac{\partial v_0}{\partial t} - b^* \cdot \nabla_x v_1 + b^s(y) \cdot (\nabla_x v_1 + \nabla_y^s v_2) - \operatorname{div}_x(D^s(y)(\nabla_x v_0 + \nabla_y^s v_1)) \\ -\operatorname{div}_y^s(D^s(y)(\nabla_x v_1 + \nabla_y^s v_2)) = \kappa \left(u_0 - \frac{v_0}{K} \right) & \text{on } \partial\Sigma^0, \\ y \rightarrow (u_2(y), v_2(y)) & Y - \text{periodic.} \end{cases} \quad (3.79)$$

The compatibility conditions for the well-posedness of (3.79) for (u_2, v_2) results in the coupled homogenized equation (3.67).

Case II: $b_1^* \neq b_2^*$

Now let us analyse the case where the bulk drift and the surface drift don't match. Upon plugging in (3.64)-(3.65) into the coupled equations (3.60)-(3.62), we find the same system as (3.77) at order ε^{-2} . Also at order ε^{-1} , we find a system similar to (3.78) except for the different drifts in the bulk and on the surface of the pore. The system we get is the following.

$$\left\{ \begin{array}{l} -b_1^* \cdot \nabla_x u_0 + b(y) \cdot (\nabla_x u_0 + \nabla_y u_1) - \operatorname{div}_y(D(y)(\nabla_x u_0 + \nabla_y u_1)) = 0 \quad \text{in } Y^0, \\ \qquad \qquad \qquad -D(y)(\nabla_x u_0 + \nabla_y u_1) \cdot n = 0 \quad \text{on } \partial\Sigma^0, \\ -b_2^* \cdot \nabla_x v_0 + b^s(y) \cdot (\nabla_x v_0 + \nabla_y^s v_1) - \operatorname{div}_y^s(D^s(y)(\nabla_x v_0 + \nabla_y^s v_1)) = 0 \quad \text{on } \partial\Sigma^0, \\ y \rightarrow (u_1(y), v_1(y)) \qquad \qquad \qquad Y\text{-periodic.} \end{array} \right. \quad (3.80)$$

The values of b_1^* and b_2^* from (3.66) guarantee the well-posedness of the above system. By invoking linearity of (3.80), we deduce that the first order correctors u_1 and v_1 can be decomposed in terms of the cell solutions and the gradient of the zero order approximation as in (3.70). The cell problems corresponding to this case of different bulk and surface drift velocities are (3.75) and (3.75).

Next, at the order ε^0 we recognize the following equations for u_2 and v_2 .

$$\left\{ \begin{array}{l} \frac{\partial u_0}{\partial t} - b^* \cdot \nabla_x u_1 + b(y) \cdot (\nabla_x u_1 + \nabla_y u_2) \\ -\operatorname{div}_x(D(y)(\nabla_x u_0 + \nabla_y u_1)) - \operatorname{div}_y(D(y)(\nabla_x u_1 + \nabla_y u_2)) = 0 \quad \text{in } Y^0, \\ -D(y)(\nabla_y u_2 + \nabla_x u_1) \cdot n = \kappa u_0 \quad \text{on } \partial\Sigma^0, \\ y \rightarrow u_2(y) \qquad \qquad \qquad Y\text{-periodic.} \end{array} \right. \quad (3.81)$$

$$\left\{ \begin{array}{l} \frac{\partial v_0}{\partial t} - b^* \cdot \nabla_x v_1 + b^s(y) \cdot (\nabla_x u_1 + \nabla_y^s u_2) - \operatorname{div}_x(D^s(y)(\nabla_x v_0 + \nabla_y^s v_1)) \\ -\operatorname{div}_y^s(D^s(y)(\nabla_x v_1 + \nabla_y^s v_2)) = -\frac{\kappa}{K} v_0 \quad \text{on } \partial\Sigma^0, \\ y \rightarrow v_2(y) \qquad \qquad \qquad Y\text{-periodic.} \end{array} \right. \quad (3.82)$$

Notice that the coupling terms haven't appeared in the above two equations (3.81) and (3.82). The compatibility condition for the well-posedness of (3.81) for u_2 results in the homogenized equation (3.73) and the compatibility condition for the well-posedness of (3.82) for v_2 results in the homogenized equation (3.73). \square

Now, we state a result that justifies the upscaling done formally in Proposition 3.11.2.

Proposition 3.11.3. *Assume that*

$$b_1^* = \frac{1}{|Y^0|} \int_{Y^0} b(y) dy = \frac{1}{|\partial\Sigma^0|} \int_{\partial\Sigma^0} b^s(y) d\sigma(y) = b_2^* = b^*(\text{say}).$$

There exists $u_0, v_0 \in L^2((0, T); H^1(\mathbb{R}^d))$, $u_1 \in L^2((0, T) \times \mathbb{R}^d; H_{\#}^1(Y^0))$ and $v_1 \in L^2((0, T) \times \mathbb{R}^d; H_{\#}^1(\partial\Sigma^0))$ such that the solution sequences $\{u_\varepsilon\}$ and $\{v_\varepsilon\}$, two-scale converge with drift b^ , in the following sense.*

$$\left\{ \begin{array}{l} u_\varepsilon \xrightarrow{2\text{-drift}} u_0(t, x) \\ v_\varepsilon \xrightarrow{2s\text{-drift}} v_0(t, x) \\ \nabla u_\varepsilon \xrightarrow{2\text{-drift}} \nabla_x u_0(t, x) + \nabla_y u_1(t, x, y) \\ \nabla^s v_\varepsilon \xrightarrow{2s\text{-drift}} \nabla_x v_0(t, x) + \nabla_y^s v_1(t, x, y) \\ \left(u_\varepsilon - \frac{v_\varepsilon}{K}\right) \xrightarrow{2s\text{-drift}} u_0(t, x) - \frac{v_0}{K}(t, x) \end{array} \right. \quad (3.83)$$

The two-scale limits u_0 and v_0 satisfy the following coupled effective equations.

$$\begin{cases} |Y^0| \frac{\partial u_0}{\partial t} + \kappa |\partial \Sigma^0| \left(u_0 - \frac{v_0}{K} \right) = \operatorname{div}(A^* \nabla_x u_0) & \text{in } \mathbb{R}^d \times (0, T), \\ |\partial \Sigma^0| \frac{\partial v_0}{\partial t} - \kappa |\partial \Sigma^0| \left(u_0 - \frac{v_0}{K} \right) = \operatorname{div}(B^* \nabla_x v_0) & \text{in } \mathbb{R}^d \times (0, T) \end{cases} \quad (3.84)$$

The dispersion tensors A^* and B^* are given by (3.68) and (3.69) respectively which are in terms of the solutions (χ_i, ω_i) for the cell problem

$$\begin{cases} b(y) \cdot \nabla_y \chi_i - \operatorname{div}_y(D(\nabla_y \chi_i + e_i)) = (b^* - b) \cdot e_i & \text{in } Y^0, \\ -D(\nabla_y \chi_i + e_i) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ b^s(y) \cdot \nabla_y^s \omega_i - \operatorname{div}_y^s(D^s(\nabla_y^s \omega_i + K e_i)) = (b^* - b^s) \cdot e_i & \text{on } \partial \Sigma^0, \\ y \rightarrow (\chi_i(y), \omega_i(y)) & Y \text{ - periodic.} \end{cases} \quad (3.85)$$

In case the drift velocities $b_1^* \neq b_2^*$, the two-scale limits as given in (3.83) hold except for the last line. The homogenized equations satisfied by u_0 and v_0 are decoupled.

$$\begin{cases} |Y^0| \frac{\partial u_0}{\partial t} + \kappa |\partial \Sigma^0| u_0 = \operatorname{div}(A^* \nabla_x u_0) & \text{in } \mathbb{R}^d \times (0, T) \end{cases} \quad (3.86)$$

$$\begin{cases} |\partial \Sigma^0| \frac{\partial v_0}{\partial t} + \frac{\kappa}{K} |\partial \Sigma^0| v_0 = \operatorname{div}(B^* \nabla_x v_0) & \text{in } \mathbb{R}^d \times (0, T) \end{cases} \quad (3.87)$$

The dispersion tensors A^* and B^* are given by (3.68) and (3.69) respectively which are in terms of the solutions (χ_i, ω_i) for the cell problems

$$\begin{cases} b(y) \cdot \nabla_y \chi_i - \operatorname{div}_y(D(\nabla_y \chi_i + e_i)) = (b_1^* - b) \cdot e_i & \text{in } Y^0, \\ -D(\nabla_y \chi_i + e_i) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \chi_i(y) & Y \text{ - periodic.} \end{cases} \quad (3.88)$$

$$\begin{cases} b^s(y) \cdot \nabla_y^s \omega_i - \operatorname{div}_y^s(D^s(\nabla_y^s \omega_i + K e_i)) = (b_2^* - b^s) \cdot e_i & \text{on } \partial \Sigma^0, \\ y \rightarrow \omega_i(y) & Y \text{ - periodic.} \end{cases} \quad (3.89)$$

Proof. Suppose $b_1^* = b_2^* = b^* \in \mathbb{R}^d$. The compactness of the sequences in (3.83) follow directly from the a priori estimates (3.63) and the compactness results of Propositions 2.3.3, 2.7.3 from Chapter 2. let us consider the variational formulation for (3.60)-(3.62) by test functions $(\phi_\varepsilon, \varepsilon K^{-1} \psi_\varepsilon)$:

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

and

$$\psi_\varepsilon(t, x) = \psi\left(t, x - \frac{b^* t}{\varepsilon}\right) + \varepsilon \psi_1\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right).$$

$$\begin{aligned} & \int_0^T \int_{\Omega_\varepsilon} \left[\frac{\partial u_\varepsilon}{\partial t} \phi_\varepsilon + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi_\varepsilon + D_\varepsilon \nabla u_\varepsilon \cdot \nabla \phi_\varepsilon \right] dx dt \\ & + \frac{\varepsilon}{K} \int_0^T \int_{\partial \Omega_\varepsilon} \left[\frac{\partial v_\varepsilon}{\partial t} \psi_\varepsilon + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon \psi_\varepsilon + D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s \psi_\varepsilon \right] d\sigma_\varepsilon(x) dt \end{aligned}$$

$$+\varepsilon\kappa \int_0^T \int_{\partial\Omega_\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K}\right) \left(\phi_\varepsilon - \frac{\psi_\varepsilon}{K}\right) d\sigma_\varepsilon(x) dt = 0.$$

We shall use the auxiliary problem (3.42) to take care of the singular terms in the above variational formulation as is done in Section 3.9. Taking $(\phi, \psi) \equiv 0$, we shall pass to the limit in the above variational formulation taking into account (3.83) resulting in the cell problem (3.85). Then we take $(\phi_1, \psi_1) \equiv 0$ in the variational formulation followed by passing to limit in arriving at a variational formulation for the coupled effective equations (3.84).

Now for the case $b_1^* \neq b_2^*$. Taking the test functions with different drifts as

$$\phi_\varepsilon(t, x) = \phi\left(t, x - \frac{b_1^* t}{\varepsilon}\right) + \varepsilon \phi_1\left(t, x - \frac{b_1^* t}{\varepsilon}, \frac{x}{\varepsilon}\right)$$

and

$$\psi_\varepsilon(t, x) = \psi\left(t, x - \frac{b_2^* t}{\varepsilon}\right) + \varepsilon \psi_1\left(t, x - \frac{b_2^* t}{\varepsilon}, \frac{x}{\varepsilon}\right).$$

The calculations carry on as before except for the coupled term

$$\begin{aligned} & \kappa\varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \left(u_\varepsilon - \frac{v_\varepsilon}{K}\right) \left(\phi\left(t, x - \frac{b_1^* t}{\varepsilon}\right) - \frac{\psi}{K}\left(t, x - \frac{b_2^* t}{\varepsilon}\right)\right) d\sigma_\varepsilon(x) dt \\ & \xrightarrow{2s\text{-drift}} \kappa \int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} u_0(t, x) \phi(t, x) d\sigma(y) dx dt + \frac{\kappa}{K^2} \int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} v_0(t, x) \psi(t, x) d\sigma(y) dx dt \end{aligned}$$

as the two-scale limit for u_ε vanishes for the test functions with drift b_2^* and the two-scale limit for v_ε vanishes for the test functions with the drift b_1^* . Taking into consideration the above two-scale limit and redoing the calculations as in the proof of the homogenization process of Section 3.9, we arrive at the homogenized equations (3.86) and (3.87) for u_0 and v_0 respectively. Also, the cell problem isn't coupled anymore. \square

3.12 Compressible flows

Until now, we have had the assumption of null divergence on the velocity fields b and b^s . In this section, we shall be ignoring this assumption. We shall, however, leave the assumption of periodicity. We present the analysis for a convection-diffusion equation of a single solute in the absence of reactions. The model we wish to analyze is the following.

$$\frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) = 0 \quad \text{in } (0, T) \times \Omega_\varepsilon, \quad (3.90)$$

$$-D_\varepsilon \nabla u_\varepsilon \cdot n = 0 \quad \text{on } (0, T) \times \partial\Omega_\varepsilon, \quad (3.91)$$

$$u_\varepsilon(0, x) = u^{in}(x) \quad \text{in } \Omega_\varepsilon \quad (3.92)$$

We make the regularity assumption $b \in L^\infty_\#(\Omega_f; \mathbb{R}^d)$ on the velocity field. Also, we assume that $\operatorname{div}(b) \in L^\infty_\#(\Omega_f; \mathbb{R})$ although this regularity can be slightly weakened. We also assume that $b(y) \cdot n \in L^\infty_\#(\partial\Omega_s; \mathbb{R})$. Let us derive energy estimates for our model. Multiplying (3.90) by the solution u_ε

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega_\varepsilon} |u_\varepsilon|^2 dx + \frac{1}{2\varepsilon} \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla |u_\varepsilon|^2 dx + \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon dx = 0$$

After an integration by parts

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega_\varepsilon} |u_\varepsilon|^2 dx - \frac{1}{2\varepsilon} \int_{\Omega_\varepsilon} \operatorname{div}(b_\varepsilon) |u_\varepsilon|^2 dx - \frac{1}{2\varepsilon} \int_{\partial\Omega_\varepsilon} b_\varepsilon \cdot n |u_\varepsilon|^2 d\sigma(x) + \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon dx = 0$$

which implies

$$\frac{1}{2} \frac{d}{dt} \|u_\varepsilon\|_{L^2}^2 + \int_{\Omega_\varepsilon} D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon dx = \frac{1}{2\varepsilon} \int_{\Omega_\varepsilon} \operatorname{div}(b_\varepsilon) |u_\varepsilon|^2 dx + \frac{1}{2\varepsilon} \int_{\partial\Omega_\varepsilon} b_\varepsilon \cdot n |u_\varepsilon|^2 d\sigma(x) \quad (3.93)$$

We have the following Poincaré type inequality (proved in [67])

$$\varepsilon \int_{\partial\Omega_\varepsilon} |u_\varepsilon|^2 d\sigma(x) \leq \delta_\varepsilon \int_{\Omega_\varepsilon} |\nabla u_\varepsilon|^2 dx + \frac{1}{\delta_\varepsilon} \int_{\Omega_\varepsilon} |u_\varepsilon|^2 dx \quad (3.94)$$

for some positive constant depending on ε . Using (3.94), we can bound the right hand side of (3.93) by

$$\begin{aligned} &\leq \frac{1}{2\varepsilon} \|\operatorname{div}(b_\varepsilon)\|_{L^\infty} \|u_\varepsilon\|_{L^2}^2 + \frac{1}{\delta_\varepsilon} \|b_\varepsilon\|_{L^\infty} \|u_\varepsilon\|_{L^2}^2 + \delta_\varepsilon \|\nabla u_\varepsilon\|_{L^2}^2 \\ &\implies \frac{1}{2} \frac{d}{dt} \|u_\varepsilon\|_{L^2}^2 \leq \frac{1}{2\varepsilon} \left(\|\operatorname{div}(b_\varepsilon)\|_{L^\infty} + \frac{1}{\delta_\varepsilon} \|b_\varepsilon\|_{L^\infty} \right) \|u_\varepsilon\|_{L^2}^2 \end{aligned}$$

Thus by Gronwall's inequality

$$\begin{aligned} \|u_\varepsilon\|^2 &\leq \|u^{in}\|^2 \exp \left(\int_0^t \left(\frac{1}{\varepsilon} \|\operatorname{div}(b_\varepsilon)\|_{L^\infty} + \frac{1}{\delta_\varepsilon} \|b_\varepsilon\|_{L^\infty} \right) ds \right) \\ &\implies \|u_\varepsilon\|^2 \leq \exp \left(\frac{t}{\varepsilon} \|\operatorname{div}(b_\varepsilon)\|_{L^\infty} + \frac{t \|b_\varepsilon\|_{L^\infty}}{\varepsilon \delta_\varepsilon} \right) \|u^{in}\|^2 \end{aligned}$$

So, it is not possible to derive a priori estimates for u_ε with constant independent of ε . However, for a fixed ε , we have the following estimates.

$$\|u_\varepsilon\|_{L^2((0,T);H^1(\Omega_\varepsilon))} \leq C_\varepsilon \quad (3.95)$$

To upscale the model at hand, we tend to employ the method of two-scale convergence. As Propositions 2.6.4 and 2.6.6 suggest, we need uniform estimates independent of ε . But the constant C_ε in (3.95) isn't independent of ε . So we cannot straightaway apply the compactness results of Chapter 2. Here we shall take cues from [25] where a method of Factorization is employed in arriving at a homogenized equation for a convection-diffusion-reaction equation with a divergent velocity flow.

The principle of the Factorization method is quite simple as explained in Section 2.8 of Chapter 2. In the formal analysis of Section 3.7, we deduced that the first term in the ansatz for the solute concentration u_ε is independent of the fast variable y . In case of some partial differential equations, however, the oscillations are present even in the first term of the ansatz. There are examples where one can factor out the oscillations from the solutions. This method was introduced in [161]. The oscillations that we factor out comes off as a eigenfunction for a spectral problem.

$$\begin{cases} b(y) \cdot \nabla_y \varphi - \operatorname{div}_y (D(y) \nabla_y \varphi) = \lambda \varphi & \text{in } Y^0, \\ -D(y) \nabla_y \varphi \cdot n = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow \varphi(y) & Y\text{-periodic.} \end{cases} \quad (3.96)$$

The adjoint of the above spectral problem.

$$\begin{cases} -\operatorname{div}_y(b(y)\varphi^*) - \operatorname{div}_y(D(y)\nabla_y\varphi^*) = \lambda\varphi^* & \text{in } Y^0, \\ D(y)\nabla_y\varphi^* \cdot n + b(y) \cdot n\varphi^* = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow \varphi^*(y) & Y\text{-periodic.} \end{cases} \quad (3.97)$$

The existence of the first simple eigenvalue $\lambda > 0$ and the first eigenfunctions $\varphi > 0$ and $\varphi^* > 0$ for the spectral and the adjoint spectral problem (3.96)-(3.97) follows from the Krein-Rutman Theorem [108], [152]. The uniqueness follows from the chosen normalization.

$$\int_{Y^0} \varphi(y)\varphi^*(y) dy = 1. \quad (3.98)$$

Using the eigenfunction associated with both the direct and the adjoint spectral cell problems (3.96) and (3.97), we define modified velocity field and diffusion matrix as

$$\tilde{b}(y) = \varphi\varphi^*b(y) + \varphi D(y)\nabla_y\varphi^* - \varphi^* D(y)\nabla_y\varphi \quad (3.99)$$

and

$$\tilde{D}(y) = \varphi\varphi^*D(y) \quad (3.100)$$

We consider the following ansatz for u_ε

$$u_\varepsilon(t, x) = \exp(-\lambda t/\varepsilon^2) \sum_{i \geq 0} \varepsilon^i u_i\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right). \quad (3.101)$$

Proposition 3.12.1. *If the ansatz for the solution u_ε of (3.90)-(3.92) in (3.101) is true, then the solution formally satisfies*

$$u_\varepsilon(t, x) \approx \exp(-\lambda t/\varepsilon^2) \varphi\left(\frac{x}{\varepsilon}\right) \left[v\left(t, x - \frac{b^*t}{\varepsilon}\right) + \varepsilon \sum_{i=1}^d \frac{\partial v}{\partial x_i}\left(t, x - \frac{b^*t}{\varepsilon}\right) \omega_i\left(\frac{x}{\varepsilon}\right) \right] \quad (3.102)$$

where $\omega_i(y)$, for every $1 \leq i \leq d$, satisfy a so called cell problem.

$$\begin{cases} \tilde{b}(y) \cdot (\nabla_y\omega_i + e_i) - \operatorname{div}_y(\tilde{D}(y)(\nabla_y\omega_i + e_i)) = \varphi\varphi^*b^* \cdot e_i & \text{in } Y^0, \\ -\tilde{D}(y)(\nabla_y\omega_i + e_i) \cdot n = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow \omega_i(y) & Y\text{-periodic} \end{cases} \quad (3.103)$$

and the effective drift is given by

$$b^* = \int_{Y^0} \tilde{b}(y) dy. \quad (3.104)$$

Further, v in (3.102) satisfies the following homogenized equation:

$$\begin{cases} \frac{\partial v}{\partial t} - \operatorname{div}(\mathcal{D}\nabla v) = 0 & \text{in } (0, T) \times \mathbb{R}^d, \\ v(0, x) = u^{in}(x) \int_{Y^0} \varphi^*(y) dy & \text{in } \mathbb{R}^d. \end{cases} \quad (3.105)$$

where \mathcal{D} is defined by

$$\mathcal{D}_{ij} = \int_{Y^0} \tilde{D}(y)(\nabla_y\omega_i + e_i) \cdot (\nabla_y\omega_j + e_j) dy. \quad (3.106)$$

We refrain from proving the above formal result as the needed arguments shall be given in the Chapter 5 on upscaling multicomponent flows where we will be employing again the method of factorization. Now we shall present the rigorous approach. Let us make the following change of unknown.

$$u_\varepsilon(t, x) = \exp(-\lambda t/\varepsilon^2) \varphi\left(\frac{x}{\varepsilon}\right) v_\varepsilon(t, x) \quad (3.107)$$

Using (3.107) in the (3.90)-(3.92), we write down the partial differential equation for v_ε .

Lemma 3.12.2. *The unknown v_ε from (3.107) satisfy*

$$\begin{cases} \varphi \varphi^* \frac{\partial v_\varepsilon}{\partial t} + \frac{1}{\varepsilon} \tilde{b}_\varepsilon \cdot \nabla v_\varepsilon - \operatorname{div} \left(\tilde{D}_\varepsilon \nabla v_\varepsilon \right) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ v_\varepsilon(0, x) = u^{in}(x) \int_{Y^0} \varphi^*(y) dy & \text{in } \Omega_\varepsilon. \end{cases} \quad (3.108)$$

Proof. Definition of the change of unknown (3.107) makes sense due to the positivity of φ , the eigenfunction for the spectral problem (3.96). In order to plug the expressions (3.107) in (3.90), we shall use the following chain rule formulae

$$\begin{aligned} \frac{\partial u_\varepsilon}{\partial t}(t, x) &= \frac{-\lambda}{\varepsilon^2} \exp(-\lambda t/\varepsilon^2) \varphi\left(\frac{x}{\varepsilon}\right) v_\varepsilon(t, x) + \exp(-\lambda t/\varepsilon^2) \varphi\left(\frac{x}{\varepsilon}\right) \frac{\partial v_\varepsilon}{\partial t}(t, x), \\ \nabla \left(u_\varepsilon(t, x) \right) &= \frac{1}{\varepsilon} \exp(-\lambda t/\varepsilon^2) v_\varepsilon(t, x) \left(\nabla_y \varphi \right) \left(\frac{x}{\varepsilon} \right) + \exp(-\lambda t/\varepsilon^2) \varphi\left(\frac{x}{\varepsilon}\right) \nabla_x v_\varepsilon(t, x). \end{aligned}$$

Upon substitution, we shall multiply the thus obtained system by the adjoint eigenfunction φ^* to arrive at (3.108). \square

We remarked earlier in (3.95) that the estimates on u_ε weren't uniform in ε . The divergence of b being non zero prevented us from having uniform estimates. The modified velocity field \tilde{b} appearing in (3.108) is however of divergence zero.

$$\begin{aligned} -\operatorname{div}_y \left(\tilde{b}(y) \right) &= -\operatorname{div}_y \left(\varphi \varphi^* b(y) \right) - \operatorname{div}_y \left(\varphi D(y) \nabla_y \varphi^* \right) + \operatorname{div}_y \left(\varphi^* D(y) \nabla_y \varphi \right) \\ &= -\varphi^* \left(b(y) \cdot \nabla_y \varphi - \operatorname{div}_y \left(D(y) \nabla_y \varphi \right) \right) + \varphi \left(-\operatorname{div}_y \left(\varphi^* b(y) \right) - \operatorname{div}_y \left(D \nabla_y \varphi^* \right) \right) = 0. \end{aligned} \quad (3.109)$$

where we used information from the spectral cell problem (3.96) and its adjoint spectral cell problem (3.97).

Lemma 3.12.3. *Let v_ε be a weak solution of (3.108). There exists a constant C , independent of ε , such that*

$$\|v_\varepsilon\|_{L^\infty((0, T); L^2(\Omega_\varepsilon))} + \|\nabla v_\varepsilon\|_{L^2((0, T) \times \Omega_\varepsilon)} \leq C \|v^{in}\|_{L^2(\mathbb{R}^d)} \quad (3.110)$$

Proof. To derive the a priori estimates, we shall multiply (3.108) by v_ε and integrate over Ω_ε to arrive at the following energy estimate.

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega_\varepsilon} \varphi \varphi^* |v_\varepsilon|^2 dx + \int_{\Omega_\varepsilon} \tilde{D}_\varepsilon \nabla v_\varepsilon \cdot \nabla v_\varepsilon dx = 0.$$

We shall now integrate over $(0, T)$. The positivity of the eigenfunctions φ and φ^* and the coercivity of \tilde{D} leads to the a priori estimate (3.110). \square

Theorem 3.12.4. *There exists $v \in L^2((0, T); H^1(\mathbb{R}^d))$ and $v_1 \in L^2((0, T) \times \mathbb{R}^d; H^1_{\#}(Y^0))$ such that the sequence of concentrations $\{v_\varepsilon\} \in L^2((0, T); H^1(\Omega_\varepsilon))$, solutions of (3.108), two-scale converge with drift b^* , up to a subsequence, as $\varepsilon \rightarrow 0$, in the following sense*

$$v_\varepsilon \xrightarrow{2\text{-drift}} v, \quad \nabla v_\varepsilon \xrightarrow{2\text{-drift}} \nabla_x v + \nabla_y v_1. \quad (3.111)$$

The two-scale limit v solves the homogenized diffusion equation (3.105) with the expression for the dispersion tensor given by (3.106) in terms of the solutions ω_i of the cell problem (3.103). Also the two-scale limit v_1 is written in terms of the cell solutions as

$$v_1(t, x, y) = \sum_{i=1}^d \omega_i(y) \frac{\partial v_0}{\partial x_i}. \quad (3.112)$$

The existence of two-scale limits follow from the compactness results of two-scale convergence with drift. The arguments to show that the limits satisfy the homogenized equation and the cell problem are similar to the ones done in the proof of Theorem 3.9.1. We shall not be repeating them here.

3.13 Numerical study

This section is devoted to the numerical computation of the cell problems and of the homogenized coefficients, given by Proposition 3.7.2, and to the study of their variations according to various parameters in the microscopic model. We have used the Freefem++ package [141] to perform some numerical tests in two dimensions. We have used Lagrange P1 finite elements with 33586 vertices (degrees of freedom) with characteristic Galerkin method for the convective term. The periodicity cell is the unit square and the solid obstacle is a disk. Table 3.1 gives the adimensionalized values of the parameters utilized in our simulations.

Parameters	Values
Radius of the obstacle r	0.2
Equilibrium constant K	1
Porosity : $ Y^0 = 1 - r^2\pi$	0.874357
Tortuosity : $ \partial\Sigma^0 = 2\pi r$	1.25664
K_d factor : $ Y^0 + K \partial\Sigma^0 $	2.13099
Surface velocity b^s	0
Mean velocity $\int_{Y^0} b(y) dy$	$(0.0385, -2.67 \times 10^{-5})$
Adsorption rate κ_0	1
Bulk molecular diffusion D	1
Surface molecular diffusion D^s	1

Table 3.1: Parameter values

The velocity profile $b(y)$ is generated by solving the following Stokes problem in the fluid part Y^0 of the unit cell.

$$\begin{cases} \nabla_y p - \Delta_y b = e_1 & \text{in } Y^0, \\ \operatorname{div}_y b = 0 & \text{in } Y^0, \\ b = 0 & \text{on } \partial\Sigma^0, \\ p, b & Y\text{-periodic.} \end{cases} \quad (3.113)$$

where e_1 is the unit vector $(1, 0)$. The drift velocity b^* is then calculated using (3.27): we found

$$b^* = (0.0180, -1.25 * 10^{-5}). \quad (3.114)$$

In a first experiment we study the behavior of the longitudinal dispersion with respect to the local Péclet number Pe_{loc} (we simply multiply the velocity field $b(y)$ by an increasing factor) for various values of D^s (see Figure 3.1). As can be expected the dispersion increases with Pe_{loc} .

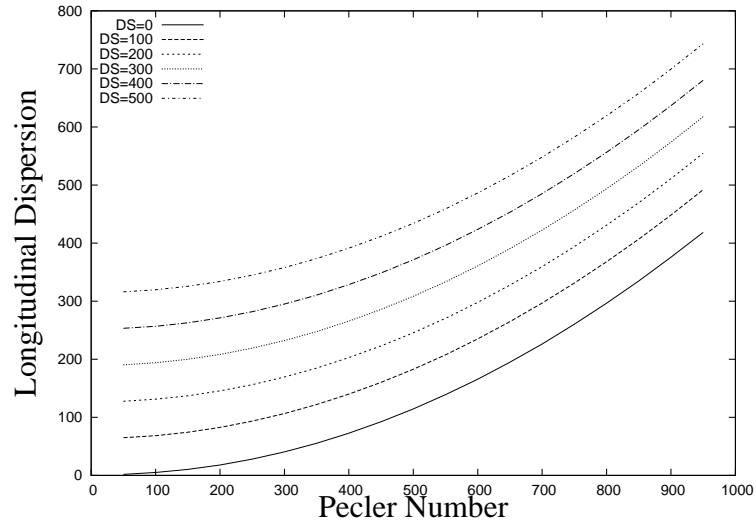


Figure 3.1: Behavior of the longitudinal dispersion with respect to Pe_{loc} for various values of the surface molecular diffusion D^s .

Clearly the dispersion increases with D^s too. However, as shown by Figure 3.2, the dispersion reaches a limit as D^s goes to infinity. This can be explained formally by the fact that, in such a case, the cell solution satisfies in the limit that $(\omega_i + Ky_i)$ is constant on the pore surface $\partial\Sigma^0$. In this limit, the bulk correctors χ_i satisfy the following limit problem

$$\begin{cases} b(y) \cdot \nabla_y \chi_i - \operatorname{div}_y (D(\nabla_y \chi_i + e_i)) = (b^* - b) \cdot e_i & \text{in } Y^0, \\ -D(\nabla_y \chi_i + e_i) \cdot n + Kb_i^* = \\ \kappa \left(\chi_i + y_i - |\partial\Sigma^0|^{-1} \int_{\partial\Sigma^0} (\chi_i + y_i) d\sigma(y) \right) & \text{on } \partial\Sigma^0, \\ y \rightarrow \chi_i(y) & Y\text{-periodic.} \end{cases} \quad (3.115)$$

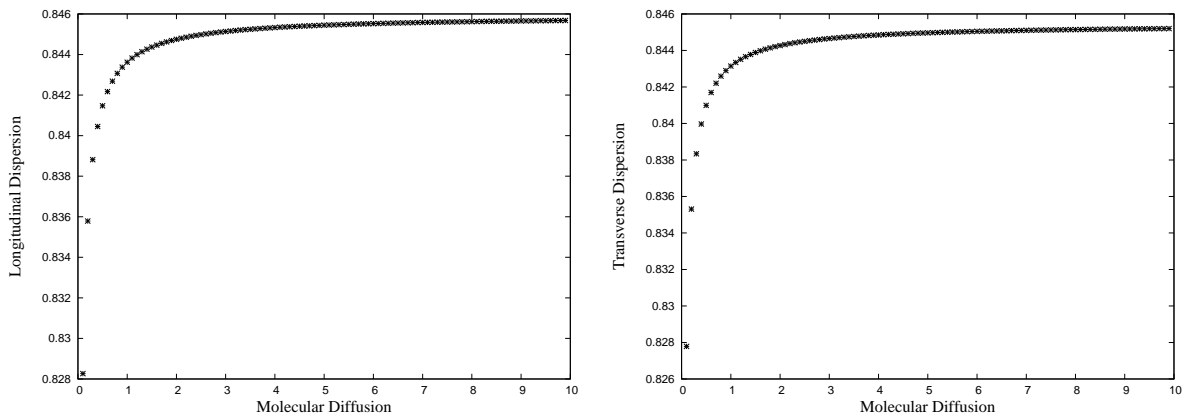


Figure 3.2: Behavior of the effective dispersion with respect to D^s : longitudinal dispersion (left), transverse dispersion (right).

In a second experiment we study the behavior of the longitudinal dispersion with respect to the reaction rate κ . Interestingly enough, we observe an inversion phenomenon on the bulk corrector χ_1 (see Figures 3.3 and 3.4 where the grey scale goes from smaller values in white to larger values in black). A similar inversion is exhibited by χ_2 too. However, this inversion phenomenon doesn't appear in the absence of surface molecular diffusion, i.e., when $D^s = 0$. For a given positive value of D^s , increasing κ implies that it may be more favorable for the solute to “travel” close to the pore surface by using the surface diffusion. Therefore, the solid pores may be seen as obstacles for small κ or attractors for large κ . It is probably easier to interpret this inversion phenomenon on the “reconstructed” solution $(\chi_1(y) + y_1)$ rather than on just on the cell solution $\chi_1(y)$ (see Figures 3.5 and 3.6). Indeed, $(\chi_1(y) + y_1)$ corresponds to a local linearization of the two first terms of the ansatz of u_ε as given in Proposition 3.7.2. As the reaction rate increases, the isolines of this reconstructed concentration start to grace off the obstacle, which implies that the orthogonal current lines of the concentration flux are more and more attracted by the obstacle. It should be remarked here that this is a handicap of performing only 2D numerical simulations. Indeed, it is only in 3D that both the fluid phase and the solid structure can be connected, which only permits a fair comparison between surface and bulk molecular diffusions.

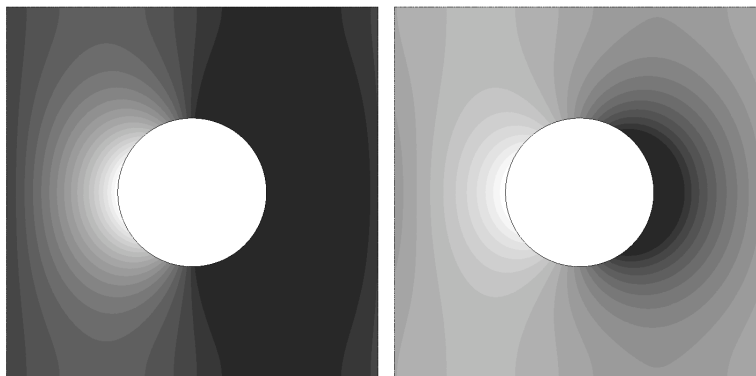


Figure 3.3: The cell solution χ_1 : Left, reference value $\kappa = \kappa^0$; Right, $\kappa = 5\kappa^0$.

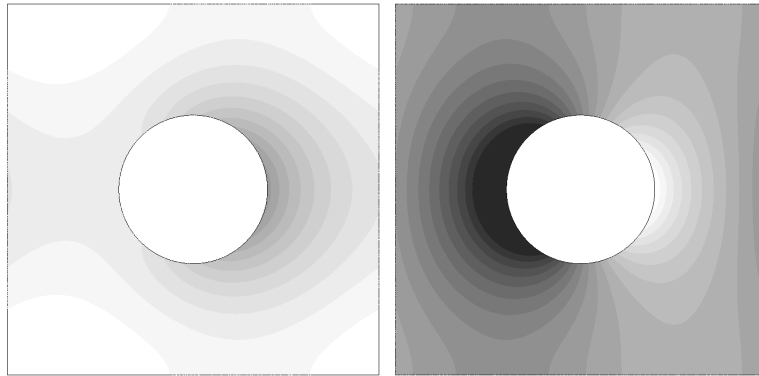


Figure 3.4: The cell solution χ_1 : Left, $\kappa = 6\kappa^0$; Right, $\kappa = 8\kappa^0$.

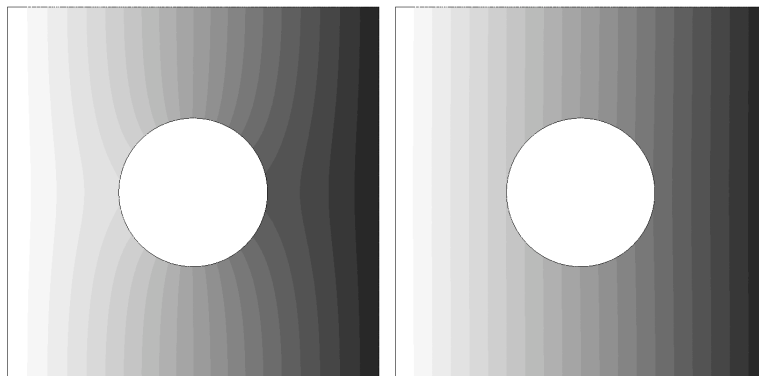


Figure 3.5: The reconstructed solution $\chi_1(y) + y_1$: Left, Reference value $\kappa = \kappa^0$; Right, $\kappa = 6\kappa^0$.

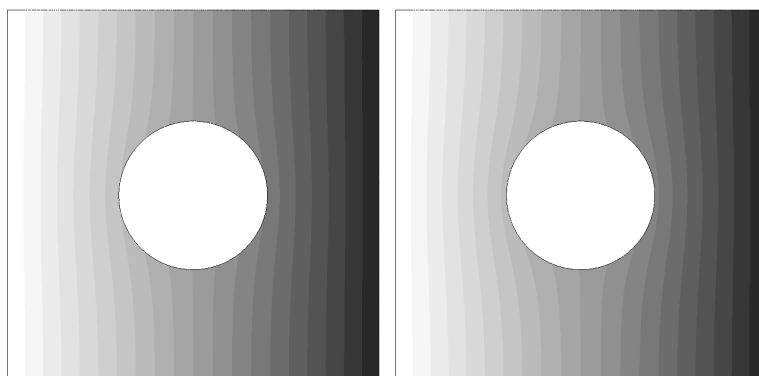


Figure 3.6: The reconstructed solution $\chi_1(y) + y_1$: Left, $\kappa = 12\kappa^0$; Right, $\kappa = 19\kappa^0$.

In Figures 3.7 and 3.8 we plot the dispersion in two asymptotic regimes: $\kappa \rightarrow 0$ and $\kappa \rightarrow \infty$. Once again when $\kappa \rightarrow \infty$ we get an asymptote for the dispersion, corresponding to a limit cell problem where $K\chi_i = \omega_i$. In this limit, the corresponding system satisfied by the bulk corrector

χ_i is

$$\begin{cases} b(y) \cdot \nabla_y \chi_i - \operatorname{div}_y(D(\nabla_y \chi_i + e_i)) = (b^* - b) \cdot e_i & \text{in } Y^0, \\ -K^{-1}D(\nabla_y \chi_i + e_i) \cdot n + (b^* - b^s) \cdot e_i = \\ \quad b^s(y) \cdot \nabla_y^s \chi_i - \operatorname{div}_y^s(D^s(\nabla_y^s \chi_i + e_i)) & \text{on } \partial \Sigma^0, \\ y \rightarrow \chi_i(y) & Y\text{-periodic.} \end{cases} \quad (3.116)$$

Of course, the transverse dispersion is always smaller than the longitudinal dispersion. Figures 3.7 and 3.8 show the blow-up behavior of both longitudinal and transverse dispersions when $\kappa \rightarrow 0$. This is due to the ill-posedness of the cell problem (3.31) in the limit $\kappa \rightarrow 0$.

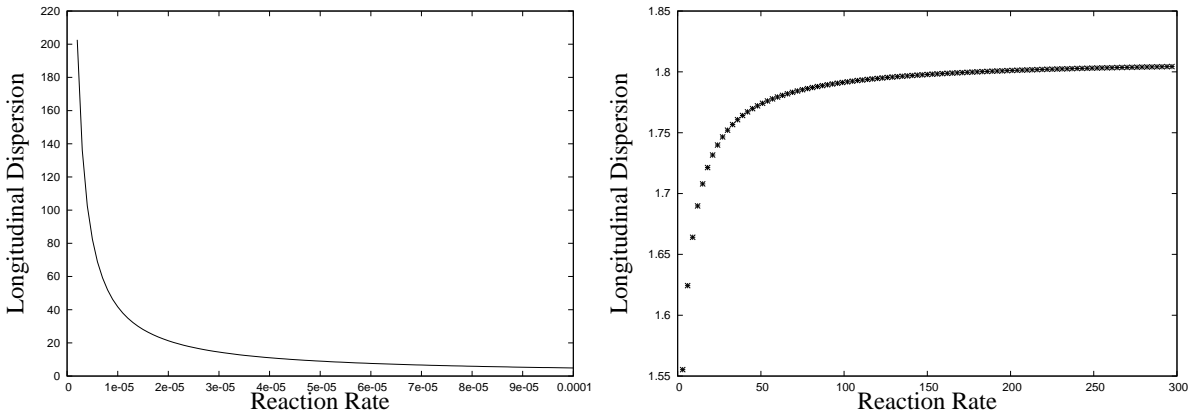


Figure 3.7: Behavior of the longitudinal dispersion with respect to κ : when κ goes to 0 (left), when κ goes to infinity (right).

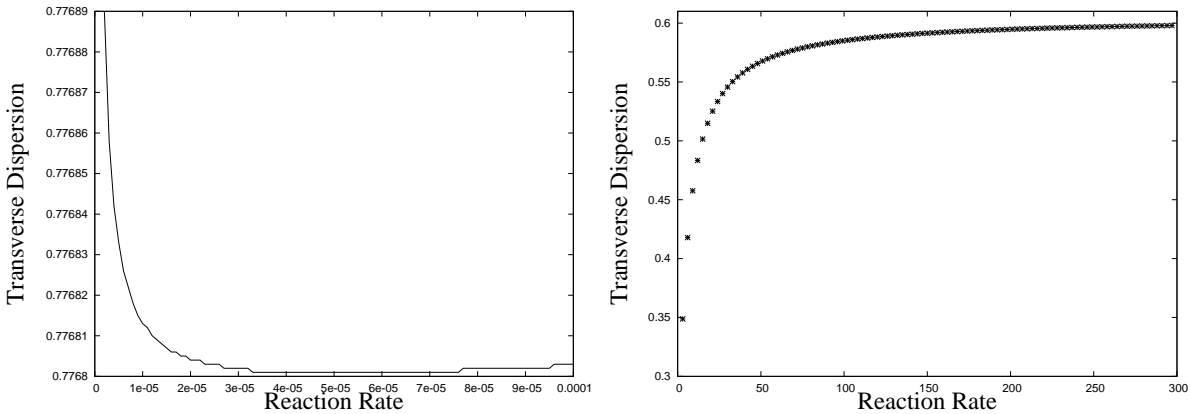


Figure 3.8: Behavior of the transverse dispersion with respect to κ : when κ goes to 0 (left), when κ goes to infinity (right).

3.14 Comments

Locally periodic coefficients

In this chapter we have analysed the reactive transport of a single solute in presence of adsorption reaction on the pore boundaries. Bulk and solute concentrations were governed by coupled

partial differential equations (3.11)-(3.13) with purely periodic coefficients i.e., $b_\varepsilon(x) = b(x/\varepsilon)$, $D_\varepsilon(x) = D(x/\varepsilon)$. The obvious question would be:

Is it possible to relax the pure periodicity assumption on the coefficients in (3.11)-(3.13) and still homogenize the microscopic model?

We can give a partial answer to this question. As far as the diffusion matrices D and D^s go, we can consider them to be locally periodic i.e., $D_\varepsilon(x) = D(x, x/\varepsilon)$, $D_\varepsilon^s(x) = D^s(x, x/\varepsilon)$ and still the homogenization techniques used in this chapter to arrive at the effective equations apply. The dispersion \mathcal{D} that we found in Section 3.7 is symmetric and constant. We symmetrized the expression for the dispersion during the process of upscaling as the Hessian matrix $\nabla^2 u_0$ is symmetric. In case of locally periodic diffusion matrices, however, we shouldn't symmetrize the expression for \mathcal{D} .

So there is a possibility of relaxing the pure periodicity assumption on the diffusion coefficients in (3.11)-(3.13). This doesn't extend to the velocity fields in (3.11)-(3.13). We are working in the strong convection regime. As we explained in Section 2.6 of Chapter 2, the classical two-scale asymptotic expansion method had to be modified by taking large drift in the slow variable. This method of two-scale asymptotic expansions with drift considers only constant values for drift. In the expression for the effective drift (3.27), if we blindly relax the pure periodicity conditions on the velocity fields then the drift velocity b^* isn't a constant and this is not admissible. This is one of the main technical reasons. Also the chain rule differentiation formulae (3.24) that we use while performing the formal calculations do not hold true anymore if b^* weren't a constant. It is to be noted that under special assumptions on the coefficients, G. Allaire and R. Orive in [22] have shown that a new localization phenomenon can occur which is completely different from the asymptotic behaviour proved in this Chapter. This highlights the need for the developments of new tools in the theory of periodic homogenization.

Quantitative analysis

Quantification of the dispersion tensor is of crucial importance. In the regime of "strong convection", some of the results on deriving upper and lower bounds for the dispersion tensor can be found in [138]. In this Chapter we have found expressions for different effective parameters in terms of the local parameters. Even though in Section 3.13, we have attempted to study the behaviour of those effective parameters with respect to local ones, it can be of value to pursue the analysis to find optimal bounds on the effective parameters. There have been some astonishing works in this regard in the absence of chemical reactions [93], [119]. In the cited references, for example, it is proved that the dispersion increases or diminishes depending on whether the mean value of the velocity field is rational or irrational. We could try to analyze if we arrive at those results in the limit of reaction rate going to zero. In the general introduction to this thesis (Chapter 1), we gathered some results on the upscaling of reactive flows in "Diffusion dominated regime" [77], [97], [78], [79], [80], [81], [69], [68]. We could compare the effective parameters obtained in that regime with those obtained in this Chapter.

Random porous media

All through this Chapter we have worked with only periodic porous medium and periodic coefficients. A. Bourgeat, A. Mikelić and S. Wright in [45] adapted the "two-scale convergence method" of periodic regime to random regimes under some suitable stationarity assumptions. In the large Péclet regime, we have learnt the need to modify the method of two-scale convergence by the introduction of large drift in the slow variable. We can try to adapt this new notion of

“two-scale convergence with drift” to random regimes in the spirit of [45]. If successful, we will be able to find effective dispersion in large Péclet regime in random porous media. J. L. Auriault in [32] argues that the random and periodic media present similar macroscopic description, when it exists. So, the analysis of the system with randomly oscillating coefficients gets interesting.

Conclusions

Finally, this Chapter has analyzed all possible scenarios for the reactive transport of single solute in periodic regime in presence of linear reaction terms. We have also seen that we recover the previous results in this regime of “strong convection” in various asymptotic regimes. In the next Chapter we move on to the homogenization problem related to a nonlinear adsorption isotherm.

Chapter 4

Langmuir isotherm in porous media

4.1 Introduction

As in Chapter 3, this chapter is devoted to the study of an adsorption process occurring at the solid-fluid interface in an ε -periodic rigid porous medium. The novelty of the mesoscale model considered in this chapter is the presence of nonlinear terms modelling the adsorption process as opposed to the linear case studied in Chapter 3. We will be working with a convection diffusion equation for the solute concentration in the bulk and a convection diffusion equation for the adsorbed concentration on the pores surface, both being coupled by a nonlinear reaction term modeling the adsorption phenomena at the solid fluid interface. We shall get into the modelling and scaling aspects of the governing equations in Section 4.3. The presence of nonlinear terms always gets interesting in the homogenization process. Starting with a linear coupled convection diffusion reaction equations in Chapter 3, we arrived at a scalar linear diffusion equation in moving coordinates. In this chapter too, we shall be employing the method for two-scale convergence with drift [121] (recalled in Section 2.6) to derive the effective equation. It would be of interest to study how the nonlinearities are going to affect the homogenization result. The drift velocity b^* associated with the linear model (3.11)-(3.13) was shown to be equal to (3.27):

$$b^* = \frac{\int_{Y^0} b(y) dy + K \int_{\partial\Sigma^0} b^s(y) d\sigma(y)}{|Y^0| + K|\partial\Sigma^0|_{d-1}}.$$

The nonlinear isotherm (4.2) with which we will be working all through this chapter is that given by Langmuir. An interesting exercise would be to derive an expression for the drift velocity associated with the convection diffusion adsorption equations with the nonlinear isotherm (4.2). In Section 2.9, we remarked that the drift velocity b^* in the method of two-scale convergence with drift has to be independent of the slow variable x . This handicap of the method necessitates a technical assumption, in the current case of Langmuir adsorption, on the velocity fields which amounts to say that the bulk and surface drifts are equal (their common value being called b^* in the sequel)

$$\frac{1}{|Y^0|} \int_{Y^0} b(y) dy = \frac{1}{|\partial\Sigma^0|} \int_{\partial\Sigma^0} b^s(y) d\sigma(y) = b^*, \quad (4.1)$$

where $b(y)$ is a Y -periodic velocity field in the bulk Ω_f and $b^s(y)$ is a Y -periodic velocity field on the pores surface $\partial\Omega_s$. Such an assumption was not necessary in the linear case [10], [20], [17] but is the price to pay for extending our previous results to the nonlinear case of the Langmuir isotherm.

Our main result (Theorem 4.8.1) says that the solution $(u_\varepsilon, v_\varepsilon)$ of the coupled convection diffusion reaction system (4.12)-(4.14) is approximatively given by the ansatz

$$\begin{aligned} u_\varepsilon(t, x) &\approx u_0\left(t, x - \frac{b^*t}{\varepsilon}\right) + \varepsilon u_1\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right), \\ v_\varepsilon(t, x) &\approx f(u_0)\left(t, x - \frac{b^*t}{\varepsilon}\right) + \varepsilon v_1\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right), \end{aligned}$$

where f is the Langmuir isotherm given in (4.2) and u_0 is the solution of the following macroscopic nonlinear monotone diffusion equation

$$\begin{cases} \left[|Y^0| + \frac{\alpha |\partial \Sigma^0|}{(1 + \beta u_0)^2} \right] \frac{\partial u_0}{\partial t} - \operatorname{div}_x(\mathcal{D}(u_0) \nabla_x u_0) = 0 & \text{in } (0, T) \times \mathbb{R}^d, \\ \left[|Y^0| u_0 + \frac{|\partial \Sigma^0| \alpha u_0}{1 + \beta u_0} \right] (0, x) = |Y^0| u^{in}(x) + |\partial \Sigma^0| v^{in}(x) & \text{in } \mathbb{R}^d, \end{cases}$$

and the correctors (u_1, v_1) are defined by

$$u_1(t, x, y) = \sum_{i=1}^d \chi_i(y, u_0(t, x)) \frac{\partial u_0}{\partial x_i}(t, x)$$

and

$$v_1(t, x, y) = \frac{\alpha}{(1 + \beta u_0(t, x))^2} \sum_{i=1}^d \omega_i(y, u_0(t, x)) \frac{\partial u_0}{\partial x_i}(t, x)$$

where $(\chi_i, \omega_i)_{1 \leq i \leq d}$ is the solution of the cell problem

$$\begin{cases} -b^* \cdot e_i + b(y) \cdot (e_i + \nabla_y \chi_i) - \operatorname{div}_y(D(e_i + \nabla_y \chi_i)) = 0 & \text{in } Y^0, \\ -D(e_i + \nabla_y \chi_i) \cdot n = \frac{\alpha \kappa}{(1 + \beta u_0)^2} (\chi_i - \omega_i) & \text{on } \partial \Sigma^0, \\ -b^* \cdot e_i + b^s(y) \cdot (e_i + \nabla_y^s \omega_i) - \operatorname{div}_y^s(D^s(e_i + \nabla_y^s \omega_i)) = \kappa (\chi_i - \omega_i) & \text{on } \partial \Sigma^0, \\ y \rightarrow (\chi_i(y), \omega_i(y)) \quad Y\text{-periodic.} \end{cases}$$

Note that the cell solution (χ, ω) depends not only on y but also on the value of $u_0(t, x)$. Furthermore, the technical assumption (4.1) is precisely the compatibility condition for solving the cell problem for any value of $u_0(t, x)$. In Chapter 3, the effective dispersion that we obtained was a constant and our upscaling method could only capture the symmetric part of the dispersion matrix. In the nonlinear case, however, the effective diffusion (or dispersion) tensor $\mathcal{D}(u_0)$ is given by

$$\begin{aligned} \mathcal{D}_{ij}(u_0) &= \int_{Y^0} D(y) (\nabla_y \chi_i + e_i) \cdot (\nabla_y \chi_j + e_j) dy + \frac{\alpha \kappa}{(1 + \beta u_0)^2} \int_{\partial \Sigma^0} [\chi_i - \omega_i] [\chi_j - \omega_j] d\sigma(y) \\ &\quad + \frac{\alpha}{(1 + \beta u_0)^2} \int_{\partial \Sigma^0} D^s(y) (\nabla_y^s \omega_i + e_i) \cdot (\nabla_y^s \omega_j + e_j) d\sigma(y) \\ &\quad + \int_{Y^0} D(y) (\nabla_y \chi_j \cdot e_i - \nabla_y \chi_i \cdot e_j) dy \\ &\quad + \frac{\alpha}{(1 + \beta u_0)^2} \int_{\partial \Sigma^0} D^s(y) (\nabla_y^s \omega_j \cdot e_i - \nabla_y^s \omega_i \cdot e_j) d\sigma(y) \\ &\quad + \int_{Y^0} (b(y) \cdot \nabla_y \chi_i) \chi_j dy + \frac{\alpha}{(1 + \beta u_0)^2} \int_{\partial \Sigma^0} (b^s(y) \cdot \nabla_y^s \omega_i) \omega_j d\sigma(y) \end{aligned}$$

which is neither symmetric nor constant. The presence of nonlinear terms in the mesoscopic equation has led to an effective behavior where the cell problem and the homogenized equation are explicitly coupled as shown by the above given expressions.

This chapter is outlined as follows. Section 4.2 introduces the Langmuir isotherm extensively used in surface chemistry and also recalls Freundlich isotherm. Having introduced the relevant isotherm that governs the chemical phenomena, in Section 4.3 we take up the task of mathematical modeling. The equations that govern the coupled phenomena of interest are rescaled to arrive at the mesoscopic system (4.12)-(4.14). Section 4.4 deals with the maximum principles (see Proposition 4.4.1) and a priori estimates for (4.12)-(4.14) which are obtained via energy estimates (see Lemma 4.4.2). Section 4.5 concerns itself with the wellposedness nature of the system (4.12)-(4.14). Finite dimensional Galerkin approximation method is employed in showing the existence of the solutions $(u_\varepsilon, v_\varepsilon)$ for (4.12)-(4.14). The main result of Section 4.5 is Proposition 4.5.1, the proof of which goes via various lemmata that are proved in Section 4.5 and relies on the monotone character of the nonlinear Langmuir isotherm. After the qualitative analysis of Sections 4.4 and 4.5, we shall get into the crux of the objective i.e., the homogenization of the mesoscopic model (4.12)-(4.14). The nonlinearity of (4.12)-(4.14) requires some strong compactness of the sequence of solutions in order to pass to the limit. This shall be the goal of Section 4.6. The needed strong compactness result is obtained in Corollary 4.6.7 which is the most technical result of the present chapter. Following the ideas of [121], [24], we first show that, in a moving frame of reference, a uniform localization of solutions holds (Lemma 4.6.1). Then a time equicontinuity type result (Lemma 4.6.2) allows us to gain compactness. These technical results are not straightforward extensions of those in [121], [24]. There are a number of additional difficulties, including the perforated character of the domain, the nonlinearity of the equations and more importantly the fact that there are two unknowns u_ε and v_ε . Section 4.7 is dedicated to the extraction of converging subsequences of the solution sequences. In this section, we intensely use the relative compactness results of Sections 2.6 and 2.7 from Chapter 2. The derivation of the homogenized equation is left to Section 4.8 (Theorem 4.8.1) using the method of two-scale convergence with drift [121], [7]. Theorems 4.7.2 and 4.8.1 give a result of weak convergence of the sequence $(u_\varepsilon, v_\varepsilon)$ to the homogenized limit $(u_0, v_0 = f(u_0))$. Although the previous Corollary 4.6.7 gives some strong compactness in the L^2 -norm, there is still room to improve the strong convergence, notably for the gradients of u_ε and v_ε . This is the purpose of Section 4.9 where we establish a strong convergence result (Theorem 4.9.1) for well prepared initial data. Eventually, Section 4.10 is devoted to some 2D numerical simulations using the FreeFem++ package [141]. In the 2D setting, assumption (4.1) implies that the homogenized drift vanishes, i.e., $b^* = 0$. We study the behaviour of the homogenized dispersion tensor with respect to variations of the magnitude of u_0 , the reaction rate κ and the surface molecular diffusion D^s . We also plot the homogenized solution u_0 and the reconstructed solution

$$\tilde{u}_\varepsilon(t, x) = u_0(t, x) + \varepsilon \sum_i^d \chi_i\left(\frac{x}{\varepsilon}, u_0\right) \frac{\partial u_0}{\partial x_i}(t, x)$$

to see the importance of the corrector term. Finally, in Section 4.11, we make some observations on the calculations done along this chapter and compare the results obtained in this chapter with those of Chapter 3 in the linear setting.

4.2 Langmuir's adsorption isotherm

Upon presenting the Henry's adsorption isotherm (linear) in Section 3.2, we did give expressions for a couple of known nonlinear isotherms (3.3) and (3.4). One among them is the following

Langmuir isotherm.

$$f(u) = \frac{\alpha u}{1 + \beta u} \quad \text{with } \alpha, \beta > 0 \quad (4.2)$$

The primitive of the Langmuir isotherm (4.2) is given by

$$F(u_\varepsilon) = \frac{\alpha}{\beta} \left[u_\varepsilon - \frac{1}{\beta} \log(1 + \beta u_\varepsilon) \right] \quad (4.3)$$

The primitive (4.3) vanishes at zero. In [111], Langmuir gave a description of the equilibrium between a single component gas and the adsorbed species at a surface. He gave a relationship between the fraction of the surface covered by adsorbed species, θ_g , and the partial pressure of the single component gas exposed to the surface, p_g .

$$\theta_g = \frac{\alpha p_g}{1 + \beta p_g} \quad (4.4)$$

The above expression can be obtained by the mass-action kinetics as demonstrated in Chapter 11 of [102]. In case of liquid-solid interface, we shall replace the partial pressure by concentration of the solute dissolved in the liquid phase and the surface fraction by the concentration of the adsorbed solute. Let u be the concentration of the dissolved solute in the bulk and v be the concentration of the same solute in the adsorbed state in the interface. Then, at chemical equilibrium we have

$$v = f(u). \quad (4.5)$$

As the interest is to study the non equilibrium reactions, we consider the following ordinary differential equation for the adsorbed concentration.

$$\frac{dv}{dt} = \kappa(f(u) - v) \quad \text{with } \kappa \text{ a positive constant.} \quad (4.6)$$

Another popular adsorption isotherm considered in the chemistry literature is due to Freundlich [88].

$$f(u) = \alpha u^\beta \quad \text{with } \alpha > 0 \text{ and } 0 < \beta < 1. \quad (4.7)$$

The expressions (4.2) and (4.7) for the two isotherms have been used quite extensively in the literature. However, the determination of the reaction coefficients is quite tedious and very case specific. In order to simplify the mathematical analysis, there was an attempt made in [78] to justify these two isotherms and generalize their notions. According to the cited reference, there are two kinds of concave isotherms : Langmuir and Freundlich. A function $f(u)$ is said to be of ‘‘Langmuir type’’ if it is strictly concave near $u = 0$ and $f'(0+) < +\infty$. The isotherm expression given in (4.2) indeed falls into this category. On the other hand, $f(u)$ is said to be of ‘‘Freundlich type’’ if it is strictly concave near $u = 0$ and $f'(0+) = +\infty$. An example of one such isotherm is (4.7).

4.3 Mathematical model

Let us consider an ε -periodic porous medium saturated with an incompressible fluid. Solutes of a kind are assumed to be dissolved in the fluid. The objective is to study the transport of the dissolved solutes. As in Chapter 3, we shall be considering transport both in the bulk of the fluid and on the porous skeleton. So we introduce two velocity fields: $b(y)$ in the bulk of the fluid Ω_f and $b^s(y)$ on the surface of the pores $\partial\Omega_s$. We shall not be analyzing any governing equations for these two velocity fields. Our hypothesis on these incompressible velocity fields

is that they are given, independent of time and Y -periodic. The incompressibility condition on both the velocity fields means

$$\operatorname{div}_y b(y) = 0 \quad \text{and} \quad \operatorname{div}_y^s b^s(y) = 0. \quad (4.8)$$

We make the following regularity assumption on both velocity fields: $b(y) \in L^\infty_{\#}(\Omega_f; \mathbb{R}^d)$, $b^s(y) \in L^\infty_{\#}(\partial\Omega_s; \mathbb{R}^d)$ and $b^s = G b^s$ is always tangential to the surface where $G(y)$ is the projection matrix on the tangent hyperplane to the surface $\partial\Omega_f = \partial\Omega_s$. The molecular diffusion associated with the dissolved solute is assumed to be periodic and different in bulk and on the surface. So, two periodic symmetric tensors $D(y) \in L^\infty_{\#}(\Omega_f)^{d \times d}$ and $D^s(y) \in L^\infty_{\#}(\partial\Omega_s)^{d \times d}$ which are assumed to be uniformly coercive, namely there exists a constant $C > 0$ such that, for any $\xi \in \mathbb{R}^d$,

$$D(y)\xi \cdot \xi \geq C|\xi|^2 \quad \text{a.e. in } \Omega_f, \quad D^s(y)\xi \cdot \xi \geq C|\xi|^2 \quad \text{a.e. on } \partial\Omega_s.$$

are introduced. The solutes in the bulk of the fluid are subjected to transport via the convective field $b(y)$ and they diffuse in the bulk, thanks to the associated diffusion matrix $D(y)$. The equation that models this combined phenomena is the following convection diffusion equation for u , the solute concentration in the fluid bulk.

$$\frac{\partial u}{\partial \tau} + b \cdot \nabla u - \operatorname{div}(D \nabla u) = 0 \quad \text{in } (0, \zeta) \times \Omega_f \quad (4.9)$$

As recalled in the introduction, we wish to study the transport of the adsorbed concentration too as in Chapter 3. Let v to the concentration of the adsorbed solutes in the interface. In Section 4.2, we have introduced an ordinary differential equation (4.6) that represents the non equilibrium chemical phenomena in terms of an isotherm. The presence of surface convective field b^s and the surface diffusion D^s associated with the solute modify (4.6) into the following partial differential equation.

$$\frac{\partial v}{\partial \tau} + b^s \cdot \nabla^s v - \operatorname{div}^s(D^s \nabla^s v) = \kappa \left(\frac{\alpha u}{1 + \beta u} - v \right) \quad \text{on } (0, \zeta) \times \partial\Omega_s. \quad (4.10)$$

To balance the mass of the system, we shall impose the right hand side of (4.10) as Neumann boundary data for u on the skeleton $\partial\Omega_s$.

$$-D \nabla u \cdot n = \kappa \left(\frac{\alpha u}{1 + \beta u} - v \right) \quad \text{on } (0, \zeta) \times \partial\Omega_s \quad (4.11)$$

The above system (4.9)-(4.11) is also supplemented with initial data. Our goal is to study the homogenization problem in the strong convection regime. So, we shall parabolically scale the system (4.9)-(4.11) i.e., by making the following change of variables: $(\tau, y) \rightarrow (\varepsilon^{-2}t, \varepsilon^{-1}x)$. The resulting adimensionalized coupled convection diffusion reaction equations for the new unknowns $u_\varepsilon(t, x) = u(\tau, y)$ and $v_\varepsilon(t, x) = v(\tau, y)$ are given by

$$\frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) = 0 \quad \text{in } (0, T) \times \Omega_\varepsilon \quad (4.12)$$

$$-\frac{D_\varepsilon}{\varepsilon} \nabla u_\varepsilon \cdot n = \frac{\partial v_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon - \operatorname{div}^s(D_\varepsilon^s \nabla^s v_\varepsilon) = \frac{\kappa}{\varepsilon^2} \left(\frac{\alpha u_\varepsilon}{1 + \beta u_\varepsilon} - v_\varepsilon \right) \quad \text{on } (0, T) \times \partial\Omega_\varepsilon \quad (4.13)$$

$$u_\varepsilon(0, x) = u^{in}(x) \quad \text{in } \Omega_\varepsilon, \quad v_\varepsilon(0, x) = v^{in}(x) \quad \text{on } \partial\Omega_\varepsilon \quad (4.14)$$

for some final time $T = \varepsilon^2 \zeta$. As $\zeta = \mathcal{O}(\varepsilon^{-2})$, the final time T is indeed of $\mathcal{O}(1)$. The initial data are chosen such that $u^{in}(x) \in L^2(\mathbb{R}^d)$ and $v^{in}(x) \in H^1(\mathbb{R}^d)$ (so that its trace is well-defined on $\partial\Omega_\varepsilon$). Remark that the coefficients in (4.12)-(4.13) are all ε -periodic with the following notations: $D_\varepsilon(x) = D(x/\varepsilon)$, $D_\varepsilon^s(x) = D^s(x/\varepsilon)$, $b_\varepsilon(x) = b(x/\varepsilon)$ and $b_\varepsilon^s(x) = b^s(x/\varepsilon)$.

4.4 Maximum principles and a priori estimates

We use the standard notations $h^+ = \max(0, h)$ and $h^- = \min(0, h)$. Recall that the function $f(u) = \alpha u / (1 + \beta u)$ is one to one and increasing from \mathbb{R}^+ to $[0, \alpha/\beta]$. Although the function $f(u)$ is not defined for $u = -1/\beta$, and since we are interested only in non negative values of u , we can modify and mollify $f(u)$ as we wish for $u < 0$ so that it is an increasing function on \mathbb{R} and all computations below make sense for negative values of u . Next, we give a result in the spirit of proving some maximum principles for (4.12)-(4.14). This result is analogous to Proposition 3.5.1 of Chapter 3. The objective of the next result is to assert that the solution $(u_\varepsilon, v_\varepsilon)$ to (4.12)-(4.13) remains non negative and bounded if one prescribes non negative and bounded initial data (u^{in}, v^{in}) in (4.14).

Proposition 4.4.1. *Let $(u_\varepsilon, v_\varepsilon)$ be a weak solution of (4.12)-(4.14). Assume that the initial data (u^{in}, v^{in}) satisfy $0 \leq u^{in} \leq M_u$, $0 \leq v^{in} \leq M_v$ for some positive constants M_u and M_v (without loss of generality consider $f(M_u) < M_v$).*

If $M_v < \alpha/\beta$, then

$$\begin{cases} 0 \leq u_\varepsilon(t, x) \leq m_u = f^{-1}(M_v) & \text{for } (t, x) \in (0, T) \times \Omega_\varepsilon, \\ 0 \leq v_\varepsilon(t, x) \leq M_v & \text{for } (t, x) \in (0, T) \times \partial\Omega_\varepsilon. \end{cases} \quad (4.15)$$

If $M_v \geq \alpha/\beta$, then there exist three positive constants τ , $M(\tau)$ and $\tilde{M}_v < \alpha/\beta$, independent of ε , such that

$$\begin{cases} 0 \leq u_\varepsilon(t, x) \leq M(\tau) & \text{for } (t, x) \in (0, \varepsilon^2\tau) \times \Omega_\varepsilon, \\ 0 \leq v_\varepsilon(t, x) \leq M_v & \text{for } (t, x) \in (0, \varepsilon^2\tau) \times \partial\Omega_\varepsilon, \end{cases} \quad (4.16)$$

and

$$\begin{cases} 0 \leq u_\varepsilon(t, x) \leq \tilde{m}_u = f^{-1}(\tilde{M}_v) & \text{for } (t, x) \in (\varepsilon^2\tau, T) \times \Omega_\varepsilon, \\ 0 \leq v_\varepsilon(t, x) \leq \tilde{M}_v & \text{for } (t, x) \in (\varepsilon^2\tau, T) \times \partial\Omega_\varepsilon. \end{cases} \quad (4.17)$$

Proof. As was done in the proof of Proposition 3.5.1, we shall be using a variational approach. To begin with, we prove that the solutions remain non negative for non negative initial data. Let us consider $(f(u_\varepsilon)^-, \varepsilon v_\varepsilon^-)$ as test functions in the variational formulation of (4.12)-(4.14).

$$\begin{aligned} & \int_0^T \frac{d}{dt} \int_{\Omega_\varepsilon} F(u_\varepsilon^-) dx dt + \frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla F(u_\varepsilon^-) dx dt - \int_0^T \int_{\Omega_\varepsilon} \operatorname{div} (D_\varepsilon \nabla u_\varepsilon) f(u_\varepsilon)^- dx dt \\ & + \frac{\varepsilon}{2} \int_0^T \frac{d}{dt} \int_{\partial\Omega_\varepsilon} |v_\varepsilon^-|^2 d\sigma(x) dt + \frac{\varepsilon}{2} \int_0^T \int_{\partial\Omega_\varepsilon} b_\varepsilon^s \cdot \nabla^s |v_\varepsilon^-|^2 d\sigma(x) dt \\ & - \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \operatorname{div}^s (D_\varepsilon^s \nabla^s v_\varepsilon) v_\varepsilon^- d\sigma(x) dt - \frac{\kappa}{\varepsilon} \int_0^T \int_{\partial\Omega_\varepsilon} [f(u_\varepsilon) - v_\varepsilon] v_\varepsilon^- d\sigma(x) dt = 0 \end{aligned} \quad (4.18)$$

where f and its primitive F are defined by (4.2) and (4.3) respectively. The divergence free assumption on the velocity fields b, b^s and the non-penetrating boundary conditions for b on the porous skeleton result in the vanishing of the convective terms in the variational formulation (4.18). Thus, we get

$$\int_{\Omega_\varepsilon} F(u_\varepsilon^-)(T) dx + \frac{\varepsilon}{2} \int_{\partial\Omega_\varepsilon} |v_\varepsilon^- (T)|^2 d\sigma(x) + \int_0^T \int_{\Omega_\varepsilon} f'(u_\varepsilon^-) D_\varepsilon \nabla u_\varepsilon^- \cdot \nabla u_\varepsilon^- dx dt$$

$$\begin{aligned}
& +\varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon^- \cdot \nabla^s v_\varepsilon^- d\sigma(x) dt + \frac{\kappa}{\varepsilon} \int_0^T \int_{\partial\Omega_\varepsilon} \left(f(u_\varepsilon) - v_\varepsilon \right) \left(f(u_\varepsilon)^- - v_\varepsilon^- \right) d\sigma(x) dt \\
& = \int_{\Omega_\varepsilon} F(u_\varepsilon^-)(0) dx + \frac{\varepsilon}{2} \int_{\partial\Omega_\varepsilon} |v_\varepsilon^-(0)|^2 d\sigma(x)
\end{aligned} \tag{4.19}$$

The function $h \rightarrow h^-$ is monotone and we know that $f'(u) > 0$. So, each one of the terms on the left hand side of (4.19) are positive. The assumption of the non negative initial data implies that the right hand side of (4.19) vanishes thus resulting in

$$u_\varepsilon^-(t, x) = 0 \quad \text{and} \quad v_\varepsilon^-(t, x) = 0 \quad \text{for all times } t \in (0, T]. \tag{4.20}$$

Next, we show that the solutions stay bounded from above if we start with a bounded initial data. The boundedness property of f adds an additional difficulty prompting us to consider two cases as below.

Case I. Assume $M_v < \alpha/\beta$ so we can define $m_u = f^{-1}(M_v) > M_u$.

We choose $((f(u_\varepsilon) - M_v)^+, \varepsilon(v_\varepsilon - M_v)^+)$ as test functions in the variational formulation of (4.12)-(4.14). Introducing the primitive function \mathcal{F} such that $\mathcal{F}'(u) = (f(u) - M_v)^+$ and $\mathcal{F}(0) = 0$, we get

$$\begin{aligned}
& \int_{\Omega_\varepsilon} \mathcal{F}(u_\varepsilon)(T) dx + \frac{\varepsilon}{2} \int_{\partial\Omega_\varepsilon} |(v_\varepsilon - M_v)^+|^2 d\sigma(x) + \int_0^T \int_{\Omega_\varepsilon} f'(u_\varepsilon) D_\varepsilon \nabla(u_\varepsilon - m_u)^+ \cdot \nabla(u_\varepsilon - m_u)^+ dx dt \\
& + \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s (v_\varepsilon - M_v)^+ \cdot \nabla^s (v_\varepsilon - M_v)^+ d\sigma(x) dt \\
& + \frac{\kappa}{\varepsilon} \int_0^T \int_{\partial\Omega_\varepsilon} \left((f(u_\varepsilon) - M_v) - (v_\varepsilon - M_v) \right) \left((f(u_\varepsilon) - M_v)^+ - (v_\varepsilon - M_v)^+ \right) d\sigma(x) dt \\
& = \int_{\Omega_\varepsilon} \mathcal{F}(u^{in}) dx + \frac{\varepsilon}{2} \int_{\partial\Omega_\varepsilon} ((v^{in} - M_v)^+)^2 d\sigma(x),
\end{aligned} \tag{4.21}$$

because $\nabla(f(u_\varepsilon) - M_v)^+ = f'(u_\varepsilon) \nabla(u_\varepsilon - m_u)^+$. The upper bound on the initial data implies that the right hand side in (4.21) vanishes. The left hand side is non-negative because $h \rightarrow h^+$ is monotone and $f'(u_\varepsilon) \geq 0$. Since $\mathcal{F}(u) = 0$ if and only if $u \leq m_u$, we deduce (4.16) that $u_\varepsilon \leq m_u$ and $v_\varepsilon \leq M_v$.

Case II. Assume $M_v \geq \alpha/\beta$.

The argument in Case I fails here because $f^{-1}(M_v)$ is not well defined. The idea is to first prove that there exists $\tau > 0$ such that, after a short time $\varepsilon^2\tau$, the solution v_ε reduces in magnitude and is uniformly smaller than α/β . Then by taking $\varepsilon^2\tau$ as a new initial time we can repeat the analysis of Case I. Whatever the value of u_ε , equation (4.13) implies the following inequality on the boundary $\partial\Omega_\varepsilon$

$$\frac{\partial v_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon - \operatorname{div}^s (D_\varepsilon^s \nabla^s v_\varepsilon) \leq \frac{\kappa}{\varepsilon^2} \left(\frac{\alpha}{\beta} - v_\varepsilon \right). \tag{4.22}$$

Choosing $q_\varepsilon = \left(v_\varepsilon - \frac{\alpha}{\beta} \right) \exp(t\kappa/\varepsilon^2)$ we get

$$\frac{\partial q_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s q_\varepsilon - \operatorname{div}^s (D_\varepsilon^s \nabla^s q_\varepsilon) \leq 0$$

with the initial data

$$q_\varepsilon(0) = v^{in} - \frac{\alpha}{\beta}.$$

Then, the maximum principle implies (see [143] for details)

$$q_\varepsilon(t) \leq \max_{x \in \partial\Omega_\varepsilon} q_\varepsilon(0) \leq M_v - \frac{\alpha}{\beta},$$

which yields the following upper bound

$$v_\varepsilon(t) \leq \exp(-t\kappa/\varepsilon^2)M_v + \left(1 - \exp(-t\kappa/\varepsilon^2)\right)\frac{\alpha}{\beta}. \quad (4.23)$$

Unfortunately (4.23) is too crude a bound which cannot reduce the initial bound M_v to a number smaller than α/β . At least, (4.23) yields $v_\varepsilon(t) \leq M_v$. We are going to use this upper bound in the equation for u_ε in order to improve (4.23).

Equations (4.12) and (4.13) give the following equation for u_ε

$$\begin{cases} \frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon}b_\varepsilon \cdot \nabla u_\varepsilon - \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) = 0 & \text{in } \Omega_\varepsilon, \\ -\frac{D_\varepsilon \nabla u_\varepsilon \cdot n}{\varepsilon} = \frac{\kappa}{\varepsilon^2} \left(\frac{\alpha u_\varepsilon}{1 + \beta u_\varepsilon} - v_\varepsilon \right) = \frac{\kappa}{\varepsilon^2} g_\varepsilon & \text{on } \partial\Omega_\varepsilon, \end{cases} \quad (4.24)$$

with g_ε satisfying, thanks to (4.23), the bound $|g_\varepsilon| \leq M_v$. Let us introduce an auxiliary problem in the unit cell

$$\begin{cases} b(y) \cdot \nabla_y \Psi - \operatorname{div}_y(D(y) \nabla_y \Psi) = \kappa M_v |\partial\Sigma^0|/|Y^0| & \text{in } Y^0, \\ -D(y) \nabla_y \Psi \cdot n = \kappa M_v & \text{on } \partial\Sigma^0, \\ y \rightarrow \Psi(y) & \text{is } Y\text{-periodic,} \end{cases} \quad (4.25)$$

where the compatibility condition for the existence and uniqueness (up to an additive constant) of Ψ is satisfied. The scaled function $\Psi_\varepsilon(x) = \Psi(x/\varepsilon)$ satisfies

$$\begin{cases} \frac{1}{\varepsilon}b_\varepsilon \cdot \nabla \Psi_\varepsilon - \operatorname{div}(D_\varepsilon \nabla \Psi_\varepsilon) = \frac{\kappa M_v}{\varepsilon^2} |\partial\Sigma^0|/|Y^0| & \text{in } \Omega_\varepsilon, \\ -\frac{1}{\varepsilon}D_\varepsilon \nabla \Psi_\varepsilon \cdot n = \frac{\kappa M_v}{\varepsilon^2} & \text{on } \partial\Omega_\varepsilon. \end{cases} \quad (4.26)$$

Let us define a function

$$p_\varepsilon = \Psi_\varepsilon + u_\varepsilon - \left(\frac{\kappa M_v}{\varepsilon^2} |\partial\Sigma^0|/|Y^0| \right) t \quad (4.27)$$

Then, p_ε satisfies

$$\begin{cases} \frac{\partial p_\varepsilon}{\partial t} + \frac{1}{\varepsilon}b_\varepsilon \cdot \nabla p_\varepsilon - \operatorname{div}(D_\varepsilon \nabla p_\varepsilon) = 0 & \text{in } (0, T) \times \Omega_\varepsilon, \\ -\frac{1}{\varepsilon}D_\varepsilon \nabla p_\varepsilon \cdot n = \frac{\kappa}{\varepsilon^2} (g_\varepsilon + M_v) \geq 0 & \text{on } (0, T) \times \partial\Omega_\varepsilon, \\ p_\varepsilon(0, x) = \Psi_\varepsilon(x) + u^{in}(x) & \text{in } \Omega_\varepsilon. \end{cases} \quad (4.28)$$

Then, the maximum principle yields (again see [143] if necessary)

$$p_\varepsilon(t) \leq \max_{\Omega_\varepsilon} (\Psi_\varepsilon + u^{in}) \leq M_u + \|\Psi\|_{L^\infty(Y^0)}. \quad (4.29)$$

From the definition (4.27) of p_ε we deduce

$$u_\varepsilon(t) \leq M_u + 2\|\Psi\|_{L^\infty(Y^0)} + \frac{\kappa M_v}{\varepsilon^2} |\partial\Sigma^0|/|Y^0|t, \quad (4.30)$$

which implies that, for any $\tau > 0$, we have

$$\max_{0 < t < \varepsilon^2\tau} u_\varepsilon(t) \leq M(\tau) = M_u + 2\|\Psi\|_{L^\infty(Y^0)} + \kappa M_v |\partial\Sigma^0|/|Y^0|\tau, \quad (4.31)$$

where $M(\tau)$ does not depend on ε and is an affine function of τ . Hence

$$\max_{0 < t < \varepsilon^2\tau} f(u_\varepsilon(t)) \leq f(M(\tau)) = \frac{\alpha M(\tau)}{1 + \beta M(\tau)} < \frac{\alpha}{\beta} \quad (4.32)$$

and (4.22) can be improved as

$$\frac{\partial v_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^S \cdot \nabla^S v_\varepsilon - \operatorname{div}^S (D_\varepsilon^S \nabla^S v_\varepsilon) \leq \frac{\kappa}{\varepsilon^2} (f(M(\tau)) - v_\varepsilon) \quad \text{for } 0 < t < \varepsilon^2\tau.$$

The same argument leading to (4.23) now gives that, for any $\tau > 0$ and $0 < t < \varepsilon^2\tau$,

$$v_\varepsilon(t) \leq \exp(-\kappa\tau)M_v + (1 - \exp(-\kappa\tau))f(M(\tau)), \quad (4.33)$$

where $f(M(\tau)) < \frac{\alpha}{\beta} - \frac{C}{\tau}$ for some positive constant $C > 0$. Thus, choosing τ large enough, we deduce that there exists \tilde{M}_v (equal to the right hand side of (4.33)) which does not depend on ε such that

$$\max_{0 < t < \varepsilon^2\tau} v_\varepsilon(t) \leq \tilde{M}_v < \frac{\alpha}{\beta}. \quad (4.34)$$

Choosing $\tilde{M}_u = M(\tau)$, we obviously have $f(\tilde{M}_u) < \tilde{M}_v$ and we can repeat the argument of Case I with the new initial time $\varepsilon^2\tau$. \square

Proposition 4.4.1 implied that the solutions to (4.12)-(4.14) are bounded in the L^∞ -norm. This information shall come in handy while deriving a priori estimates on the solution $(u_\varepsilon, v_\varepsilon)$. Next, we state a lemma that gives the a priori estimates on the solution to our mesoscopic model.

Lemma 4.4.2. *Let $(u_\varepsilon, v_\varepsilon)$ be a weak solution of (4.12)-(4.14) and the initial data (u^{in}, v^{in}) be such that $0 \leq u^{in} \leq M_u$, $0 \leq v^{in} \leq M_v$. There exists a constant C that depends on M_u and M_v but not on ε such that*

$$\begin{aligned} & \|u_\varepsilon\|_{L^\infty((0,T);L^2(\Omega_\varepsilon))} + \sqrt{\varepsilon}\|v_\varepsilon\|_{L^\infty((0,T);L^2(\partial\Omega_\varepsilon))} \\ & + \|\nabla u_\varepsilon\|_{L^2((0,T)\times\Omega_\varepsilon)} + \sqrt{\varepsilon}\|\nabla^s v_\varepsilon\|_{L^2((0,T)\times\partial\Omega_\varepsilon)} \\ & + \sqrt{\varepsilon}\|w_\varepsilon\|_{L^\infty((0,T);L^2(\partial\Omega_\varepsilon))} \leq C \left(\|u^{in}\|_{L^2(\mathbb{R}^d)} + \|v^{in}\|_{H^1(\mathbb{R}^d)} \right), \end{aligned} \quad (4.35)$$

where $w_\varepsilon = \varepsilon^{-1} \left(\frac{\alpha u_\varepsilon}{1 + \beta u_\varepsilon} - v_\varepsilon \right)$.

Proof. To obtain an energy equality we multiply (4.12) by $f(u_\varepsilon)$ and integrate over Ω_ε

$$\frac{d}{dt} \int_{\Omega_\varepsilon} F(u_\varepsilon) dx + \int_{\Omega_\varepsilon} f'(u_\varepsilon) D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon dx + \frac{\kappa}{\varepsilon} \int_{\partial\Omega_\varepsilon} (f(u_\varepsilon) - v_\varepsilon) f(u_\varepsilon) d\sigma(x) = 0,$$

where F is the primitive of f , defined by (4.3), which satisfies $F(u) \geq 0$ for $u \geq 0$. We next multiply (4.13) by $\varepsilon v_\varepsilon$ and integrate over $\partial\Omega_\varepsilon$

$$\frac{\varepsilon}{2} \frac{d}{dt} \int_{\partial\Omega_\varepsilon} |v_\varepsilon|^2 d\sigma(x) + \varepsilon \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s v_\varepsilon d\sigma(x) - \frac{\kappa}{\varepsilon} \int_{\partial\Omega_\varepsilon} (f(u_\varepsilon) - v_\varepsilon) v_\varepsilon d\sigma(x) = 0.$$

Adding the above two expressions leads to the following energy equality

$$\begin{aligned} & \frac{d}{dt} \int_{\Omega_\varepsilon} F(u_\varepsilon) dx + \frac{\varepsilon}{2} \frac{d}{dt} \int_{\partial\Omega_\varepsilon} |v_\varepsilon|^2 d\sigma(x) + \int_{\Omega_\varepsilon} f'(u_\varepsilon) D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon dx \\ & + \varepsilon \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s v_\varepsilon d\sigma(x) + \frac{\kappa}{\varepsilon} \int_{\partial\Omega_\varepsilon} (f(u_\varepsilon) - v_\varepsilon)^2 d\sigma(x) = 0. \end{aligned} \quad (4.36)$$

Recalling that, because of the maximum principle of Proposition 4.4.1, $F(u_\varepsilon) \geq 0$ and $f'(u_\varepsilon) \geq 0$, and integrating over time yields

$$\begin{aligned} & \|F(u_\varepsilon)\|_{L^\infty((0,T);L^1(\Omega_\varepsilon))} + \varepsilon \|v_\varepsilon\|_{L^\infty((0,T);L^2(\partial\Omega_\varepsilon))}^2 + \varepsilon \left\| \frac{1}{\varepsilon} (f(u_\varepsilon) - v_\varepsilon) \right\|_{L^2(\partial\Omega_\varepsilon \times (0,T))}^2 \\ & + \left\| \sqrt{f'(u_\varepsilon)} \nabla u_\varepsilon \right\|_{L^2(\Omega_\varepsilon \times (0,T))}^2 + \varepsilon \|\nabla^s v_\varepsilon\|_{L^2(\partial\Omega_\varepsilon \times (0,T))}^2 \leq C \left(\|F(u^{in})\|_{L^1(\mathbb{R}^d)} + \|v^{in}\|_{H^1(\mathbb{R}^d)}^2 \right) \end{aligned} \quad (4.37)$$

A second-order Taylor expansion at 0 yields $F(u) = \frac{1}{2}u^2 f'(c)$ for some $c \in (0, u)$. By the maximum principle we have $0 \leq u_\varepsilon \leq M$ so that

$$0 < \frac{\alpha}{1 + \beta M} \leq f'(u_\varepsilon) \leq \alpha, \quad (4.38)$$

and $\|F(u^{in})\|_{L^1(\mathbb{R}^d)} \leq C \|u^{in}\|_{L^2(\mathbb{R}^d)}^2$ while

$$\|F(u_\varepsilon)\|_{L^\infty((0,T);L^1(\Omega_\varepsilon))} + \left\| \sqrt{f'(u_\varepsilon)} \nabla u_\varepsilon \right\|_{L^2(\Omega_\varepsilon \times (0,T))}^2 \geq C \left(\|u_\varepsilon\|_{L^\infty((0,T);L^2(\Omega_\varepsilon))}^2 + \|\nabla u_\varepsilon\|_{L^2(\Omega_\varepsilon \times (0,T))}^2 \right) \quad (4.39)$$

from which we deduce (4.35). \square

4.5 Existence and uniqueness

Establishing the wellposedness of the coupled system (4.12)-(4.14) follows by the arguments of the finite dimensional Galerkin approximations [110], [114], [115], [84]. We shall be taking some cues from [127] where an adsorption/desorption model is studied in a different geometric and chemical setting. The method of finite Galerkin approximations, as the name suggests, is to construct finite dimensional approximations to the solution. After constructing the finite dimensional approximations, we shall tend the dimensions of the approximation spaces to infinity hoping to find a limit. The next step shall be to show that the limit does exist. The final step would be to prove that the limit is, indeed, the solution that we are looking for. The presence of the nonlinear terms in (4.12)-(4.14) dictate the need for strong compactness type results in order to pass to the limit. Additional difficulty arises due to the unbounded nature of our porous domain Ω_ε as the Rellich's theorem doesn't apply. So we shall construct a sequence $\{u_\varepsilon^{N,A}\}$ of finite dimensional approximations to the solution where A is the size of a bounded cube in \mathbb{R}^d and N is the dimension of the finite dimensional approximation space. As a first step, we

shall keep A fixed and prove that $u_\varepsilon^{N,A}$ attains a limit u_ε^A as $N \rightarrow \infty$. To this effect, we shall derive a priori estimates on the time derivative of the approximate solutions in order to apply Aubin's lemma [31], [114]. Our next step would be to consider the sequence $\{u_\varepsilon^A\}$ and prove that it is relatively compact in $L^2((0, T) \times \Omega_\varepsilon)$. As the ε -periodic porous medium Ω_ε that we are considering is unbounded, we need to prove a localization result in the following sense: for a given $\delta > 0$, we can find a cube $Q_{R(\delta)} =] - R(\delta), +R(\delta)[^d \subset \mathbb{R}^d$ such that the L^2 -norm of u_ε^A is inferior to δ outside the cube $Q_{R(\delta)}$ for every $A > R(\delta)$. After obtaining the compactness of the sequence of approximate solutions, we pass to the limit in the variational formulation as $A \rightarrow \infty$. Thus, we will be able to prove the wellposedness result for (4.12)-(4.14). Proposition 4.5.1 states this result on existence and uniqueness of the solution.

The limits considered in this section are $N \rightarrow \infty$ and $A \rightarrow \infty$ where N is the dimension of the finite dimensional approximation space and A is the size of a bounded cube in \mathbb{R}^d . In the present section the scale parameter ε is fixed. The compactness is obtained in a fixed frame of reference. Section 4.6 is concerned with the study of the limit $\varepsilon \rightarrow 0$ where we obtain compactness result in a moving frame of reference. It is to be noted that the results in this section and the next section may look similar at a passing glance. But both are, in essence, quite different.

Proposition 4.5.1. *Assume that the initial data (u^{in}, v^{in}) belong to the space $L^2(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d) \times H^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ and are non negative. For any given $\varepsilon > 0$, there exists a unique solution $(u_\varepsilon, v_\varepsilon)$ of (4.12)-(4.14) in the energy space, namely*

$$u_\varepsilon \in L^\infty((0, T); L^2(\Omega_\varepsilon)), \quad \nabla u_\varepsilon \in L^2((0, T) \times \Omega_\varepsilon),$$

and

$$v_\varepsilon \in L^\infty((0, T); L^2(\partial\Omega_\varepsilon)), \quad \nabla^s v_\varepsilon \in L^2((0, T) \times \partial\Omega_\varepsilon).$$

Before we give the proof for the Proposition 4.5.1, we shall prepare the ground work for the proof. To begin with, we shall adopt an approach from (Chapter 1, Section 6 of [114]) in the context of proving existence of solutions for unsteady Navier-Stokes equations. Let us consider the following spectral problem

$$\begin{cases} -\Delta\varphi + \varphi = \lambda\varphi & \text{in } \Omega_\varepsilon \cap Q_A \\ -\nabla\varphi \cdot n = 0 & \text{on } \partial\Omega_\varepsilon \cap Q_A \end{cases} \quad (4.40)$$

with periodic boundary conditions on ∂Q_A where $Q_A =] - A, +A[^d \subset \mathbb{R}^d$ is a cube. Associated with (4.40) we have a sequence of eigenfunctions $\{\varphi_j^\varepsilon\}_{j \in \mathbb{N}}$ corresponding to a sequence of eigenvalues $\{\lambda_j\}_{j \in \mathbb{N}}$:

$$\int_{\Omega_\varepsilon \cap Q_A} (\nabla\varphi_j^\varepsilon \cdot \nabla\theta + \varphi_j^\varepsilon\theta) dx = \lambda_j \int_{\Omega_\varepsilon \cap Q_A} \varphi_j^\varepsilon\theta dx \quad \text{for } \theta \in H_{\#}^1(\Omega_\varepsilon \cap Q_A), \lambda_j > 0. \quad (4.41)$$

We shall be using $\{\varphi_j^\varepsilon\}_{j \in \mathbb{N}}$ as basis functions to construct finite dimensional approximation spaces for the bulk concentration u_ε . As done in (4.40) and (4.41), we shall be introducing another set of basis eigenfunctions with the help of Laplace Beltrami operator to approximate the surface concentration v_ε . Consider the sequence of eigenfunctions $\{\psi_j^\varepsilon\}_{j \in \mathbb{N}}$ corresponding to a sequence of eigenvalues $\{\nu_j\}_{j \in \mathbb{N}}$ obtained via

$$\int_{\partial\Omega_\varepsilon \cap Q_A} (\nabla^s\psi_j^\varepsilon \cdot \nabla^s\Theta + \psi_j^\varepsilon\Theta) d\sigma(x) = \nu_j \int_{\partial\Omega_\varepsilon \cap Q_A} \psi_j^\varepsilon\Theta d\sigma(x) \quad \text{for } \Theta \in H_{\#}^1(\partial\Omega_\varepsilon \cap Q_A), \nu_j > 0. \quad (4.42)$$

Let us consider the following finite dimensional subspaces of $H^1(\Omega_\varepsilon \cap Q_A)$

$$D_\varepsilon^N = \text{span}\{\varphi_1^\varepsilon, \varphi_2^\varepsilon, \dots, \varphi_N^\varepsilon\} \quad (4.43)$$

and that of $H^1(\partial\Omega_\varepsilon \cap Q_A)$

$$B_\varepsilon^N = \text{span}\{\psi_1^\varepsilon, \psi_2^\varepsilon, \dots, \psi_N^\varepsilon\}. \quad (4.44)$$

Consider the L^2 projection P_N from $H^1(\Omega_\varepsilon \cap Q_A)$ to D_ε^N i.e.,

$$P_N w = \sum_{i=1}^N \left(\int_{\Omega_\varepsilon \cap Q_A} w \varphi_i^\varepsilon dx \right) \varphi_i^\varepsilon \quad \text{for } w \in H^1(\Omega_\varepsilon \cap Q_A). \quad (4.45)$$

Similarly consider the L^2 projection \mathcal{P}_N from $H^1(\partial\Omega_\varepsilon \cap Q_A)$ to B_ε^N i.e.,

$$\mathcal{P}_N w = \sum_{i=1}^N \left(\int_{\partial\Omega_\varepsilon \cap Q_A} w \psi_i^\varepsilon dx \right) \psi_i^\varepsilon \quad \text{for } w \in H^1(\Omega_\varepsilon \cap Q_A). \quad (4.46)$$

Thanks to the orthonormal property of φ_j^ε in L^2 , the operator norm of the projection P_N

$$\|P_N\|_{\mathcal{L}(H^1, D_\varepsilon^N)} = \inf_{w \neq 0} \frac{\|P_N w\|_{L^2}}{\|w\|_{H^1}} \leq 1. \quad (4.47)$$

We define $(u_\varepsilon^{N,A}(t), v_\varepsilon^{N,A}(t)) \in D_\varepsilon^N \times B_\varepsilon^N$ an approximate solution of order N to (4.12)-(4.14) posed in $(0, T) \times \Omega_\varepsilon \cap Q_A$ as

$$u_\varepsilon^{N,A}(t, x) = \sum_{j=1}^N c_j^{N,A}(t) \varphi_j^\varepsilon(x), \quad v_\varepsilon^{N,A}(t, x) = \sum_{j=1}^N d_j^{N,A}(t) \psi_j^\varepsilon(x), \quad (4.48)$$

$$\begin{aligned} & \int_{\Omega_\varepsilon \cap Q_A} \frac{\partial u_\varepsilon^{N,A}}{\partial t} u dx + \frac{1}{\varepsilon} \int_{\Omega_\varepsilon \cap Q_A} b_\varepsilon \cdot \nabla u_\varepsilon^{N,A} u dx + \int_{\Omega_\varepsilon \cap Q_A} D_\varepsilon \nabla u_\varepsilon^{N,A} \cdot \nabla u dx \\ & + \varepsilon \int_{\partial\Omega_\varepsilon \cap Q_A} \frac{\partial v_\varepsilon^{N,A}}{\partial t} v d\sigma(x) + \int_{\partial\Omega_\varepsilon \cap Q_A} b_\varepsilon^s \cdot \nabla^s v_\varepsilon^{N,A} v d\sigma(x) \\ & + \varepsilon \int_{\partial\Omega_\varepsilon \cap Q_A} D_\varepsilon^s \nabla^s v_\varepsilon^{N,A} \cdot \nabla^s v d\sigma(x) + \frac{\kappa}{\varepsilon} \int_{\partial\Omega_\varepsilon \cap Q_A} \left(f(u_\varepsilon^{N,A}) - v_\varepsilon^{N,A} \right) (u - v) d\sigma(x) = 0 \end{aligned} \quad (4.49)$$

for every $(u, v) \in D_\varepsilon^N \times B_\varepsilon^N$. The Fourier coefficients $c_j^{N,A}$ and $d_j^{N,A}$ in (4.48) do depend on the scaling parameter ε . As far as the purpose of the wellposedness result (Proposition 4.5.1) is concerned, we have a fixed $\varepsilon > 0$. Not to complicate the notation for the Fourier coefficients, we shall not mention explicitly their dependence on ε but shall admit that they do. The above Cauchy problem (4.49) is supplemented with initial data that are nothing but the projections of the initial data (u^{in}, v^{in}) on to the finite dimensional space:

$$u_\varepsilon^{N,A}(0) = P_N u^{in} \quad \text{and} \quad v_\varepsilon^{N,A}(0) = \mathcal{P}_N v^{in}. \quad (4.50)$$

Upon applying the classical Cauchy-Lipschitz-Picard theorem [66], the existence of a continuously differentiable solution $(c_j^{N,A}(t), d_j^{N,A}(t))$ on $[0, T_m]$ for the Cauchy problem (4.49) follows. The interval of existence $[0, T_m]$ as given by the Cauchy-Lipschitz-Picard theorem forces us to show that T_m is indeed T . The maximum principles that we obtained on the weak solutions

of (4.12)-(4.14) in Proposition 4.4.1 carry on to the approximate solutions $(u_\varepsilon^{N,A}, v_\varepsilon^{N,A})$ as well. Next, we shall state a lemma giving a priori estimates on the finite dimensional approximations $(u_\varepsilon^{N,A}, v_\varepsilon^{N,A})$. The proof follows line to line the same arguments as in Lemma 4.4.2 where we obtained the a priori estimates on the solution $(u_\varepsilon, v_\varepsilon)$. As usual variational approach is employed and the proof goes via the derivation of the energy estimate. So, we will simply state the result giving the a priori estimates on the approximations with no proof.

Lemma 4.5.2. *Let $\{(u_\varepsilon^{N,A}, v_\varepsilon^{N,A})\}_{N \in \mathbb{N}}$ be the finite dimensional approximations to the solution $(u_\varepsilon, v_\varepsilon)$ for (4.12)-(4.14) posed in $(0, T) \times \Omega_\varepsilon \cap Q_A$. Let us choose the initial data (u^{in}, v^{in}) to be non negative and bounded. Then, there exists a constant C depending on the bounds of the initial data but not on N such that*

$$\begin{aligned} & \|u_\varepsilon^{N,A}\|_{L^\infty((0,T);L^2(\Omega_\varepsilon \cap Q_A))} + \sqrt{\varepsilon} \|v_\varepsilon^{N,A}\|_{L^\infty((0,T);L^2(\partial\Omega_\varepsilon \cap Q_A))} \\ & + \|\nabla u_\varepsilon^{N,A}\|_{L^2((0,T) \times \Omega_\varepsilon \cap Q_A)} + \sqrt{\varepsilon} \|\nabla^s v_\varepsilon^{N,A}\|_{L^2((0,T) \times \partial\Omega_\varepsilon \cap Q_A)} \\ & + \sqrt{\varepsilon} \|w_\varepsilon^{N,A}\|_{L^\infty((0,T);L^2(\partial\Omega_\varepsilon \cap Q_A))} \leq C \left(\|u^{in}\|_{L^2(\mathbb{R}^d)} + \|v^{in}\|_{H^1(\mathbb{R}^d)} \right), \end{aligned} \quad (4.51)$$

$$\text{where } w_\varepsilon^{N,A} = \varepsilon^{-1} \left(\frac{\alpha u_\varepsilon^{N,A}}{1 + \beta u_\varepsilon^{N,A}} - v_\varepsilon^{N,A} \right).$$

The a priori estimates (4.51) imply that the energy associated with (4.49) is bounded and any possibility of a blow up of the solutions at time T_m doesn't arise. Thus the existence of solution $(c_j^{N,A}(t), d_j^{N,A}(t))$ on $[0, T]$ for any time $T < \infty$. As explained in the beginning of this section the idea here is to tend N towards infinity in order to arrive at a solution $(u_\varepsilon, v_\varepsilon)$ of (4.12)-(4.14). The estimates from (4.51) helps us extract convergent subsequences off $\{u_\varepsilon^{N,A}\}$ and $\{v_\varepsilon^{N,A}\}$. But the presence of the nonlinear term f in (4.49) demands strong compactness for $u_\varepsilon^{N,A}$. So, in addition to the a priori estimates (4.51), we shall look for an a priori estimate on the time derivative of $\{u_\varepsilon^{N,A}\}$. As only $u_\varepsilon^{N,A}$ appears as an argument in the nonlinear term of (4.49), we shall try to obtain a strong compactness result for $\{u_\varepsilon^{N,A}\}_{N \in \mathbb{N}}$. So let us take the test function v to be zero in (4.49). Then using the projection P_N , the Cauchy problem (4.49) can be rewritten as

$$\begin{aligned} & \int_{\Omega_\varepsilon \cap Q_A} \frac{\partial u_\varepsilon^{N,A}}{\partial t} P_N u \, dx + \frac{1}{\varepsilon} \int_{\Omega_\varepsilon \cap Q_A} b_\varepsilon \cdot \nabla u_\varepsilon^{N,A} P_N u \, dx \\ & + \int_{\Omega_\varepsilon \cap Q_A} D_\varepsilon \nabla u_\varepsilon^{N,A} \cdot \nabla P_N u \, dx + \frac{\kappa}{\varepsilon} \int_{\partial\Omega_\varepsilon \cap Q_A} \left(f(u_\varepsilon^{N,A}) - v_\varepsilon^{N,A} \right) P_N u \, d\sigma(x) = 0 \end{aligned}$$

for $u \in H^1(\Omega_\varepsilon)$ which implies

$$\begin{aligned} & \int_{\Omega_\varepsilon \cap Q_A} \frac{\partial P_N^* u_\varepsilon^{N,A}}{\partial t} u \, dx = -\frac{1}{\varepsilon} \int_{\Omega_\varepsilon \cap Q_A} b_\varepsilon \cdot \nabla u_\varepsilon^{N,A} P_N u \, dx \\ & - \int_{\Omega_\varepsilon \cap Q_A} D_\varepsilon \nabla u_\varepsilon^{N,A} \cdot \nabla P_N u \, dx - \frac{\kappa}{\varepsilon} \int_{\partial\Omega_\varepsilon \cap Q_A} \left(f(u_\varepsilon^{N,A}) - v_\varepsilon^{N,A} \right) P_N u \, d\sigma(x) \end{aligned} \quad (4.52)$$

Let us integrate (4.52) over the time interval $(0, T)$ leading to

$$\int_0^T \int_{\Omega_\varepsilon \cap Q_A} \frac{\partial P_N^* u_\varepsilon^{N,A}}{\partial t} u \, dx = -\frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon \cap Q_A} b_\varepsilon \cdot \nabla u_\varepsilon^{N,A} P_N u \, dx$$

$$-\int_0^T \int_{\Omega_\varepsilon \cap Q_A} D_\varepsilon \nabla u_\varepsilon^{N,A} \cdot \nabla P_N u \, dx - \frac{\kappa}{\varepsilon} \int_0^T \int_{\partial\Omega_\varepsilon \cap Q_A} \left(f(u_\varepsilon^{N,A}) - v_\varepsilon^{N,A} \right) P_N u \, d\sigma(x) \quad (4.53)$$

Using the hypothesis that $b, b^s \in L^\infty$ and that the nonlinear term has at most a linear growth i.e., $f(u_\varepsilon^{N,A}) \leq \alpha u_\varepsilon^{N,A}$, the projection P_N has bounded norm (4.47) and invoking the Trace theorem for the coupled term we can bound the right hand side of (4.53) as follows

$$\begin{aligned} & \left| \frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon \cap Q_A} b_\varepsilon \cdot \nabla u_\varepsilon^{N,A} P_N u \, dx \right| + \left| \int_0^T \int_{\Omega_\varepsilon \cap Q_A} D_\varepsilon \nabla u_\varepsilon^{N,A} \cdot \nabla P_N u \, dx \right| \\ & \quad + \left| \frac{\kappa}{\varepsilon} \int_0^T \int_{\partial\Omega_\varepsilon \cap Q_A} \left(f(u_\varepsilon^{N,A}) - v_\varepsilon^{N,A} \right) P_N u \right| \\ & \leq C_\varepsilon \|b\|_{L^\infty} \|\nabla u_\varepsilon^{N,A}\|_{L^2(\Omega_\varepsilon \cap Q_A)} \|u\|_{H^1(\Omega_\varepsilon \cap Q_A)} + C \|\nabla u_\varepsilon^{N,A}\|_{L^2(\Omega_\varepsilon \cap Q_A)} \|u\|_{H^1(\Omega_\varepsilon \cap Q_A)} \\ & \quad + \frac{\kappa}{\varepsilon^2} \left(\|u_\varepsilon^{N,A}\|_{H^1(\Omega_\varepsilon \cap Q_A)} + \sqrt{\varepsilon} \|v_\varepsilon^{N,A}\|_{L^2(\partial\Omega_\varepsilon \cap Q_A)} \right) \|u\|_{H^1(\Omega_\varepsilon \cap Q_A)} \end{aligned} \quad (4.54)$$

From (4.54) we have shown that, for every $u \in H^1(\Omega_\varepsilon \cap Q_A)$,

$$\left| \int_0^T \int_{\Omega_\varepsilon \cap Q_A} \frac{\partial P_N^* u_\varepsilon^{N,A}}{\partial t} u \, dx \right| \leq C. \quad (4.55)$$

From (4.55), we deduce that

$$\left\| \frac{\partial u_\varepsilon^{N,A}}{\partial t} \right\|_{L^2((0,T); H^{-1}(\Omega_\varepsilon \cap Q_A))} \leq C. \quad (4.56)$$

Now, we consider the a priori estimates from (4.51) and the estimate obtained on the first order time derivative (4.56). It follows from Aubin's lemma [31], [114] that $\{u_\varepsilon^{N,A}\}_{N \in \mathbb{N}}$ is relatively compact in $L^2((0,T) \times (\Omega_\varepsilon \cap Q_A))$. That is, there exists a $u_\varepsilon^A \in L^2((0,T) \times (\Omega_\varepsilon \cap Q_A))$ such that

$$\lim_{N \rightarrow \infty} \int_0^T \int_{\Omega_\varepsilon \cap Q_A} \left| u_\varepsilon^{N,A} - u_\varepsilon^A \right|^2 \, dx \, dt = 0. \quad (4.57)$$

Similarly we have the existence of $v_\varepsilon^A \in L^2((0,T) \times (\partial\Omega_\varepsilon \cap Q_A))$ such that

$$\lim_{N \rightarrow \infty} \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon \cap Q_A} \left| v_\varepsilon^{N,A} - v_\varepsilon^A \right|^2 \, dx \, dt = 0. \quad (4.58)$$

So far we have shown the compactness of $\{u_\varepsilon^{N,A}\}_{N \in \mathbb{N}}$ in a cube Q_A . Next we shall prove a localization result for $(u_\varepsilon^A, v_\varepsilon^A)$. This result is essential to prove compactness of the solution sequence $\{u_\varepsilon^{N,A}\}$ as our domain Ω_ε is unbounded.

Lemma 4.5.3. *Let $\{(u_\varepsilon^A, v_\varepsilon^A)\}$ be the limit of the approximate solutions $\{(u_\varepsilon^{N,A}, v_\varepsilon^{N,A})\}$ of (4.12)-(4.14) in the cube Q_A . Fix a final time $T < +\infty$. Then, for any $\delta > 0$, there exists $R(\delta) > 0$ such that, for all $A > R(\delta)$ and for any $t \in [0, T]$,*

$$\|u_\varepsilon^A(t, x)\|_{L^2(\Omega_\varepsilon \cap Q^c(R(\delta)))} \leq \delta \quad (4.59)$$

$$\sqrt{\varepsilon} \|v_\varepsilon^A(t, x)\|_{L^2(\partial\Omega_\varepsilon \cap Q^c(R(\delta)))} \leq \delta \quad (4.60)$$

where $Q_{R(\delta)}^c$ is the complementary of the cube $Q_{R(\delta)} =]-R(\delta), +R(\delta)[^d \subset \mathbb{R}^d$.

Proof. The proof will take into consideration the structure of (4.12)-(4.14) of which $(u_\varepsilon^{N,A}, v_\varepsilon^{N,A})$ is supposed to be a finite dimensional approximation of the solution. As the goal is to derive a localization result, let $\phi \in C^\infty(\mathbb{R})$ be a smooth cut-off function such that

$$0 \leq \phi(r) \leq 1, \phi = 0 \text{ for } r \leq 1, \phi = 1 \text{ for } r \geq 2.$$

For $x \in \mathbb{R}^d$, denote $\phi_R(x) = \phi(|x|/R)$ with $R \ll A$. Consider the variational formulation of (4.49) in the full domain with $(f(u_\varepsilon^A)\phi_R, \varepsilon v_\varepsilon^A \phi_R)$ as test functions. The choice of the test functions suggest that the cut-off function $\phi_R(x)$ appear as weight.

$$\begin{aligned} & \int_0^t \frac{d}{dt} \int_{\Omega_\varepsilon \cap Q_A} F(u_\varepsilon^A)(s, x) \phi_R(x) ds dx + \frac{1}{\varepsilon} \int_0^t \int_{\Omega_\varepsilon \cap Q_A} b_\varepsilon \cdot \nabla F(u_\varepsilon^A)(s, x) \phi_R(x) dx ds \\ & - \int_0^t \int_{\Omega_\varepsilon \cap Q_A} \operatorname{div} \left(D_\varepsilon \nabla u_\varepsilon^A(s, x) \right) f(u_\varepsilon^A)(s, x) \phi_R(x) dx ds + \frac{\varepsilon}{2} \int_0^t \frac{d}{dt} \int_{\partial \Omega_\varepsilon \cap Q_A} |v_\varepsilon^A(s, x)|^2 \phi_R(x) ds d\sigma(x) \\ & \quad + \frac{1}{2} \int_0^t \int_{\partial \Omega_\varepsilon \cap Q_A} b_\varepsilon^s \cdot \nabla^s |v_\varepsilon^A(s, x)|^2 \phi_R(x) ds d\sigma(x) \\ & \quad - \varepsilon \int_0^t \int_{\partial \Omega_\varepsilon \cap Q_A} \operatorname{div}^s \left(D_\varepsilon^s \nabla^s v_\varepsilon^A(s, x) \right) v_\varepsilon^A(s, x) \phi_R(x) d\sigma(x) ds \\ & \quad + \frac{\kappa}{\varepsilon} \int_0^t \int_{\partial \Omega_\varepsilon \cap Q_A} \left(f(u_\varepsilon^A) - v_\varepsilon^A \right)^2(s, x) \phi_R(x) d\sigma(x) ds = 0 \end{aligned}$$

Upon integration by parts, we arrive at

$$\begin{aligned} & \int_{\Omega_\varepsilon \cap Q_A} F(u_\varepsilon^A)(t, x) \phi_R(x) dx + \int_0^t \int_{\Omega_\varepsilon \cap Q_A} f'(u_\varepsilon^A)(s, x) D_\varepsilon \nabla u_\varepsilon^A(s, x) \cdot \nabla u_\varepsilon^A(s, x) \phi_R(x) dx ds \\ & + \frac{\varepsilon}{2} \int_{\partial \Omega_\varepsilon \cap Q_A} \phi_R(x) |v_\varepsilon^A(t, x)|^2 d\sigma(x) + \varepsilon \int_0^t \int_{\partial \Omega_\varepsilon \cap Q_A} D_\varepsilon^s \nabla^s v_\varepsilon^A(s, x) \cdot \nabla^s v_\varepsilon^A(s, x) \phi_R(x) d\sigma(x) ds \\ & \quad + \frac{\kappa}{\varepsilon} \int_0^t \int_{\partial \Omega_\varepsilon \cap Q_A} \left(f(u_\varepsilon^A) - v_\varepsilon^A \right)^2(s, x) \phi_R(x) d\sigma(x) ds \\ & = \int_{\Omega_\varepsilon \cap Q_A} F(u^{in}) \phi_R(x) dx + \frac{\varepsilon}{2} \int_{\partial \Omega_\varepsilon \cap Q_A} \phi_R(x) |v^{in}(x)|^2 d\sigma(x) \\ & \quad + \frac{1}{\varepsilon} \int_0^t \int_{\Omega_\varepsilon \cap Q_A} b_\varepsilon \cdot \nabla \phi_R(x) F(u_\varepsilon^A)(s, x) dx ds + \frac{1}{2} \int_0^t \int_{\partial \Omega_\varepsilon \cap Q_A} |v_\varepsilon^A(s, x)|^2 b_\varepsilon^s \cdot \nabla^s \phi_R(x) ds d\sigma(x) \end{aligned}$$

$$\begin{aligned}
& - \int_0^t \int_{\Omega_\varepsilon \cap Q_A} f(u_\varepsilon^A)(s, x) D_\varepsilon \nabla u_\varepsilon^A(s, x) \cdot \nabla \phi_R(x) dx ds \\
& - \varepsilon \int_0^t \int_{\partial \Omega_\varepsilon \cap Q_A} v_\varepsilon^A(s, x) D_\varepsilon^s \nabla^s v_\varepsilon^A(s, x) \cdot \nabla^s \phi_R(x) d\sigma(x) ds
\end{aligned} \tag{4.61}$$

To arrive at the result, we need to bound the right hand side terms in the relation (4.61). The first two terms in (4.61), involving the initial data (u^{in}, v^{in}) , tend to zero as R tends to ∞ . Now let us turn our attention to the last two terms in (4.61). Recall that $f(u_\varepsilon^A) \leq \alpha u_\varepsilon^A$. By definition of ϕ_R we have $\|\nabla \phi_R\|_{L^\infty(\Omega_\varepsilon)} \leq C/R$, so last two terms in (4.61) are bounded by

$$\begin{aligned}
& \frac{C}{R} \left(\|u_\varepsilon^A\|_{L^2((0,T) \times \Omega_\varepsilon \cap Q_A)} \|\nabla u_\varepsilon^A\|_{L^2((0,T) \times \Omega_\varepsilon \cap Q_A)} \right. \\
& \left. + \varepsilon \|v_\varepsilon^A\|_{L^2((0,T) \times \partial \Omega_\varepsilon \cap Q_A)} \|\nabla^s v_\varepsilon^A\|_{L^2((0,T) \times \partial \Omega_\varepsilon \cap Q_A)} \right) \leq \frac{C}{R}
\end{aligned} \tag{4.62}$$

by virtue of Lemma 4.5.2. Finally, the second and the third terms in (4.61). The primitive F has quadratic growth for a bounded u_ε^A which is guaranteed by the maximum principles. Next we invoke the a priori estimates from Lemma 4.5.2 which result in a bound similar to (4.62) for the second and third terms in (4.61). So, for any given $\delta > 0$, we can always choose a $R(\delta) \in \mathbb{R}$, large enough, such that we have, for any $t \in [0, T]$ and for all $A > R(\delta)$,

$$\|u_\varepsilon^A\|_{L^2(\Omega_\varepsilon \cap Q_{R(\delta)}^c)} \leq \delta \text{ and } \sqrt{\varepsilon} \|v_\varepsilon^A\|_{L^2(\partial \Omega_\varepsilon \cap Q_{R(\delta)}^c)} \leq \delta,$$

This observation is nothing but the assertions (4.59) and (4.60). \square

We have laid out enough ground work through Lemmata 4.5.2, 4.5.3 to prove that the compactness of the sequence $\{u_\varepsilon^A\}$.

Proposition 4.5.4. *There exists a subsequence, still denoted by A , such that*

$$\lim_{A \rightarrow \infty} \int_0^T \int_{\Omega_\varepsilon} |u_\varepsilon^A(t, x) - u_\varepsilon(t, x)| dx dt = 0 \tag{4.63}$$

Proof. As a consequence of the localization lemma 4.5.3, for a given $\delta > 0$, there exists a $R(\delta)$ such that, for all $A > R(\delta)$, we have

$$\left\| u_\varepsilon^A(t, x) - u_\varepsilon^A(t, x) \chi_{Q(R(\delta))} \right\|_{L^2((0,T) \times \Omega_\varepsilon)} \leq \frac{\delta}{2} \tag{4.64}$$

From (4.51) we have that $\{u_\varepsilon^A\}$ is relatively compact in $L^2((0, T) \times \Omega_\varepsilon \cap Q_A)$. Thus, by choosing big enough $R(\delta)$, if necessary, we have

$$\left\| u_\varepsilon^A(t, x) \chi_{Q(R(\delta))} - u_\varepsilon(t, x) \right\|_{L^2((0,T) \times \Omega_\varepsilon)} \leq \frac{\delta}{2} \tag{4.65}$$

Telescoping through the inequalities (4.64)-(4.65), we indeed arrive at (4.63). \square

Let us denote the limit of v_ε^A by v_ε obtained by the a priori estimates (4.51). It turns out that the solutions envisaged in Proposition 4.5.1 turn out to be the two limits $(u_\varepsilon, v_\varepsilon)$. Now, we shall give the proof of the Proposition 4.5.1.

Proof of Proposition 4.5.1. We have the strong compactness result for the sequence $u_\varepsilon^{N,A}$ from Proposition 4.5.4. Let us consider (4.49) and integrate it over time interval $(0, T)$ to arrive at

$$\begin{aligned} & \int_0^T \int_{\Omega_\varepsilon \cap Q_A} \frac{\partial u_\varepsilon^{N,A}}{\partial t} u \, dx \, dt + \frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon \cap Q_A} b_\varepsilon \cdot \nabla u_\varepsilon^{N,A} u \, dx \, dt + \int_0^T \int_{\Omega_\varepsilon \cap Q_A} D_\varepsilon \nabla u_\varepsilon^{N,A} \cdot \nabla u \, dx \, dt \\ & + \varepsilon \int_0^T \int_{\partial \Omega_\varepsilon \cap Q_A} \frac{\partial v_\varepsilon^{N,A}}{\partial t} v \, d\sigma(x) \, dt + \int_0^T \int_{\partial \Omega_\varepsilon \cap Q_A} b_\varepsilon^s \cdot \nabla^s v_\varepsilon^{N,A} v \, d\sigma(x) \, dt + \\ & \varepsilon \int_0^T \int_{\partial \Omega_\varepsilon \cap Q_A} D_\varepsilon^s \nabla^s v_\varepsilon^{N,A} \cdot \nabla^s v \, d\sigma(x) \, dt + \frac{\kappa}{\varepsilon} \int_0^T \int_{\partial \Omega_\varepsilon \cap Q_A} \left(f(u_\varepsilon^{N,A}) - v_\varepsilon^{N,A} \right) (u - v) \, d\sigma(x) \, dt = 0 \end{aligned} \quad (4.66)$$

Now we need to tend N and A towards infinity. Thanks to our compactness result, Proposition 4.5.4, we can pass to the limit in the variational formulation (4.66) as $N \rightarrow \infty$ and $A \rightarrow \infty$. The limit variational formulation that we arrive at shall be a variational formulation for (4.12)-(4.14) with the limit $(u_\varepsilon, v_\varepsilon)$ as the solution. Thus the existence of the solutions.

We are still left to prove the uniqueness of the solution. On the contrary, let us suppose that there are at least two solutions to our coupled convection diffusion reaction equations (4.12)-(4.14), say $u_{1,\varepsilon}$, $u_{2,\varepsilon}$ two bulk concentrations and $v_{1,\varepsilon}$, $v_{2,\varepsilon}$ two surface concentrations. Let us denote the differences by U_ε and V_ε respectively for bulk and surface concentrations. We shall write down the coupled equations satisfied by the differences $(U_\varepsilon, V_\varepsilon)$.

$$\frac{\partial U_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla U_\varepsilon - \operatorname{div} (D_\varepsilon \nabla U_\varepsilon) = 0 \text{ in } (0, T) \times \Omega_\varepsilon \quad (4.67)$$

$$\begin{aligned} -\frac{D_\varepsilon}{\varepsilon} \nabla U_\varepsilon \cdot n &= \frac{\partial V_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s V_\varepsilon - \operatorname{div}^s (D_\varepsilon^s \nabla^s V_\varepsilon) \\ &= \frac{\kappa}{\varepsilon^2} \left(\left(f(u_{1,\varepsilon}) - v_{1,\varepsilon} \right) - \left(f(u_{2,\varepsilon}) - v_{2,\varepsilon} \right) \right) \text{ on } (0, T) \times \partial \Omega_\varepsilon \end{aligned} \quad (4.68)$$

$$U_\varepsilon(0, x) = 0 \text{ in } \Omega_\varepsilon, \quad V_\varepsilon(0, x) = 0 \text{ on } \partial \Omega_\varepsilon \quad (4.69)$$

The initial data are zero by construction. This approach is very classical. The idea is to derive the energy estimate for the above system. To that effect, let us multiply (4.67) by U_ε followed by an integration over Ω_ε and multiply the second part of 4.68 by $\varepsilon V_\varepsilon$ followed by an integration over $\partial \Omega_\varepsilon$. The resulting expression is

$$\begin{aligned} & \frac{d}{dt} \int_{\Omega_\varepsilon} |U_\varepsilon|^2 \, dx + \int_{\Omega_\varepsilon} D_\varepsilon \nabla U_\varepsilon \cdot \nabla U_\varepsilon \, dx + \frac{d}{dt} \varepsilon \int_{\partial \Omega_\varepsilon} |V_\varepsilon|^2 \, d\sigma(x) + \varepsilon \int_{\partial \Omega_\varepsilon} D_\varepsilon^s \nabla^s V_\varepsilon \cdot \nabla^s V_\varepsilon \, d\sigma(x) + \\ & \frac{\kappa}{\varepsilon} \int_{\partial \Omega_\varepsilon} \left(\left(f(u_{1,\varepsilon}) - v_{1,\varepsilon} \right) - \left(f(u_{2,\varepsilon}) - v_{2,\varepsilon} \right) \right) (U_\varepsilon - V_\varepsilon) \, d\sigma(x) = 0 \end{aligned} \quad (4.70)$$

The term of interest in (4.70) is the coupled term.

$$\frac{\kappa}{\varepsilon} \int_{\partial \Omega_\varepsilon} \left(\left(f(u_{1,\varepsilon}) - v_{1,\varepsilon} \right) - \left(f(u_{2,\varepsilon}) - v_{2,\varepsilon} \right) \right) (U_\varepsilon - V_\varepsilon) \, d\sigma(x) = \frac{\kappa}{\varepsilon} \int_{\partial \Omega_\varepsilon} \left(f'(\bar{U}) U_\varepsilon - V_\varepsilon \right) (U_\varepsilon - V_\varepsilon) \, d\sigma(x) \quad (4.71)$$

for some $u_{1,\varepsilon}(t, x) \leq \bar{U}(t, x) \leq u_{2,\varepsilon}(t, x)$. As the first derivative of f is bounded, the coupled term (4.71) in the variational formulation (4.70) is can be bounded from above as

$$\left| \frac{\kappa}{\varepsilon} \int_{\partial\Omega_\varepsilon} \left((f(u_{1,\varepsilon}) - v_{1,\varepsilon}) - (f(u_{2,\varepsilon}) - v_{2,\varepsilon}) \right) (U_\varepsilon - V_\varepsilon) d\sigma(x) \right| \leq \frac{\kappa}{\varepsilon} \int_{\partial\Omega_\varepsilon} (|U_\varepsilon| + |V_\varepsilon|)^2 d\sigma(x) \quad (4.72)$$

Now let us integrate (4.70) over $(0, T)$. Considering the inequality (4.72) for the coupled term and a simple application of Young's inequality leads to

$$\begin{aligned} \int_{\Omega_\varepsilon} |U_\varepsilon(T, x)|^2 dx + \varepsilon \int_{\partial\Omega_\varepsilon} |V_\varepsilon(T, x)|^2 d\sigma(x) + \int_0^T \int_{\Omega_\varepsilon} D_\varepsilon \nabla U_\varepsilon \cdot \nabla U_\varepsilon dx dt + \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s V_\varepsilon \cdot \nabla^s V_\varepsilon d\sigma(x) dt \\ \leq \frac{3\kappa}{2\varepsilon} \int_0^T \int_{\partial\Omega_\varepsilon} U_\varepsilon^2(t, x) d\sigma(x) dt + \frac{3\kappa}{2\varepsilon} \int_0^T \int_{\partial\Omega_\varepsilon} V_\varepsilon^2(t, x) d\sigma(x) dt \end{aligned} \quad (4.73)$$

Thanks to the inequality (4.73). We can apply Gronwall's lemma to deduce that $U_\varepsilon(t, x) = 0$ and $V_\varepsilon(t, x) = 0$ for almost every (t, x) . Hence the unicity follows. \square

4.6 Localization in moving coordinates and compactness

Our objective is to find the effective behavior of our convection diffusion reaction model (4.12)-(4.14). This can be achieved, as explained in Chapter 2, by tending the heterogeneities' length scale ε to zero. As we are in the strong convection regime, we take cues from Section 2.6 to employ the method of two-scale convergence with drift. The a priori estimates of Lemma 4.4.2 allow us to extract weakly converging subsequences but they do not give any strong compactness for the sequence $(u_\varepsilon, v_\varepsilon)$ since a priori estimates on their time derivatives are lacking. Passing to the limit in system (4.12)-(4.14), which is nonlinear, requires some strong compactness. Furthermore, since Ω_ε is unbounded, Rellich theorem does not hold in Ω_ε and a localization result is thus required to get compactness. This is the goal of the results to follow for the rest of this section which culminate in Corollary 4.6.7. Their proof rely on the use of the equations (4.12)-(4.14). Similar results were obtained for a sequence of approximate solutions in Section 4.5 where we wished to pass to the limit when the dimension of the approximation spaces tends to infinity. In the regime $\varepsilon \rightarrow 0$, there is however one additional hurdle which is the large convective terms of order ε^{-1} . In order to compensate this large drift, following the lead of [121], we shall prove these compactness and localization results, not for the original sequence $(u_\varepsilon, v_\varepsilon)$, but for its counterpart defined in a moving frame of reference. For $\varphi_\varepsilon(t, x)$, let us define its counterpart in moving coordinates as

$$\widehat{\varphi}_\varepsilon(t, x) = \varphi_\varepsilon \left(t, x + \frac{b^*t}{\varepsilon} \right) \quad \text{and} \quad \check{\varphi}_\varepsilon(t, x) = \varphi_\varepsilon \left(t, x - \frac{b^*t}{\varepsilon} \right), \quad (4.74)$$

where b^* is the effective drift defined by (4.1). Of course, definition (4.74) is consistent with the notion of two-scale convergence with drift which is briefly recalled in Section 2.6 of Chapter 2. As we consider functions in moving coordinates, the underlying porous domain Ω_ε does move with the same velocity. Let us define

$$\widehat{\Omega}_\varepsilon(t) = \left\{ x + \frac{b^*t}{\varepsilon} : x \in \Omega_\varepsilon \right\}. \quad (4.75)$$

The following first lemma of this section gives the localization in space for the solution sequences in moving coordinates.

Lemma 4.6.1. *Let $(u_\varepsilon, v_\varepsilon)$ be the solution of (4.12)-(4.14). Fix a final time $T < +\infty$. Then, for any $\delta > 0$, there exists $R(\delta) > 0$ such that, for any $t \in [0, T]$,*

$$\left\| \widehat{u}_\varepsilon(t, x) \right\|_{L^2(\widehat{\Omega}_\varepsilon(t) \cap Q_{R(\delta)}^c)} \leq \delta, \quad \left\| \widehat{v}_\varepsilon(t, x) \right\|_{L^2(\partial \widehat{\Omega}_\varepsilon(t) \cap Q_{R(\delta)}^c)} \leq \delta,$$

where $Q_{R(\delta)}^c$ is the complementary of the cube $Q_{R(\delta)} =]-R(\delta), +R(\delta)[^d$ in \mathbb{R}^d .

Proof. We rely on an idea of [121], [24]. The proof runs almost similar to the proof of Lemma 4.5.3 except for the construction of the test functions. Attributing to the inevitable large drift, we shall take the test functions in the moving coordinates as defined in (4.74). Let $\phi \in C^\infty(\mathbb{R})$ be a smooth cut-off function such that

$$0 \leq \phi(r) \leq 1, \quad \phi = 0 \text{ for } r \leq 1, \quad \phi = 1 \text{ for } r \geq 2.$$

For $x \in \mathbb{R}^d$, denote $\phi_R(x) = \phi(|x|/R)$. Let us consider the variational formulation of (4.12)-(4.14) with test functions $(f(u_\varepsilon)\check{\phi}_R, \varepsilon v_\varepsilon \check{\phi}_R)$ where the $\check{\cdot}$ -notation is defined by (4.74). Upon integration by parts in time, the first bulk term is

$$\begin{aligned} \int_0^t \int_{\Omega_\varepsilon} \frac{\partial u_\varepsilon}{\partial t}(s, x) f(u_\varepsilon)(s, x) \check{\phi}_R(s, x) dx ds &= \frac{1}{\varepsilon} \int_0^t \int_{\Omega_\varepsilon} F(u_\varepsilon)(s, x) b^* \cdot \nabla \check{\phi}_R(s, x) dx ds \\ &+ \int_{\Omega_\varepsilon} F(u_\varepsilon)(t, x) \check{\phi}_R(t, x) dx - \int_{\Omega_\varepsilon} F(u^{in})(x) \phi_R(x) dx, \end{aligned}$$

while, by integration by parts in space, the convective term is

$$\frac{1}{\varepsilon} \int_0^t \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon f(u_\varepsilon) \check{\phi}_R dx ds = -\frac{1}{\varepsilon} \int_0^t \int_{\Omega_\varepsilon} F(u_\varepsilon) b_\varepsilon \cdot \nabla \check{\phi}_R dx ds,$$

and the diffusive term is

$$\begin{aligned} - \int_0^t \int_{\Omega_\varepsilon} \operatorname{div}(D_\varepsilon \nabla u_\varepsilon) f(u_\varepsilon) \check{\phi}_R dx ds &= \int_0^t \int_{\Omega_\varepsilon} f'(u_\varepsilon) D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon \check{\phi}_R dx ds \\ &+ \int_0^t \int_{\Omega_\varepsilon} f(u_\varepsilon) D_\varepsilon \nabla u_\varepsilon \cdot \nabla \check{\phi}_R dx ds + \frac{\kappa}{\varepsilon} \int_0^t \int_{\partial \Omega_\varepsilon} (f(u_\varepsilon) - v_\varepsilon) f(u_\varepsilon) \check{\phi}_R dx ds. \end{aligned}$$

On the other hand, the surface terms are

$$\begin{aligned} 2\varepsilon \int_0^t \int_{\partial \Omega_\varepsilon} \frac{\partial v_\varepsilon}{\partial t} \check{\phi}_R v_\varepsilon ds d\sigma(x) &= \int_0^t \int_{\partial \Omega_\varepsilon} b^* \cdot \nabla \check{\phi}_R |v_\varepsilon|^2 ds d\sigma(x) \\ &+ \varepsilon \int_{\partial \Omega_\varepsilon} \check{\phi}_R(t, x) |v_\varepsilon(t, x)|^2 d\sigma(x) - \varepsilon \int_{\partial \Omega_\varepsilon} \phi_R(x) |v^{in}(x)|^2 d\sigma(x), \\ 2 \int_0^t \int_{\partial \Omega_\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon v_\varepsilon \check{\phi}_R ds d\sigma(x) &= - \int_0^t \int_{\partial \Omega_\varepsilon} |v_\varepsilon|^2 b_\varepsilon^s \cdot \nabla^s \check{\phi}_R ds d\sigma(x), \end{aligned}$$

and

$$\begin{aligned} -\varepsilon \int_0^t \int_{\partial\Omega_\varepsilon} \operatorname{div}^s(D_\varepsilon^s \nabla^s v_\varepsilon) v_\varepsilon \check{\phi}_R d\sigma(x) ds &= \varepsilon \int_0^t \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s v_\varepsilon \check{\phi}_R d\sigma(x) ds \\ +\varepsilon \int_0^t \int_{\partial\Omega_\varepsilon} v_\varepsilon D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s \check{\phi}_R d\sigma(x) ds &- \frac{\kappa}{\varepsilon} \int_0^t \int_{\partial\Omega_\varepsilon} (f(u_\varepsilon) - v_\varepsilon) v_\varepsilon \check{\phi}_R d\sigma(x) ds. \end{aligned}$$

Adding these terms together yields

$$\begin{aligned} &\int_{\Omega_\varepsilon} F(u_\varepsilon)(t, x) \check{\phi}_R(t, x) dx + \int_0^t \int_{\Omega_\varepsilon} f'(u_\varepsilon) D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon \check{\phi}_R dx ds \\ &+ \frac{\varepsilon}{2} \int_{\partial\Omega_\varepsilon} |v_\varepsilon(t, x)|^2 \check{\phi}_R(t, x) d\sigma(x) + \varepsilon \int_0^t \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s v_\varepsilon \check{\phi}_R d\sigma(x) ds \\ &\quad + \frac{\kappa}{\varepsilon} \int_0^t \int_{\partial\Omega_\varepsilon} \check{\phi}_R (f(u_\varepsilon) - v_\varepsilon)^2 d\sigma(x) ds \\ &= - \int_0^t \int_{\Omega_\varepsilon} f(u_\varepsilon) D_\varepsilon \nabla u_\varepsilon \cdot \nabla \check{\phi}_R dx ds - \varepsilon \int_0^t \int_{\partial\Omega_\varepsilon} v_\varepsilon D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s \check{\phi}_R d\sigma(x) ds \end{aligned} \quad (4.76)$$

$$+ \frac{1}{\varepsilon} \int_0^t \int_{\Omega_\varepsilon} F(u_\varepsilon) (b_\varepsilon - b^*) \cdot \nabla \check{\phi}_R dx ds + \int_0^t \int_{\partial\Omega_\varepsilon} |v_\varepsilon|^2 (b_\varepsilon^s - b^*) \cdot \nabla^s \check{\phi}_R d\sigma(x) ds \quad (4.77)$$

$$+ \int_{\Omega_\varepsilon} F(u^{in})(x) \phi_R(x) dx + \frac{\varepsilon}{2} \int_{\partial\Omega_\varepsilon} \phi_R(x) |v^{in}(x)|^2 d\sigma(x). \quad (4.78)$$

To arrive at the result, we need to bound the right hand side terms. Recall that $f(u_\varepsilon) \leq \alpha u_\varepsilon$. By definition of ϕ_R we have $\|\nabla \check{\phi}_R\|_{L^\infty(\Omega_\varepsilon)} \leq C/R$, so that the first and second terms in (4.76) are bounded by

$$\frac{C}{R} \left(\|u_\varepsilon\|_{L^2((0,T) \times \Omega_\varepsilon)} \|\nabla u_\varepsilon\|_{L^2((0,T) \times \Omega_\varepsilon)} + \varepsilon \|v_\varepsilon\|_{L^2((0,T) \times \partial\Omega_\varepsilon)} \|\nabla^s v_\varepsilon\|_{L^2((0,T) \times \partial\Omega_\varepsilon)} \right) \leq \frac{C}{R} \quad (4.79)$$

by virtue of Lemma 4.4.2. The two last terms in (4.78), involving the initial data (u^{in}, v^{in}) , do not depend on ε and tend to zero as R tends to ∞ . In the proof of Lemma 4.5.3, we bounded the terms similar to (4.77) just by using the regularity hypothesis on the velocity fields and the a priori estimates (4.51) as the ε factor in (4.61) was a constant. In (4.77), however, we cannot argue the same way. To cope with the terms in (4.77), we introduce two auxiliary problems

$$\begin{cases} -\Delta \xi_i(y) = b_i^* - b_i(y) & \text{in } Y^0, \\ -\nabla \xi_i \cdot n = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow \xi_i(y) & \text{is } Y\text{-periodic,} \end{cases} \quad (4.80)$$

$$\begin{cases} -\Delta^s \Xi_i(y) = b_i^* - b_i^s(y) & \text{on } \partial\Sigma^0, \\ y \rightarrow \Xi_i(y) & \text{is } Y\text{-periodic,} \end{cases} \quad (4.81)$$

which both admit a unique solution (up to an additive constant) since, by definition (4.1) of b^* , the source terms in (4.80) and (4.81) are in equilibrium. Substitution of the above auxiliary functions in (4.77) and integration by parts yields

$$\sum_{i=1}^d \int_0^t \left(\int_{\Omega_\varepsilon} \varepsilon \nabla \xi_i^\varepsilon \cdot \nabla \left(F(u_\varepsilon) \partial_{x_i} \check{\phi}_R \right) dx + \varepsilon \int_{\partial\Omega_\varepsilon} \varepsilon \nabla^s \Xi_i^\varepsilon \cdot \nabla^s \left(|v_\varepsilon|^2 \partial_{x_i} \check{\phi}_R \right) d\sigma(x) \right) ds.$$

Since $\varepsilon \nabla \xi_i^\varepsilon(x) = (\nabla_y \xi_i)(x/\varepsilon)$ and $\varepsilon \nabla^s \Xi_i^\varepsilon(x) = (\nabla_y^s \Xi_i)(x/\varepsilon)$, using again the fact that $F(u_\varepsilon)$ has quadratic growth for bounded u_ε , the a priori estimates from Lemma 4.4.2 imply that (4.77) is bounded by a term similar to (4.79). A final change of frame of reference and letting R go to infinity leads to the desired result. \square

We now prepare the ground for the final compactness result by proving some type of equicontinuity in time. The next result tries to obtain some type of equicontinuity in time in order to prove relative compactness in L^2 for the Fourier coefficients. Again, the following lemma considers the concentration sequences in moving coordinates as opposed to the fixed frame of reference in Section 4.5. Let us introduce an orthonormal basis $\{e_j\}_{j \in \mathbb{N}} \in L^2((0,1)^d)$ such that $\{e_j\} \in C_0^\infty([0,1]^d)$. Then the functions $\{e_{jk}\}_{j \in \mathbb{N}, k \in \mathbb{Z}^d}$, where $e_{jk}(x) = e_j(x - k)$, form an orthonormal basis in $L^2(\mathbb{R}^d)$.

Lemma 4.6.2. *Let $h > 0$ be a small parameter representing time translation. There exists a positive constant C_{jk} independent of ε and h such that*

$$\begin{aligned} & \left| \int_0^{T-h} \left\{ \int_{\widehat{\Omega}_\varepsilon(t+h)} \left(\widehat{u}_\varepsilon + \eta f(\widehat{u}_\varepsilon) \right) (t+h, x) e_{jk}(x) dx - \int_{\widehat{\Omega}_\varepsilon(t)} \left(\widehat{u}_\varepsilon + \eta f(\widehat{u}_\varepsilon) \right) (t, x) e_{jk}(x) dx \right\} dt \right| \\ & \leq C_{jk} \left(\sqrt{h} + \varepsilon \right) \end{aligned} \quad (4.82)$$

where $\eta = |\partial\Sigma^0|/|Y^0|$.

Proof. We compute the difference

$$\begin{aligned} & \left(\widehat{u}_\varepsilon(t+h, x), e_{jk}(x) \right)_{L^2(\widehat{\Omega}_\varepsilon(t+h))} - \left(\widehat{u}_\varepsilon(t, x), e_{jk}(x) \right)_{L^2(\widehat{\Omega}_\varepsilon(t))} \\ & + \varepsilon \left(\widehat{v}_\varepsilon(t+h, x), e_{jk}(x) \right)_{L^2(\partial\widehat{\Omega}_\varepsilon(t+h))} - \varepsilon \left(\widehat{v}_\varepsilon(t, x), e_{jk}(x) \right)_{L^2(\partial\widehat{\Omega}_\varepsilon(t))} \\ & = \int_t^{t+h} \frac{d}{ds} \left\{ \int_{\widehat{\Omega}_\varepsilon(s)} \widehat{u}_\varepsilon(s, x) e_{jk}(x) dx + \varepsilon \int_{\partial\widehat{\Omega}_\varepsilon(s)} \widehat{v}_\varepsilon(s, x) e_{jk}(x) d\sigma(x) \right\} ds \\ & = \int_t^{t+h} \frac{d}{ds} \left\{ \int_{\Omega_\varepsilon} u_\varepsilon(s, x) \check{e}_{jk}(x) dx + \varepsilon \int_{\partial\Omega_\varepsilon} v_\varepsilon(s, x) \check{e}_{jk}(x) d\sigma(x) \right\} ds \\ & = \int_t^{t+h} \int_{\Omega_\varepsilon} \left\{ \frac{\partial u_\varepsilon}{\partial s}(s, x) \check{e}_{jk}(x) - \frac{b^*}{\varepsilon} \cdot \nabla \check{e}_{jk}(x) u_\varepsilon(s, x) \right\} dx ds \\ & + \int_t^{t+h} \varepsilon \int_{\partial\Omega_\varepsilon} \left\{ \frac{\partial v_\varepsilon}{\partial s}(s, x) \check{e}_{jk}(x) - \frac{b^*}{\varepsilon} \cdot \nabla \check{e}_{jk}(x) v_\varepsilon(s, x) \right\} d\sigma(x) ds \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{\varepsilon} \int_t^{t+h} \int_{\Omega_\varepsilon} \left\{ (b_\varepsilon - b^*) \cdot \nabla \check{e}_{jk}(x) u_\varepsilon(s, x) - D_\varepsilon \nabla u_\varepsilon(s, x) \cdot \nabla \check{e}_{jk}(x) \right\} dx ds \\
&+ \varepsilon \int_t^{t+h} \int_{\partial\Omega_\varepsilon} \left\{ \frac{1}{\varepsilon} (b_\varepsilon^s - b^*) \cdot \nabla \check{e}_{jk}(x) v_\varepsilon(s, x) - D_\varepsilon^s \nabla^s v_\varepsilon(s, x) \cdot \nabla^s \check{e}_{jk}(x) \right\} d\sigma(x) ds \quad (4.83)
\end{aligned}$$

In (4.83), we have terms similar to (4.77). We handled those singular terms in (4.77) with the introduction of two auxiliary problems (4.80) and (4.81). We shall use the auxiliary problems to handle the problematic terms in (4.83) too. Then (4.83) becomes

$$\begin{aligned}
&\int_t^{t+h} \int_{\Omega_\varepsilon} \left\{ \varepsilon \Delta \xi_i^\varepsilon(x) \partial_{x_i} \check{e}_{jk}(x) u_\varepsilon(s, x) - D_\varepsilon \nabla u_\varepsilon(s, x) \cdot \nabla \check{e}_{jk}(x) \right\} dx ds \\
&+ \int_t^{t+h} \int_{\partial\Omega_\varepsilon} \left\{ \varepsilon^2 \Delta^s \Xi_i^\varepsilon(x) \partial_{x_i} \check{e}_{jk}(x) v_\varepsilon(s, x) - \varepsilon D_\varepsilon^s \nabla^s v_\varepsilon(s, x) \cdot \nabla^s \check{e}_{jk}(x) \right\} d\sigma(x) ds \\
&= - \int_t^{t+h} \int_{\Omega_\varepsilon} \left\{ \nabla_y \xi_i^\varepsilon(x) \cdot \nabla \left(\partial_{x_i} \check{e}_{jk}(x) u_\varepsilon(s, x) \right) + D_\varepsilon \nabla u_\varepsilon(s, x) \cdot \nabla \check{e}_{jk}(x) \right\} dx ds \\
&- \varepsilon \int_t^{t+h} \int_{\partial\Omega_\varepsilon} \left\{ \nabla_y^s \Xi_i^\varepsilon(x) \cdot \nabla^s \left(\partial_{x_i} \check{e}_{jk}(x) v_\varepsilon(s, x) \right) + D_\varepsilon^s \nabla^s v_\varepsilon(s, x) \cdot \nabla^s \check{e}_{jk}(x) \right\} d\sigma(x) ds \leq C_{jk} \sqrt{h}.
\end{aligned}$$

The above bound follows from the a priori estimates (4.35). By the definition of w_ε , we have $\widehat{v}_\varepsilon = f(\widehat{u}_\varepsilon) - \varepsilon \widehat{w}_\varepsilon$. Substituting for \widehat{v}_ε in the above inequality yields

$$\begin{aligned}
&\left| \left(\widehat{u}_\varepsilon(t+h, x), e_{jk}(x) \right)_{L^2(\widehat{\Omega}_\varepsilon(t+h))} + \varepsilon \left(f(\widehat{u}_\varepsilon)(t+h, x), e_{jk}(x) \right)_{L^2(\partial\widehat{\Omega}_\varepsilon(t+h))} \right. \\
&\quad \left. - \left(\widehat{u}_\varepsilon(t, x), e_{jk}(x) \right)_{L^2(\widehat{\Omega}_\varepsilon(t))} - \varepsilon \left(f(\widehat{u}_\varepsilon)(t, x), e_{jk}(x) \right)_{L^2(\partial\widehat{\Omega}_\varepsilon(t))} \right| \\
&\leq C_{jk} \sqrt{h} + \left| \varepsilon^2 \left(\widehat{w}_\varepsilon(t+h, x), e_{jk}(x) \right)_{L^2(\partial\widehat{\Omega}_\varepsilon(t+h))} \right| + \left| \varepsilon^2 \left(\widehat{w}_\varepsilon(t, x), e_{jk}(x) \right)_{L^2(\partial\widehat{\Omega}_\varepsilon(t))} \right|.
\end{aligned}$$

We now replace the boundary integrals involving the nonlinear term with volume integrals. We achieve this with the help of an auxiliary problem.

$$\begin{cases} \operatorname{div}_y \Upsilon(y) = \eta = |\partial\Sigma^0|/Y^0 & \text{in } Y^0, \\ \Upsilon \cdot n = 1 & \text{on } \partial\Sigma^0, \\ y \rightarrow \Upsilon(y) & \text{is } Y\text{-periodic,} \end{cases} \quad (4.84)$$

which admits a smooth Y -periodic vector solution Υ . Then,

$$\begin{aligned}
\varepsilon \int_{\partial\widehat{\Omega}_\varepsilon(t)} f(\widehat{u}_\varepsilon)(t, x) e_{jk}(x) d\sigma(x) &= \varepsilon \int_{\partial\Omega_\varepsilon} f(u_\varepsilon)(t, x) \check{e}_{jk}(x) d\sigma(x) \\
&= \varepsilon \int_{\partial\Omega_\varepsilon} f(u_\varepsilon)(t, x) \check{e}_{jk}(x) \left(\Upsilon^\varepsilon(x) \cdot n \right) d\sigma(x)
\end{aligned}$$

$$\begin{aligned}
&= \varepsilon \int_{\Omega_\varepsilon} \operatorname{div} \left(f(u_\varepsilon)(t, x) \check{e}_{jk}(x) \Upsilon^\varepsilon(x) \right) dx = \varepsilon \int_{\Omega_\varepsilon} f'(u_\varepsilon)(t, x) \nabla u_\varepsilon(t, x) \cdot \Upsilon^\varepsilon(x) \check{e}_{jk}(x) dx + \\
&\quad \varepsilon \int_{\Omega_\varepsilon} \nabla \check{e}_{jk}(x) \cdot \Upsilon^\varepsilon(x) f(u_\varepsilon)(t, x) dx + \eta \int_{\Omega_\varepsilon} \check{e}_{jk}(x) f(u_\varepsilon)(t, x) dx.
\end{aligned}$$

The above calculation leads to

$$\begin{aligned}
&\left| \int_t^{t+h} \frac{d}{ds} \int_{\widehat{\Omega}_\varepsilon(s)} \left(\widehat{u}_\varepsilon + \eta f(\widehat{u}_\varepsilon) \right)(s, x) e_{jk}(x) dx ds \right| \leq C_{jk} \sqrt{h} \\
&+ \left| \varepsilon^2 \int_{\partial\Omega_\varepsilon} w_\varepsilon(t+h, x) e_{jk} \left(x - \frac{b^*(t+h)}{\varepsilon} \right) d\sigma(x) \right| + \left| \varepsilon^2 \int_{\partial\Omega_\varepsilon} w_\varepsilon(t, x) e_{jk} \left(x - \frac{b^*t}{\varepsilon} \right) d\sigma(x) \right| \\
&+ \left| \varepsilon \int_{\Omega_\varepsilon} f'(u_\varepsilon)(t, x) \nabla u_\varepsilon(t, x) \cdot \Upsilon^\varepsilon(x) e_{jk} \left(x - \frac{b^*t}{\varepsilon} \right) dx \right| + \left| \varepsilon \int_{\Omega_\varepsilon} \nabla e_{jk} \left(x - \frac{b^*t}{\varepsilon} \right) \cdot \Upsilon^\varepsilon(x) f(u_\varepsilon)(t, x) dx \right| \\
&+ \left| \varepsilon \int_{\Omega_\varepsilon} f'(u_\varepsilon)(t, x) \nabla u_\varepsilon(t, x) \cdot \Upsilon^\varepsilon(x) e_{jk} \left(x - \frac{b^*(t+h)}{\varepsilon} \right) dx \right| \\
&+ \left| \varepsilon \int_{\Omega_\varepsilon} \nabla e_{jk} \left(x - \frac{b^*(t+h)}{\varepsilon} \right) \cdot \Upsilon^\varepsilon(x) f(u_\varepsilon)(t, x) dx \right|.
\end{aligned}$$

We integrate the above inequality over $(0, T-h)$. As $0 \leq f(u_\varepsilon) \leq \alpha u_\varepsilon$ and $0 \leq f'(u_\varepsilon) \leq \alpha$, the a priori estimates in (4.35) lead to (with a possibly different constant C_{jk})

$$\int_0^{T-h} \left| \int_t^{t+h} \frac{d}{ds} \int_{\widehat{\Omega}_\varepsilon(s)} \left(\widehat{u}_\varepsilon + \eta f(\widehat{u}_\varepsilon) \right)(s, x) e_{jk}(x) dx ds \right| dt \leq C_{jk} (\sqrt{h} + \varepsilon)$$

which is nothing but (4.82). \square

To prove the compactness of u_ε , an intermediate result is to prove the compactness of the sequence z_ε defined by

$$z_\varepsilon(t, x) = u_\varepsilon(t, x) + \eta f(u_\varepsilon)(t, x) \quad \text{for } (t, x) \in (0, T) \times \Omega_\varepsilon. \quad (4.85)$$

In view of the a priori estimates (4.35), z_ε satisfies the following estimates

$$\begin{aligned}
\int_{\Omega_\varepsilon} |z_\varepsilon|^2 dx &\leq \int_{\Omega_\varepsilon} (1 + \eta\alpha)^2 |u_\varepsilon|^2 dx \leq C \quad \forall t \in (0, T), \\
\int_0^T \int_{\Omega_\varepsilon} |\nabla z_\varepsilon|^2 dx &= \int_0^T \int_{\Omega_\varepsilon} (1 + \eta f'(u_\varepsilon))^2 |\nabla u_\varepsilon|^2 dx \leq C.
\end{aligned} \quad (4.86)$$

We recall that the extension operator $E_\varepsilon : H^1(\Omega_\varepsilon) \rightarrow H^1(\mathbb{R}^d)$ of [1] satisfies the following property: there exists a constant C , independent of ε , such that, for any function $\phi_\varepsilon \in H^1(\Omega_\varepsilon)$, $E_\varepsilon \phi_\varepsilon \Big|_{\Omega_\varepsilon} = \phi_\varepsilon$ and

$$\|E_\varepsilon \phi_\varepsilon\|_{L^2(\mathbb{R}^d)} \leq C \|\phi_\varepsilon\|_{L^2(\Omega_\varepsilon)}, \quad \|\nabla E_\varepsilon \phi_\varepsilon\|_{L^2(\mathbb{R}^d)} \leq C \|\nabla \phi_\varepsilon\|_{L^2(\Omega_\varepsilon)}. \quad (4.87)$$

As we are proving compactness in moving coordinates, we consider the sequences \widehat{z}_ε and $\widehat{E_\varepsilon z_\varepsilon}$ where the $\widehat{\cdot}$ -operator is defined by (4.74). The decomposition of these two functions in terms of the orthonormal basis $\{e_{jk}\}$ of $L^2(\mathbb{R}^d)$ yields

$$\widehat{z}_\varepsilon(t, x) = \sum_{j \in \mathbb{N}} \sum_{k \in \mathbb{Z}^d} \mu_{jk}^\varepsilon(t) e_{jk}(x) \quad \text{with} \quad \mu_{jk}^\varepsilon(t) = \int_{\widehat{\Omega}_\varepsilon(t)} \widehat{z}_\varepsilon(t, x) e_{jk}(x) dx, \quad (4.88)$$

$$\widehat{E_\varepsilon z_\varepsilon}(t, x) = \sum_{j \in \mathbb{N}} \sum_{k \in \mathbb{Z}^d} \nu_{jk}^\varepsilon(t) e_{jk}(x) \quad \text{with} \quad \nu_{jk}^\varepsilon(t) = \int_{\mathbb{R}^d} \widehat{E_\varepsilon z_\varepsilon}(t, x) e_{jk}(x) dx, \quad (4.89)$$

where $\mu_{jk}^\varepsilon(t)$ and $\nu_{jk}^\varepsilon(t)$ are the time dependent Fourier coefficients.

Lemma 4.6.3. *Let $\{\mu_{jk}^\varepsilon\}_\varepsilon$ be the Fourier coefficients defined in (4.88). There exists a subsequence, still denoted by ε , such that*

$$\mu_{jk}^\varepsilon \rightarrow \mu_{jk} \quad \text{in } L^2(0, T) \quad \forall j \in \mathbb{N}, k \in \mathbb{Z}^d,$$

for some $\mu_{jk} \in L^2(0, T)$. Further, the function

$$z_0(t, x) = \sum_{j \in \mathbb{N}} \sum_{k \in \mathbb{Z}^d} \mu_{jk}(t) e_{jk}(x) \quad (4.90)$$

is an element of $L^2((0, T) \times \mathbb{R}^d)$.

Proof. From Lemma 4.6.2, we have

$$\int_0^{T-h} \left| \mu_{jk}^\varepsilon(t+h) - \mu_{jk}^\varepsilon(t) \right| dt \leq C_{jk} (\sqrt{h} + \varepsilon). \quad (4.91)$$

Inequality (4.91) is a variant of the Riesz-Fréchet-Kolmogorov criterion for (strong) compactness in $L^1(0, T)$ (see e.g. [50], page 72, Theorem IV.25), the variant being caused by the additional ε -term in the right hand side. It is not difficult to check that the proof of compactness is still valid with this additional term. Therefore, for any $j \in \mathbb{N}, k \in \mathbb{Z}^d$, there is a subsequence $\varepsilon_{jk} \rightarrow 0$ and a limit $\mu_{jk} \in L^1(0, T)$ such that

$$\mu_{jk}^{\varepsilon_{jk}} \rightarrow \mu_{jk} \quad \text{in } L^1(0, T).$$

A diagonalization procedure yields another subsequence ε such that the above convergence in L^1 holds for all indices j, k . The a priori estimates (4.35) on u_ε in turn implies that the Fourier coefficients are bounded in $L^\infty(0, T)$ too. Thus, the above strong compactness property is true in every L^p , $1 \leq p < +\infty$, and, in particular, in $L^2(0, T)$. The assertion that $z_0 \in L^2((0, T) \times \mathbb{R}^d)$ follows from the observation that

$$\begin{aligned} \left\| z_0 \right\|_{L^2((0, T) \times \mathbb{R}^d)}^2 &= \sum_{j \in \mathbb{N}} \sum_{k \in \mathbb{Z}^d} \int_0^T |\mu_{jk}(t)|^2 dt \\ &\leq \sum_{j \in \mathbb{N}} \sum_{k \in \mathbb{Z}^d} \liminf_{\varepsilon \rightarrow 0} \int_0^T |\mu_{jk}^\varepsilon|^2 dt \leq \liminf_{\varepsilon \rightarrow 0} \left\| \widehat{z}_\varepsilon \right\|_{L^2((0, T) \times \widehat{\Omega}_\varepsilon(t))}^2 < \infty. \end{aligned}$$

□

The next result states that there is not much difference between the time Fourier coefficients of \widehat{z}_ε (defined in the perforated domain $\widehat{\Omega}_\varepsilon(t)$) and of its extension $\widehat{E_\varepsilon z_\varepsilon}$.

Lemma 4.6.4. *Let $\theta = |Y^0|/|Y| \in (0, 1)$. There exists a constant C_{jk} independent of ε such that*

$$\left| \mu_{jk}^\varepsilon(t) - \theta \nu_{jk}^\varepsilon(t) \right| \leq C_{jk} \varepsilon. \quad (4.92)$$

Proof. By definition of the Fourier coefficients (4.88)-(4.89), we have

$$\begin{aligned} \mu_{jk}^\varepsilon(t) - \theta \nu_{jk}^\varepsilon(t) &= \int_{\widehat{\Omega}_\varepsilon(t)} \widehat{z}_\varepsilon(t, x) e_{jk}(x) dx - \theta \int_{\mathbb{R}^d} \widehat{E_\varepsilon z_\varepsilon}(t, x) e_{jk}(x) dx \\ &= \int_{\mathbb{R}^d} E_\varepsilon z_\varepsilon(t, x) \check{e}_{jk}(x) (\chi(x/\varepsilon) - \theta) dx \end{aligned} \quad (4.93)$$

where $\chi(x/\varepsilon)$ is the characteristic function of Ω_ε , or equivalently $\chi(y)$ is the characteristic function of Y^0 . Let us introduce the following auxiliary problem

$$\begin{cases} -\operatorname{div}_y(\nabla_y \Phi(y)) = \chi(y) - \theta & \text{in } Y, \\ y \rightarrow \Phi(y) & \text{is } Y\text{-periodic.} \end{cases} \quad (4.94)$$

Using (4.94) in (4.93) leads to

$$\left| \mu_{jk}^\varepsilon(t) - \theta \nu_{jk}^\varepsilon(t) \right| \leq \varepsilon \int_{\mathbb{R}^d} \left| \nabla_y \Phi(x/\varepsilon) \cdot \nabla (E_\varepsilon z_\varepsilon(t, x) \check{e}_{jk}(x)) \right| dx.$$

The properties (4.87) of the extension operator E_ε and the estimates (4.86) lead to (4.92). \square

A last technical result is the possibility of truncating the modal series (with respect to j) of a sequence which is bounded in $L^2(0, T; H^1(\mathbb{R}^d))$. This result has also appeared in [121], [27], [28]. Here we give a proof of the same as it hasn't been fully done in the references cited.

Lemma 4.6.5. *Let $\phi_\varepsilon(t, x)$ be a bounded sequence in $L^2(0, T; H^1(\mathbb{R}^d))$. For any $\delta > 0$, there exists a $J(\delta)$ such that for all ε*

$$\left\| \phi_\varepsilon \chi_{Q_{R(\delta)}} - \sum_{|k| \leq R(\delta)} \sum_{|j| \leq J(\delta)} \lambda_{jk}^\varepsilon(t) e_{jk}(x) \right\|_{L^2((0, T) \times \mathbb{R}^d)} \leq \delta, \quad (4.95)$$

where $Q_{R(\delta)}$ is the cube defined in Lemma 4.6.1 and $\lambda_{jk}^\varepsilon(t)$ are the time dependent Fourier coefficients of ϕ_ε defined as

$$\lambda_{jk}^\varepsilon(t) = \int_{\mathbb{R}^d} \phi_\varepsilon(t, x) e_{jk}(x) dx. \quad (4.96)$$

Proof. As $Q_{R(\delta)}$ is a bounded domain, the expansion of $\phi_\varepsilon \chi_{Q_{R(\delta)}}$ in the basis $\{e_{jk}\}$ can be truncated in k with $|k| \leq R(\delta)$ and is still exact. Let us consider the unit ball

$$B = \{v \in H^1(Q_{R(\delta)}) : \|v\|_{H^1(Q_{R(\delta)})} \leq 1\}.$$

We know that $H^1(Q_{R(\delta)})$ is pre-compact in $L^2(Q_{R(\delta)})$ [50]. Hence for a given $\delta > 0$ and for all $v \in B$, there exists $J(\delta)$ such that

$$\left\| \sum_{|k| \leq R(\delta)} \sum_{j > J(\delta)} (v, e_{jk})_{L^2(Q_{R(\delta)})} e_{jk} \right\|_{L^2(Q_{R(\delta)})}^2 \leq \delta$$

Now, given $\phi_\varepsilon \in L^2(0, T; H^1(Q_{R(\delta)}))$, we have $\phi_\varepsilon(t) \in H^1(Q_{R(\delta)})$ for almost every $t \in (0, T)$. Thus for a given $\delta > 0$, there exists a $J(\delta)$ such that

$$\left\| \sum_{|k| \leq R(\delta)} \sum_{j > J(\delta)} (\phi_\varepsilon(t), e_{jk})_{L^2(Q_{R(\delta)})} e_{jk} \right\|_{L^2(Q_{R(\delta)})}^2 \leq \delta \|\phi_\varepsilon(t)\|_{H^1(Q_{R(\delta)})}^2$$

for almost every $t \in (0, T)$. Integrating the above expression over $(0, T)$, we arrive at

$$\left\| \sum_{|k| \leq R(\delta)} \sum_{j > J(\delta)} (\phi_\varepsilon(t), e_{jk})_{L^2((0, T) \times Q_{R(\delta)})} e_{jk} \right\|_{L^2(Q_{R(\delta)})}^2 \leq \delta \|\phi_\varepsilon(t)\|_{L^2(0, T; H^1(Q_{R(\delta)}))}^2,$$

which implies the result (4.95). \square

We are now ready to state the compactness of the sequence z_ε . Note that the limit is not z_0 but z_0/θ since z_0 was the limit of the sequence z_ε extended by zero outside the porous domain $\widehat{\Omega}_\varepsilon(t)$.

Theorem 4.6.6. *There exists a subsequence ε such that*

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\widehat{\Omega}_\varepsilon(t)} \left| \widehat{z}_\varepsilon(t, x) - \theta^{-1} z_0(t, x) \right|^2 dx dt = 0 \quad (4.97)$$

where z_ε is defined in (4.85).

Proof. The estimates (4.86) for $\{\widehat{z}_\varepsilon\}$, being similar to (4.35), imply that the localization principle, Lemma 4.6.1, holds true for the sequence $\{\widehat{z}_\varepsilon\}$ too. Thus, for a given $\delta > 0$, there exists a $R(\delta) > 0$ big enough such that

$$\left\| \widehat{z}_\varepsilon - \widehat{z}_\varepsilon \chi_{Q_{R(\delta)}} \right\|_{L^2((0, T) \times \widehat{\Omega}_\varepsilon(t))} \leq \frac{\delta}{5}. \quad (4.98)$$

Applying Lemma 4.6.5 to $\widehat{E}_\varepsilon \widehat{z}_\varepsilon \chi_{Q_{R(\delta)}}$, for any $\delta > 0$, there exists $J(\delta)$ such that, for any small $\varepsilon > 0$,

$$\left\| \widehat{E}_\varepsilon \widehat{z}_\varepsilon \chi_{Q_{R(\delta)}} - \sum_{|k| \leq R(\delta)} \sum_{|j| \leq J(\delta)} \nu_{jk}^\varepsilon(t) e_{jk}(x) \right\|_{L^2((0, T) \times \mathbb{R}^d)} \leq \frac{\delta}{5}. \quad (4.99)$$

As $\widehat{E}_\varepsilon \widehat{z}_\varepsilon$ is an extension of \widehat{z}_ε , we deduce from (4.99) that

$$\left\| \widehat{z}_\varepsilon \chi_{Q_{R(\delta)}} - \sum_{|k| \leq R(\delta)} \sum_{|j| \leq J(\delta)} \nu_{jk}^\varepsilon(t) e_{jk}(x) \right\|_{L^2((0, T) \times \widehat{\Omega}_\varepsilon(t))} \leq \frac{\delta}{5}. \quad (4.100)$$

From Lemma 4.6.4, for a given $\delta > 0$ and ε small enough, we have

$$\left\| \sum_{|k| \leq R(\delta)} \sum_{|j| \leq J(\delta)} \nu_{jk}^\varepsilon(t) e_{jk}(x) - \frac{1}{\theta} \sum_{|k| \leq R(\delta), |j| \leq J(\delta)} \mu_{jk}^\varepsilon(t) e_{jk}(x) \right\|_{L^2((0, T) \times \widehat{\Omega}_\varepsilon(t))} \leq \frac{\delta}{5}. \quad (4.101)$$

Lemma 4.6.3 asserted that the Fourier coefficients are relatively compact in $L^2(0, T)$. Thus, for ε small enough, we have

$$\left\| \sum_{|k| \leq R(\delta)} \sum_{|j| \leq J(\delta)} \mu_{jk}^\varepsilon(t) e_{jk}(x) - \sum_{|k| \leq R(\delta), |j| \leq J(\delta)} \mu_{jk}(t) e_{jk}(x) \right\|_{L^2((0, T) \times \widehat{\Omega}_\varepsilon(t))} \leq \theta \frac{\delta}{5}. \quad (4.102)$$

By Lemma 4.6.3 we know that $z_0 \in L^2((0, T) \times \mathbb{R}^d)$ so, by choosing a large enough $J(\delta)$, we have

$$\left\| \sum_{|k| \leq R(\delta)} \sum_{|j| \leq J(\delta)} \mu_{jk}(t) e_{jk}(x) - z_0(t, x) \right\|_{L^2((0, T) \times Q_{R(\delta)})} \leq \frac{\delta}{5} \quad (4.103)$$

Thus summing up (4.98), (4.100), (4.101), (4.102) and (4.103) we arrive at

$$\left\| \widehat{z}_\varepsilon(t, x) - \theta^{-1} z_0(t, x) \right\|_{L^2((0, T) \times \widehat{\Omega}_\varepsilon(t))} \leq \delta \quad (4.104)$$

which is (4.97). □

Eventually, we deduce the desired compactness of the sequence u_ε from that of z_ε .

Corollary 4.6.7. *There exists a subsequence ε and a limit $u_0 \in L^2((0, T) \times \mathbb{R}^d)$ such that*

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\widehat{\Omega}_\varepsilon(t)} |\widehat{u}_\varepsilon(t, x) - u_0(t, x)|^2 dx dt = 0. \quad (4.105)$$

Proof. Since the nonlinear isotherm f is bounded and monotone, the application $(I + \eta f)$ is globally invertible with linear growth. We have $u_\varepsilon(t, x) = (I + \eta f)^{-1} z_\varepsilon(t, x)$ and the compactness property of $\{\widehat{z}_\varepsilon\}$, as stated in Theorem 4.6.6, immediately translates to $\{\widehat{u}_\varepsilon\}$ by a standard application of the Lebesgue dominated convergence theorem. □

Compactness results are crucial in nonlinear parabolic equations. Another approach sharing some similarities with us can be found in [28]. A standard approach in proving compactness for sequences defined in porous domains is to make use of the extension operators of [1]. This approach has been employed, for example, in [28] with regard to homogenization of nonlinear degenerate parabolic convection diffusion equation for the water saturation in the study of two-phase flows. Our approach deviates from this standard approach.

4.7 Two-scale compactness

This section is concerned with obtaining the two-scale limits for the the solutions sequences $\{u_\varepsilon\}$, $\{v_\varepsilon\}$ and the coupled sequence $\{w_\varepsilon\}$ with $w_\varepsilon = \frac{1}{\varepsilon} (f(u_\varepsilon) - v_\varepsilon)$ where f is given by (4.2). The two-scale convergence with drift is a weak type of convergence for the sequences since it relies on the use of test functions. However, by virtue of Corollary 4.6.7 the convergence is strong for u_ε in the sense that

$$\lim_{\varepsilon \rightarrow 0} \left\| u_\varepsilon(t, x) - u_0 \left(t, x - \frac{b^*}{\varepsilon} t \right) \right\|_{L^2((0, T) \times \Omega_\varepsilon)} = 0.$$

We still have to find the two-scale with drift limits of $\{v_\varepsilon\}$ and $\{w_\varepsilon\}$. In Section 3.8 of Chapter 3 we managed to find the two-scale with drift of a coupled sequence, thanks to the auxiliary problem (3.36) introduced in Lemma 3.8.1. We shall be using the same lemma here to find the limit of the coupled sequence $\{w_\varepsilon\}$. For easy reference we shall restate the Lemma 3.8.1, the proof of which can be found in Section 3.8.

Lemma 4.7.1. *Let $\phi(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times \partial\Sigma^0)$ be such that $\int_{\partial\Sigma^0} \phi(t, x, y) d\sigma(y) = 0$ for a.e. $(t, x) \in (0, T) \times \mathbb{R}^d$. There exist two periodic vector fields $\theta(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times Y)^d$*

and $\Theta(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times \partial\Sigma^0)^d$ such that

$$\begin{cases} \operatorname{div}_y \theta = 0 & \text{in } Y^0, \\ \theta \cdot n = \phi & \text{on } \partial\Sigma^0, \\ \operatorname{div}_y^s \Theta = \phi & \text{on } \partial\Sigma^0. \end{cases} \quad (4.106)$$

We now apply the compactness results on two-scale convergence with drift from Chapter 2 to the homogenization of (4.12)-(4.14) to deduce our main result.

Theorem 4.7.2. *Under assumption (4.1) which defines a common average value b^* for the bulk and surface velocities, the sequence of bulk and surface concentrations $(u_\varepsilon, v_\varepsilon)$, solutions of system (4.12)-(4.14), two-scale converge with drift b^* , as $\varepsilon \rightarrow 0$, in the following sense*

$$\begin{cases} u_\varepsilon \xrightarrow{2\text{-drift}} u_0(t, x) \\ v_\varepsilon \xrightarrow{2s\text{-drift}} f(u_0)(t, x) \\ \nabla u_\varepsilon \xrightarrow{2\text{-drift}} \nabla_x u_0(t, x) + \nabla_y u_1(t, x, y) \\ \nabla^s v_\varepsilon \xrightarrow{2s\text{-drift}} f'(u_0)G(y)\nabla_x u_0(t, x) + \nabla_y^s v_1(t, x, y) \\ \frac{1}{\varepsilon} (f(u_\varepsilon) - v_\varepsilon) \xrightarrow{2s\text{-drift}} f'(u_0)u_1(t, x, y) - v_1(t, x, y) \end{cases} \quad (4.107)$$

where f is the Langmuir isotherm defined in (4.2), the two-scale limit $u_0 \in L^2((0, T); H^1(\mathbb{R}^d))$ and the corrector terms $u_1 \in L^2((0, T) \times \mathbb{R}^d; H_{\#}^1(Y^0))$ and $v_1 \in L^2((0, T) \times \mathbb{R}^d; H_{\#}^1(\partial\Sigma^0))$.

Proof. Lemma 4.4.2 furnishes a priori estimates so that, up to a subsequence, all sequences in (4.107) have two-scale limits with drift, thanks to the Propositions 2.6.6, 2.7.2 and 2.7.3 in Chapter 2. The first task is to identify those limits. Similar computations were performed in the proof of Theorem 3.8.2 in Chapter 3 and in [20], so we content ourselves in explaining how to derive the limit of the most delicate term, that is $w_\varepsilon = \frac{1}{\varepsilon} (f(u_\varepsilon) - v_\varepsilon)$, assuming that the other limits are already characterized. As opposed to the proof of Theorem 3.8.2 in Chapter 3 and the calculations in [20], where only linear terms were involved, we have to identify the weak two-scale drift limit of $f(u_\varepsilon)$. In view of Corollary 4.6.7 which states the compactness of $\widehat{u}_\varepsilon(t, x)$, and since $f(u) \leq \alpha u$, it is easily deduced that $f(u_\varepsilon)$ two-scale converges with drift to $f(u_0)$.

Let us denote by $q(t, x, y)$ the two-scale drift limit of w_ε and let us choose a test function ϕ as in Lemma 4.7.1, i.e., $\int_{\partial\Sigma^0} \phi(t, x, y) d\sigma(y) = 0$. By Definition 2.7.1

$$\lim_{\varepsilon \rightarrow 0} \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} w_\varepsilon(t, x) \phi \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) d\sigma(x) dt = \int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} q \phi d\sigma(y) dx dt.$$

Replacing w_ε by the difference between $f(u_\varepsilon)$ and v_ε we get a different two-scale limit which will allows us to characterize $q(t, x, y)$. In view of (4.106), we first have

$$\begin{aligned} \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \frac{1}{\varepsilon} f(u_\varepsilon) \phi \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) d\sigma(x) dt &= \int_0^T \int_{\Omega_\varepsilon} \operatorname{div} \left(f(u_\varepsilon) \theta \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) \right) dx dt, \\ &= \int_0^T \int_{\Omega_\varepsilon} \left[f'(u_\varepsilon) \nabla u_\varepsilon \cdot \theta \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) + f(u_\varepsilon) (\operatorname{div}_x \theta) \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) \right] dx dt, \end{aligned}$$

which, using again the compactness of Corollary 4.6.7, converges, as ε goes to 0, to

$$\begin{aligned} & \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} f'(u_0) \left[(\nabla_x u_0 + \nabla_y u_1) \cdot \theta + f(u_0) \operatorname{div}_x \theta \right] dy dx dt \\ &= \int_0^T \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} f'(u_0) u_1 \theta \cdot n d\sigma(y) dx dt = \int_0^T \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} f'(u_0) u_1 \phi d\sigma(y) dx dt. \end{aligned} \quad (4.108)$$

On the other hand, the second term is

$$\begin{aligned} & \varepsilon \int_0^T \int_{\partial \Omega_\varepsilon} \frac{1}{\varepsilon} v_\varepsilon \phi \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) d\sigma(x) dt = \int_0^T \int_{\partial \Omega_\varepsilon} v_\varepsilon (\operatorname{div}_y^s \Theta) \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) d\sigma(x) dt \\ &= \varepsilon \int_0^T \int_{\partial \Omega_\varepsilon} v_\varepsilon \left[\operatorname{div}^s \left(\Theta \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \right) - \operatorname{div}_x (G\Theta) \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \right] d\sigma(x) dt \\ &= -\varepsilon \int_0^T \int_{\partial \Omega_\varepsilon} \left[\Theta \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \cdot \nabla^s v_\varepsilon + \operatorname{div}_x (G\Theta) \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) v_\varepsilon \right] d\sigma(x) dt \end{aligned}$$

which converges, as ε goes to 0, to

$$\begin{aligned} & - \int_0^T \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} \left[\Theta \cdot (G(y) \nabla_x f(u_0) + \nabla_y^s v_1) + \operatorname{div}_x (G(y) \Theta) f(u_0) \right] d\sigma(y) dx dt \\ &= \int_0^T \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} v_1 \operatorname{div}_y^s \Theta d\sigma(y) dx dt = \int_0^T \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} v_1 \phi d\sigma(y) dx dt. \end{aligned} \quad (4.109)$$

Subtracting the two limit terms (4.108) and (4.109), we have shown that

$$\int_0^T \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} q \phi d\sigma(y) dx dt = \int_0^T \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} (f'(u_0) u_1 - v_1) \phi d\sigma(y) dx dt,$$

for all ϕ such that $\int_{\partial \Sigma^0} \phi dy = 0$. Thus,

$$q(t, x, y) = f'(u_0)(t, x) u_1(t, x, y) - v_1(t, x, y) + l(t, x)$$

for some function $l(t, x)$ which does not depend on y . Since, u_1 and v_1 are also defined up to the addition of a function solely dependent on (t, x) , we can get rid of $l(t, x)$ and we recover indeed the last line of (4.107). \square

4.8 Proof of the homogenization result

This section tries to characterize the two-scale limits obtained in Theorem 4.7.2. Chapter 3 had a separate section, Section 3.7, dedicated to the formal derivation of the homogenized equation using the method of two-scale asymptotic expansions with drift. In the present chapter, we shall avoid the details on the formal derivation. The calculations are almost similar to the ones found in Section 3.7. Our mesoscopic equation (4.12)-(4.14) has got a zero order nonlinear term. As usual in the two-scale asymptotic analysis with drift, consult Section 2.6 and Section 2.7 if necessary, we start with an assumption that the solutions can be written as an ansatz

$$u_\varepsilon(t, x) = \sum_{i \geq 0} \varepsilon^i u_i \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right). \quad (4.110)$$

As u_ε enters as an argument of the nonlinear term, the formal idea would be to approximate the nonlinear term by its Taylor expansion.

$$f(u_\varepsilon) = f(u_0) + \varepsilon f'(u_0) u_1 + \varepsilon^2 \left(u_2 f'(u_0) + \frac{u_1^2}{2} f''(u_0) \right) + \mathcal{O}(\varepsilon) \quad (4.111)$$

We shall use the proposed ansatz (4.110) for u_ε (a similar ansatz for the surface concentration v_ε) and use (4.111) in place of the nonlinear term and perform the asymptotic analysis as in Section 3.7. Now we shall state a result that gives the effective behavior of the mesoscopic model (4.12)-(4.14) in terms of the two-scale limits (4.107).

Theorem 4.8.1. *The two-scale drift limit u_0 of Theorem 4.7.2 satisfies the following nonlinear effective diffusion equation*

$$\begin{cases} [|Y^0| + |\partial\Sigma^0| f'(u_0)] \frac{\partial u_0}{\partial t} - \operatorname{div}_x(\mathcal{D}(u_0) \nabla_x u_0) = 0 & \text{in } (0, T) \times \mathbb{R}^d, \\ [|Y^0| u_0 + |\partial\Sigma^0| f(u_0)](0, x) = |Y^0| u^{in}(x) + |\partial\Sigma^0| v^{in}(x) & \text{in } \mathbb{R}^d, \end{cases} \quad (4.112)$$

where the dispersion tensor \mathcal{D} is given by its entries

$$\begin{aligned} \mathcal{D}_{ij}(u_0) = & \int_{Y^0} D(y) (\nabla_y \chi_i + e_i) \cdot (\nabla_y \chi_j + e_j) dy + \frac{\alpha \kappa}{(1 + \beta u_0)^2} \int_{\partial\Sigma^0} [\chi_i - \omega_i] [\chi_j - \omega_j] d\sigma(y) \\ & + \frac{\alpha}{(1 + \beta u_0)^2} \int_{\partial\Sigma^0} D^s(y) (\nabla_y^s \omega_i + e_i) \cdot (\nabla_y^s \omega_j + e_j) d\sigma(y) \\ & + \int_{Y^0} D(y) (\nabla_y \chi_j \cdot e_i - \nabla_y \chi_i \cdot e_j) dy \\ & + \frac{\alpha}{(1 + \beta u_0)^2} \int_{\partial\Sigma^0} D^s(y) (\nabla_y^s \omega_j \cdot e_i - \nabla_y^s \omega_i \cdot e_j) d\sigma(y) \\ & + \int_{Y^0} (b(y) \cdot \nabla_y \chi_i) \chi_j dy + \frac{\alpha}{(1 + \beta u_0)^2} \int_{\partial\Sigma^0} (b^s(y) \cdot \nabla_y^s \omega_i) \omega_j d\sigma(y) \end{aligned} \quad (4.113)$$

with $(\chi, \omega) = (\chi_i, \omega_i)_{1 \leq i \leq d}$ being the solution of the cell problem

$$\begin{cases} -b^* \cdot e_i + b(y) \cdot (e_i + \nabla_y \chi_i) - \operatorname{div}_y(D(e_i + \nabla_y \chi_i)) = 0 & \text{in } Y^0, \\ -D(y) (e_i + \nabla_y \chi_i) \cdot n = \kappa f'(u_0) (\chi_i - \omega_i) & \text{on } \partial\Sigma^0, \\ -b^* \cdot e_i + b^s(y) \cdot (e_i + \nabla_y^s \omega_i) - \operatorname{div}_y^s(D^s(e_i + \nabla_y^s \omega_i)) = \kappa (\chi_i - \omega_i) & \text{on } \partial\Sigma^0, \\ y \rightarrow (\chi_i(y), \omega_i(y)) & Y\text{-periodic.} \end{cases} \quad (4.114)$$

Before proving Theorem 4.8.1 we establish the well-posed character of the homogenized equation (4.112) and cell problems (4.114).

Lemma 4.8.2. *For any given value of $u_0(t, x) \geq 0$, the cell problem (4.114) admits a unique solution $(\chi_i, \omega_i) \in H_{\#}^1(Y^0) \times H_{\#}^1(\partial\Sigma^0)$, up to the addition of a constant vector (C, C) if and only if the drift velocity is chosen from (4.1)*

The homogenized problem (4.112) admits a unique solution

$$u_0 \in C([0, T]; L^2(\mathbb{R}^d)) \quad \text{and} \quad \nabla u_0 \in L^2((0, T) \times \mathbb{R}^d)^d.$$

Proof. The variational formulation of (4.114) is

$$\begin{aligned} & \int_{Y^0} (b(y) \cdot \nabla_y \chi_i) \varphi \, dy + \int_{Y^0} D(e_i + \nabla_y \chi_i) \cdot \nabla_y \varphi \, dy + f'(u_0) \int_{\partial\Sigma^0} (b^s(y) \cdot \nabla_y^s \omega_i) \psi \, d\sigma(y) \\ & + f'(u_0) \int_{\partial\Sigma^0} D^s(e_i + \nabla_y^s \omega_i) \cdot \nabla_y^s \psi \, d\sigma(y) + \kappa f'(u_0) \int_{\partial\Sigma^0} (\chi_i - \omega_i) (\varphi - \psi) \, d\sigma(y) \\ & = \int_{Y^0} (b^* - b(y)) \cdot e_i \varphi \, dy + f'(u_0) \int_{\partial\Sigma^0} (b^* - b^s(y)) \cdot e_i \psi \, d\sigma(y). \end{aligned} \quad (4.115)$$

Given the drift velocity b^* is (4.1), the Lax-Milgram lemma can be easily applied. Upon symmetrization, the dispersion tensor \mathcal{D} takes the following form

$$\begin{aligned} \mathcal{D}_{ij}^{sym}(u_0) &= \int_{Y^0} D(y) (\nabla_y \chi_i + e_i) \cdot (\nabla_y \chi_j + e_j) \, dy \\ &+ f'(u_0) \int_{\partial\Sigma^0} D^s(y) (\nabla_y^s \omega_i + e_i) \cdot (\nabla_y^s \omega_j + e_j) \, d\sigma(y) \\ &+ \kappa f'(u_0) \int_{\partial\Sigma^0} (\chi_i - \omega_i) (\chi_j - \omega_j) \, d\sigma(y) \end{aligned} \quad (4.116)$$

Since $f'(u_0) \geq 0$, (4.116) implies that $\mathcal{D}(u_0) \geq \int_{Y^0} D(y) \, dy$ and thus the dispersion tensor is uniformly coercive. On the other hand, since $f'(u_0) \leq \alpha$, $\mathcal{D}(u_0)$ is uniformly bounded from above. Then, it is a standard process to prove existence and uniqueness of (4.112) (see [110] if necessary). \square

Proof of Theorem 4.8.1. The proof is to show that $u_0(t, x)$ is the solution of the homogenized equation (4.112). For that goal, we shall pass to the limit in the coupled variational formulation of (4.12)-(4.14),

$$\begin{aligned} & \int_0^T \int_{\Omega_\varepsilon} \left[\frac{\partial u_\varepsilon}{\partial t} \phi_\varepsilon + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi_\varepsilon + D_\varepsilon \nabla u_\varepsilon \cdot \nabla \phi_\varepsilon \right] \, dx \, dt \\ & + \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \left[\frac{\partial v_\varepsilon}{\partial t} \psi_\varepsilon + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon \psi_\varepsilon + D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s \psi_\varepsilon \right] \, d\sigma(x) \, dt \\ & + \frac{\kappa}{\varepsilon} \int_0^T \int_{\partial\Omega_\varepsilon} (f(u_\varepsilon) - v_\varepsilon) (\phi_\varepsilon - \psi_\varepsilon) \, d\sigma(x) \, dt = 0, \end{aligned} \quad (4.117)$$

with the test functions

$$\begin{aligned}\phi_\varepsilon &= \phi\left(t, x - \frac{b^*t}{\varepsilon}\right) + \varepsilon\phi_1\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right), \\ \psi_\varepsilon &= \phi\left(t, x - \frac{b^*t}{\varepsilon}\right) + \varepsilon\psi_1\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right).\end{aligned}$$

Here $\phi(t, x)$, $\phi_1(t, x, y)$ and $\psi_1(t, x, y)$ are smooth compactly supported functions which vanish at $t = T$. Let us consider the convective terms in (3.40) and perform integrations by parts:

$$\begin{aligned}& \int_0^T \int_{\Omega_\varepsilon} \left(\frac{\partial u_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \right) \phi_\varepsilon dx dt + \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \left(\frac{\partial v_\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon \right) \psi_\varepsilon d\sigma(x) dt \\ &= - \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon \frac{\partial \phi}{\partial t} \left(t, x - \frac{b^*t}{\varepsilon} \right) dx dt + \frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon b^* \cdot \nabla_x \phi \left(t, x - \frac{b^*t}{\varepsilon} \right) dx dt \\ &\quad + \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon b^* \cdot \nabla_x \phi_1 \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt - \int_{\Omega_\varepsilon} u^{in}(x) \phi(0, x) dx + \mathcal{O}(\varepsilon) \\ &\quad - \frac{1}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon b_\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^*t}{\varepsilon} \right) dx dt + \int_0^T \int_{\Omega_\varepsilon} b_\varepsilon \cdot \nabla u_\varepsilon \phi_1 \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt \\ &\quad - \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon \frac{\partial \phi}{\partial t} \left(t, x - \frac{b^*t}{\varepsilon} \right) d\sigma(x) dt + \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon b^* \cdot \nabla_x \phi \left(t, x - \frac{b^*t}{\varepsilon} \right) d\sigma(x) dt \\ &\quad + \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon b^* \cdot \nabla_x \psi_1 \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) d\sigma(x) dt - \varepsilon \int_{\partial\Omega_\varepsilon} v^{in}(x) \phi(0, x) d\sigma(x) + \mathcal{O}(\varepsilon) \\ &\quad - \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon b_\varepsilon^s \cdot \nabla_x \phi \left(t, x - \frac{b^*t}{\varepsilon} \right) d\sigma(x) dt + \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} b_\varepsilon^s \cdot \nabla^s v_\varepsilon \psi_1 \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) d\sigma(x) dt.\end{aligned}$$

We cannot directly pass to the two-scale limit since there are terms which apparently are of order ε^{-1} . We thus regroup them and, recalling definition (4.74) of the transported function $\check{\phi}$ and using the two auxiliary problems (4.80) and (4.81), we deduce

$$\begin{aligned}& \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon \frac{b^* - b_\varepsilon}{\varepsilon} \cdot \nabla_x \check{\phi} dx dt + \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon (b^* - b_\varepsilon^s) \cdot \nabla_x \check{\phi} d\sigma(x) dt \\ &= \varepsilon \sum_{i=1}^d \int_0^T \int_{\Omega_\varepsilon} u_\varepsilon \Delta \xi_i^\varepsilon \partial_{x_i} \check{\phi} dx dt + \varepsilon^2 \sum_{i=1}^d \int_0^T \int_{\partial\Omega_\varepsilon} v_\varepsilon \Delta \Xi_i^\varepsilon \partial_{x_i} \check{\phi} d\sigma(x) dt \\ &= -\varepsilon \sum_{i=1}^d \int_0^T \int_{\Omega_\varepsilon} \nabla \xi_i^\varepsilon \cdot \nabla (u_\varepsilon \partial_{x_i} \check{\phi}) dx dt - \varepsilon^2 \sum_{i=1}^d \int_0^T \int_{\partial\Omega_\varepsilon} \nabla \Xi_i^\varepsilon \cdot \nabla (v_\varepsilon \partial_{x_i} \check{\phi}) d\sigma(x) dt,\end{aligned}$$

for which we can pass to the two-scale limit. The above simplification of the singular terms already appeared in the proof of the localization result, Lemma 4.6.1, in Section 4.6 where the auxiliary problems (4.80) and (4.81) were introduced.

In a first step towards obtaining the homogenized result, we choose $\phi \equiv 0$ and we pass to the two-scale limit with drift in (4.117). It yields

$$\begin{aligned}
& \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} u_0(t, x) b^* \cdot \nabla_x \phi_1(t, x, y) dy dx dt \\
& + \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} b(y) \cdot (\nabla_x u_0(t, x) + \nabla_y u_1(t, x, y)) \phi_1(t, x, y) dy dx dt \\
& + \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} D(y) (\nabla_x u_0(t, x) + \nabla_y u_1(t, x, y)) \cdot \nabla_y \phi_1(t, x, y) dy dx dt \\
& + \int_0^T \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} f(u_0) b^* \cdot \nabla_x \psi_1(t, x, y) d\sigma(y) dx dt \\
& + \int_0^T \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} b^s(y) \cdot (f'(u_0) G \nabla_x u_0(t, x) + \nabla_y^s v_1(t, x, y)) \psi_1(t, x, y) d\sigma(y) dx dt \\
& + \int_0^T \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} D^s(y) (f'(u_0) G \nabla_x u_0(t, x) + \nabla_y^s v_1(t, x, y)) \cdot \nabla_y^s \psi_1(t, x, y) d\sigma(y) dx dt \\
& + \kappa \int_0^T \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} (f'(u_0) u_1 - v_1) (\phi_1 - \psi_1) d\sigma(y) dx dt = 0,
\end{aligned}$$

which is nothing but the variational formulation of

$$\left\{ \begin{array}{ll}
-b^* \cdot \nabla_x u_0 + b \cdot (\nabla_x u_0 + \nabla_y u_1) - \operatorname{div}_y (D(\nabla_x u_0 + \nabla_y u_1)) = 0 & \text{in } Y^0, \\
-D(\nabla_x u_0 + \nabla_y u_1) \cdot n = \frac{\kappa}{(1 + \beta u_0)^2} (\alpha u_1 - (1 + \beta u_0)^2 v_1) & \text{on } \partial \Sigma^0, \\
-b^* \cdot \alpha \nabla_x u_0 + b^s(y) \cdot (\alpha \nabla_x u_0 + (1 + \beta u_0)^2 \nabla_y^s u_1) & \\
-\operatorname{div}_y^s (D^s(\alpha \nabla_x u_0 + (1 + \beta u_0)^2 \nabla_y^s v_1)) = \kappa (\alpha u_1 - (1 + \beta u_0)^2 v_1) & \text{on } \partial \Sigma^0, \\
y \rightarrow (u_1(y), v_1(y)) & Y\text{-periodic,}
\end{array} \right. \quad (4.118)$$

which implies that

$$u_1(t, x, y) = \sum_{i=1}^d \chi_i(y) \frac{\partial u_0}{\partial x_i}(t, x) \quad \text{and} \quad v_1 = f'(u_0) \sum_{i=1}^d \omega_i(y) \frac{\partial u_0}{\partial x_i}(t, x)$$

where $(\chi_i, \omega_i)_{1 \leq i \leq d}$ is the solution of the cell problem (4.114).

In a second step, we choose $\phi_1 \equiv 0$, $\psi_1 \equiv 0$ and we pass to the two-scale limit with drift in (4.117). It yields

$$|Y^0| \int_{\mathbb{R}^d} \frac{\partial u_0}{\partial t} \phi dx dt + \sum_{i,j=1}^d \int_{\mathbb{R}^d} \int_{Y^0} D_{ij}(y) \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} dx dt$$

$$\begin{aligned}
& -|Y^0| \int_{\mathbb{R}^d} u^{in}(x) \phi(0, x) dx + \int_{\mathbb{R}^d} \int_{Y^0} \sum_{i,j=1}^d \sum_{l=1}^d D_{il}(y) \frac{\partial \chi_j(y)}{\partial y_l} \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} dx dt \\
& + |\partial \Sigma^0| \int_{\mathbb{R}^d} f'(u_0) \frac{\partial u_0}{\partial t} \phi dx dt + \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} \sum_{i,j=1}^d \sum_{l=1}^d f'(u_0) D_{il}^s(y) G_{lj}(y) \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} d\sigma(y) dx dt \\
& - |\partial \Sigma^0| \int_{\mathbb{R}^d} v^{in}(x) \phi(0, x) dx + \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} \sum_{i,j=1}^d \sum_{l=1}^d f'(u_0) D_{il}^s(y) \frac{\partial u_0}{\partial x_j} \frac{\partial^s \omega_j(y)}{\partial y_l} \frac{\partial \phi}{\partial x_i} d\sigma(y) dx dt \\
& \quad + \int_{\mathbb{R}^d} \int_{Y^0} \sum_{i,j=1}^d \sum_{l=1}^d \frac{\partial \xi_i(y)}{\partial y_l} \frac{\partial \chi_j(y)}{\partial y_l} \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} dy dx dt \\
& \quad + \int_{\mathbb{R}^d} \int_{\partial \Sigma^0} \sum_{i,j=1}^d \sum_{l=1}^d f'(u_0) \frac{\partial^s \Xi_i(y)}{\partial y_l} \frac{\partial^s \omega_j(y)}{\partial y_l} \frac{\partial u_0}{\partial x_j} \frac{\partial \phi}{\partial x_i} d\sigma(y) dx dt = 0,
\end{aligned}$$

which is precisely the variational formulation of the homogenized problem (4.112) where the elements of \mathcal{D} are given by

$$\begin{aligned}
\mathcal{D}_{ij} = & \int_{Y^0} D e_i \cdot e_j dy + \int_{Y^0} D \nabla_y \chi_j \cdot e_i dy + f'(u_0) \int_{\partial \Sigma^0} D^s e_i \cdot e_j d\sigma(y) + f'(u_0) \int_{\partial \Sigma^0} D^s \nabla_y^s \omega_j \cdot e_i d\sigma(y) \\
& + \int_{Y^0} \nabla_y \xi_i \cdot \nabla_y \chi_j dy + f'(u_0) \int_{\partial \Sigma^0} \nabla_y^s \Xi_i \cdot \nabla_y^s \omega_j d\sigma(y) \tag{4.119}
\end{aligned}$$

It remains to prove that formula (4.119) is equivalent to that announced in (4.113). Note that we haven't symmetrized the expression for the dispersion tensor. In Section 3.7 we did symmetrize the homogenized matrix as the dispersion matrix (3.29) was a constant matrix. Our upscaling method could recognize the role played only by the symmetric part of the dispersion matrix. In the current case, however, the dispersion matrix depends on the homogenized solution u_0 and the observation (2.51) we made in Chapter 2 is no longer valid. So, the non-symmetric nature of the dispersion matrix in (4.113). In (4.119) we recognize the solutions to the auxiliary problems (4.80) and (4.81) that we used to take care of the singular terms in the variational formulation (4.117). So the two auxiliary problems (4.80) and (4.81) have to be used for transforming (4.119) into (4.113). Let us test (4.80) for ξ_i by the cell solution χ_j followed by testing (4.81) for Ξ_i by $f'(u_0)\omega_j$. Adding the thus obtained expressions leads to

$$\int_{Y^0} \nabla_y \xi_i \cdot \nabla_y \chi_j dy + f'(u_0) \int_{\partial \Sigma^0} \nabla_y^s \Xi_i \cdot \nabla_y^s \omega_j d\sigma(y) = \int_{Y^0} (b_i^* - b_i) \chi_j dy + f'(u_0) \int_{\partial \Sigma^0} (b_i^* - b_i^s) \omega_j d\sigma(y) \tag{4.120}$$

Next, in the variational formulation (4.115) for (χ_i, ω_i) , we shall replace the test functions by (χ_j, ω_j) leading to

$$\begin{aligned}
& \int_{Y^0} (b_i^* - b_i(y)) \chi_j(y) dy + f'(u_0) \int_{\partial \Sigma^0} (b_i^* - b_i^s(y)) \omega_j(y) d\sigma(y) \\
& = \int_{Y^0} D(y) \nabla_y \chi_i \cdot \nabla_y \chi_j dy + f'(u_0) \int_{\partial \Sigma^0} D^s(y) \nabla_y^s \omega_i \cdot \nabla_y^s \omega_j d\sigma(y) + \int_{Y^0} D \nabla_y \chi_j \cdot e_i dy
\end{aligned}$$

$$+f'(u_0) \int_{\partial\Sigma^0} D^s \nabla_y^s \omega_j \cdot e_i d\sigma(y) + \kappa f'(u_0) \int_{\partial\Sigma^0} (\chi_i - \omega_i) (\chi_j - \omega_j) d\sigma(y). \quad (4.121)$$

Finally, using (4.120) and (4.121) in (4.119) shows that both formulas (4.119) and (4.113) for the dispersion tensor \mathcal{D} are equivalent. Therefore, we have indeed obtained the variational formulation of the homogenized problem (4.112) which, by Lemma 4.8.2, admits a uniqueness solution. As a consequence of uniqueness, the entire sequence converges, not merely a subsequence. \square

4.9 Strong convergence

Theorem 4.7.2 gives a weak type convergence result for the sequences u_ε and v_ε in the sense of two-scale convergence with drift. Thanks to the strong compactness of Corollary 4.6.7 it was immediately improved as a strong convergence result for u_ε in the L^2 -norm.

$$\lim_{\varepsilon \rightarrow 0} \left\| u_\varepsilon(t, x) - u_0 \left(t, x - \frac{b^*}{\varepsilon} t \right) \right\|_{L^2((0,T) \times \Omega_\varepsilon)} = 0.$$

In the present section, we recover this result and additionally prove the strong convergence of v_ε and of their gradients, up to the addition of some corrector terms. The main idea is to show that the energy associated with (4.12)-(4.14) converges to that of the homogenized equation (4.112). This is shown to work under a specific constraint on the initial data (u^{in}, v^{in}) which must be well prepared (see below). Then, our argument relies on the notion of strong two-scale convergence which is recalled in Proposition 2.6.7 of Chapter 2. Theorem 4.9.1 is the main result of the section. Following ideas of [20], [17], its proof relies on the lower semicontinuity property of the norms with respect to the (weak) two-scale convergence. The additional difficulty is the nonlinear terms which arise in the energy equality (4.36). Lemma 4.9.3 is a technical result of strong two-scale convergence adapted to our nonlinear setting.

Let us explain the assumption on the well prepared character of the initial data and its origin. We denote by $u_0^0(x)$ the initial data of the homogenized problem (4.112), which is defined on \mathbb{R}^d by

$$|Y^0|u_0^0 + |\partial\Sigma^0|f(u_0^0) = |Y^0|u^{in} + |\partial\Sigma^0|v^{in}. \quad (4.122)$$

Since f is non negative and increasing, (4.122) uniquely defines u_0^0 as a nonlinear function of (u^{in}, v^{in}) . It will turn out that, passing to the limit in the energy equality, and thus deducing strong convergence, requires another constraint for u_0^0 which is

$$|Y^0|F(u_0^0) + \frac{1}{2}|\partial\Sigma^0|f^2(u_0^0) = |Y^0|F(u^{in}) + \frac{1}{2}|\partial\Sigma^0|(v^{in})^2, \quad (4.123)$$

where F is the primitive of f . In general, (4.122) and (4.123) are not compatible, except if the initial data (u^{in}, v^{in}) satisfies a compatibility condition which, for the moment, we admittedly write as a nonlinear relationship

$$\mathcal{H}(u^{in}, v^{in}) = 0. \quad (4.124)$$

Typically, if u^{in} is known, (4.124) prescribes a given value for v^{in} . Lemma 4.9.4 will investigate the existence and uniqueness of a solution v^{in} in terms of given u^{in} . In the linear case, namely $f(u) = \alpha u$, (4.124) reduces to the explicit relationship $v^{in} = \alpha u^{in}$ which was indeed the object of Theorem 3.10.1 of Section 3.10 in Chapter 3.

Theorem 4.9.1. *Let the initial data (u^{in}, v^{in}) satisfy the nonlinear equation (4.124). Then the sequences $u_\varepsilon(t, x)$ and $v_\varepsilon(t, x)$ strongly two-scale converge with drift in the sense that*

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \left\| u_\varepsilon(t, x) - u_0 \left(t, x - \frac{b^*}{\varepsilon} t \right) \right\|_{L^2((0, T) \times \Omega_\varepsilon)} &= 0, \\ \lim_{\varepsilon \rightarrow 0} \sqrt{\varepsilon} \left\| v_\varepsilon(t, x) - f(u_0) \left(t, x - \frac{b^*}{\varepsilon} t \right) \right\|_{L^2((0, T) \times \partial\Omega_\varepsilon)} &= 0. \end{aligned} \quad (4.125)$$

Similarly, the gradients of $u_\varepsilon(t, x)$ and $v_\varepsilon(t, x)$ strongly two-scale converge with drift in the sense that

$$\lim_{\varepsilon \rightarrow 0} \left\| \nabla u_\varepsilon(t, x) - \nabla u_0 \left(t, x - \frac{b^*}{\varepsilon} t \right) - \nabla_y u_1 \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) \right\|_{L^2((0, T) \times \Omega_\varepsilon)} = 0, \quad (4.126)$$

with $u_1(t, x, y) = \chi(y) \cdot \nabla_x u_0(t, x)$, and

$$\lim_{\varepsilon \rightarrow 0} \sqrt{\varepsilon} \left\| \nabla^S v_\varepsilon(t, x) - G \left(\frac{x}{\varepsilon} \right) \nabla f(u_0) - \nabla_y^S v_1 \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) \right\|_{L^2((0, T) \times \partial\Omega_\varepsilon)} = 0. \quad (4.127)$$

with $v_1(t, x, y) = \omega(y) \cdot \nabla_x f(u_0)(t, x)$.

Remark 4.9.2. *If the well prepared assumption (4.124) is not satisfied we believe that strong convergence, in the sense of Theorem 4.9.1, still holds true. This was indeed proved for the linear case in [20], [17] (details of which can be found in Theorem 3.10.1 of Section 3.10 in Chapter 3). The mechanism is that, after a time t_0 as small as we wish, diffusion relaxes any initial data to an almost well prepared solution $(u_\varepsilon(\cdot, t_0), v_\varepsilon(\cdot, t_0))$ which can serve as a well prepared initial data starting at time t_0 . There are technical difficulties for proving such a result in the nonlinear case which we are unable to overcome.*

To prove Theorem 4.9.1 we need the notion of strong two-scale convergence which was originally introduced in Theorem 1.8 in [5]. It was further extended to the case of sequences on periodic surfaces in [14] and to the case of two-scale convergence with drift in [7] (Proposition 2.6.7). Of course, we can blend these two ingredients and extend the notion of strong convergence to sequences defined on periodic surfaces. This was done in 2.7.4.

We now prove a technical result which amounts to say that the L^2 -norm can be replaced by a convex functional in the criterion of strong two-scale convergence (2.61) of Proposition 2.6.7.

Lemma 4.9.3. *Let $\mathcal{A} : \mathbb{R} \rightarrow \mathbb{R}$ be a strongly convex function in the sense that there exists a constant $a > 0$ such that, for any $u, v \in \mathbb{R}$ and any $\theta \in [0, 1]$, it satisfies*

$$\mathcal{A}(\theta u + (1 - \theta)v) \leq \theta \mathcal{A}(u) + (1 - \theta) \mathcal{A}(v) - \frac{a}{2} \theta(1 - \theta) |u - v|^2.$$

Let $\{U_\varepsilon(t, x)\}$ be a sequence that two-scale converges with drift to $U_0(t, x, y)$. If

$$\lim_{\varepsilon \rightarrow 0} \|\mathcal{A}(U_\varepsilon)(t, x)\|_{L^1((0, T) \times \Omega_\varepsilon)} = \|\mathcal{A}(U_0)(t, x, y)\|_{L^1((0, T) \times \mathbb{R}^d \times Y^0)} \quad (4.128)$$

then

$$\lim_{\varepsilon \rightarrow 0} \left\| U_\varepsilon(t, x) - U_0 \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) \right\|_{L^2((0, T) \times \Omega_\varepsilon)} = 0. \quad (4.129)$$

Proof. Since \mathcal{A} is convex and proper (finite), it is continuous and thus, up to an additive constant which plays no role, non negative. The strong convexity of \mathcal{A} yields

$$\mathcal{A} \left(\theta U_\varepsilon(t, x) + (1 - \theta) U_0 \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) \right) \leq \theta \mathcal{A}(U_\varepsilon)(t, x)$$

$$+(1-\theta)\mathcal{A}(U_0)\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right) - \frac{a}{2}\theta(1-\theta)\left|U_\varepsilon(t, x) - U_0\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right)\right|^2.$$

Taking $\theta = \frac{1}{2}$ and integrating over $\Omega_\varepsilon \times (0, T)$, we get

$$\begin{aligned} & \int_0^T \int_{\Omega_\varepsilon} \mathcal{A}\left(\frac{U_\varepsilon(t, x) + U_0\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right)}{2}\right) + \frac{a}{8} \int_0^T \int_{\Omega_\varepsilon} \left|U_\varepsilon(t, x) - U_0\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right)\right|^2 \\ & \leq \frac{1}{2} \int_0^T \int_{\Omega_\varepsilon} \mathcal{A}(U_\varepsilon)(t, x) + \frac{1}{2} \int_0^T \int_{\Omega_\varepsilon} \mathcal{A}(U_0)\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right). \end{aligned} \quad (4.130)$$

Because of the lower semi-continuity property of convex functions with respect to the weak two-scale convergence with drift, we have

$$\int_0^T \int_{\mathbb{R}^d} \int_{Y^0} \mathcal{A}(U_0)(t, x, y) \leq \int_0^T \int_{\Omega_\varepsilon} \mathcal{A}\left(\frac{U_\varepsilon(t, x) + U_0\left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon}\right)}{2}\right).$$

Upon passing to the limit, as $\varepsilon \rightarrow 0$, the right hand side of (4.130) is exactly equal to the left hand side of the above inequality because of our hypothesis (4.128) on $\mathcal{A}(U_\varepsilon)$, which yields the desired result (4.129). \square

The criterion (4.128) is that in the context of convex functional to (2.61) in the L^2 setting (Proposition 2.6.7). This adoption to convex functional is called for as we encounter nonlinear terms in the energy estimate (4.36) of (4.12)-(4.14). We now are ready to prove the main result of this section.

Proof of Theorem 4.9.1. Following an idea from [17], [20], we prove that the energy associated with (4.12)-(4.14) converges to the that of the homogenized equation (4.112) under assumption (4.124). Integrating the energy equality (4.36) over $(0, t)$ yields

$$\begin{aligned} & \int_{\Omega_\varepsilon} F(u_\varepsilon)(t) dx + \frac{\varepsilon}{2} \int_{\partial\Omega_\varepsilon} |v_\varepsilon(t)|^2 d\sigma(x) + \int_0^t \int_{\Omega_\varepsilon} f'(u_\varepsilon) D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon dx ds \\ & + \varepsilon \int_0^t \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s v_\varepsilon d\sigma(x) ds + \kappa \varepsilon \int_0^t \int_{\partial\Omega_\varepsilon} (w_\varepsilon)^2 d\sigma(x) ds = \int_{\Omega_\varepsilon} F(u^{in}) dx + \frac{\varepsilon}{2} \int_{\partial\Omega_\varepsilon} |v^{in}|^2 d\sigma(x), \end{aligned}$$

with $w_\varepsilon = (f(u_\varepsilon) - v_\varepsilon)/\varepsilon$. Since two-scale convergence with drift holds only in a time-space product interval, we integrate again the above expression over $(0, T)$ to get

$$\begin{aligned} & \int_0^T \int_{\Omega_\varepsilon} F(u_\varepsilon)(t) dx dt + \frac{\varepsilon}{2} \int_0^T \int_{\partial\Omega_\varepsilon} |v_\varepsilon(t)|^2 d\sigma(x) dt + \int_0^T \int_0^t \int_{\Omega_\varepsilon} f'(u_\varepsilon) D_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon dx ds dt \\ & + \varepsilon \int_0^T \int_0^t \int_{\partial\Omega_\varepsilon} D_\varepsilon^s \nabla^s v_\varepsilon \cdot \nabla^s v_\varepsilon d\sigma(x) ds dt + \kappa \varepsilon \int_0^T \int_0^t \int_{\partial\Omega_\varepsilon} (w_\varepsilon)^2 d\sigma(x) ds dt \\ & = T \int_{\Omega_\varepsilon} F(u^{in}) dx + \frac{T\varepsilon}{2} \int_{\partial\Omega_\varepsilon} |v^{in}|^2 d\sigma(x). \end{aligned} \quad (4.131)$$

We pass to the two-scale limit in all terms of the left hand side of (4.131) by using the lower semi-continuity property of norms and of the convex function F . The only delicate term is the third one, involving the nonlinear term $f'(u_\varepsilon)$, where we use again the compactness of Corollary 4.6.7. Passing to the limit yields the following inequality

$$\begin{aligned}
& |Y^0| \int_0^T \int_{\mathbb{R}^d} F(u_0) dx dt + \frac{1}{2} |\partial\Sigma^0| \int_0^T \int_{\mathbb{R}^d} (f(u_0))^2 dx dt \\
& + \kappa \int_0^T \int_0^t \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} |(\chi(y) - \omega(y)) \cdot \nabla_x f(u_0)(s, x)|^2 d\sigma(y) dx ds dt. \\
& + \int_0^T \int_0^t \int_{\mathbb{R}^d} \int_{Y^0} f'(u_0) D(y) |\nabla_x u_0(s, x) + \nabla_y (\chi(y) \cdot \nabla_x u_0(s, x))|^2 dy dx ds dt. \\
& + \int_0^T \int_0^t \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} D^s(y) |G(y) \nabla_x f(u_0)(s, x) + \nabla_y^s (\omega(y) \cdot \nabla_x f(u_0)(s, x))|^2 d\sigma(y) dx ds dt \\
& \leq T |Y^0| \int_{\mathbb{R}^d} F(u^{in}) dx + \frac{T}{2} |\partial\Sigma^0| \int_{\mathbb{R}^d} |v^{in}|^2 dx.
\end{aligned}$$

Recognizing formula (4.116) for \mathcal{D}^{sym} leads to

$$\begin{aligned}
|Y^0| \int_0^T \int_{\mathbb{R}^d} F(u_0) dx dt + \frac{1}{2} |\partial\Sigma^0| \int_0^T \int_{\mathbb{R}^d} (f(u_0))^2 dx dt + \int_0^T \int_0^t \int_{\mathbb{R}^d} \mathcal{D}^{sym}(u_0) \nabla_x u_0 \cdot \nabla_x (f(u_0)) dx ds dt \\
\leq T |Y^0| \int_{\mathbb{R}^d} F(u^{in}) dx + \frac{T}{2} |\partial\Sigma^0| \int_{\mathbb{R}^d} |v^{in}|^2 dx. \tag{4.132}
\end{aligned}$$

As we are dealing with the energy estimates, the non symmetric part of \mathcal{D} doesn't play any role in the left hand side of the inequality (4.132). So we can replace \mathcal{D}^{sym} in the third term of the left hand side of (4.132). This leads to

$$\begin{aligned}
|Y^0| \int_0^T \int_{\mathbb{R}^d} F(u_0) dx dt + \frac{1}{2} |\partial\Sigma^0| \int_0^T \int_{\mathbb{R}^d} (f(u_0))^2 dx dt + \int_0^T \int_0^t \int_{\mathbb{R}^d} \mathcal{D}(u_0) \nabla_x u_0 \cdot \nabla_x (f(u_0)) dx ds dt \\
\leq T |Y^0| \int_{\mathbb{R}^d} F(u^{in}) dx + \frac{T}{2} |\partial\Sigma^0| \int_{\mathbb{R}^d} |v^{in}|^2 dx. \tag{4.133}
\end{aligned}$$

We now compare inequality (4.133) with the (time integral of the) energy equality for the homogenized equation (4.112) with $f(u_0)$ as a test function

$$\begin{aligned}
|Y^0| \int_0^T \int_{\mathbb{R}^d} F(u_0) dx dt + \frac{1}{2} |\partial\Sigma^0| \int_0^T \int_{\mathbb{R}^d} (f(u_0))^2 dx dt + \int_0^T \int_0^t \int_{\mathbb{R}^d} \mathcal{D}(u_0) \nabla_x u_0 \cdot \nabla_x (f(u_0)) dx ds dt \\
= T |Y^0| \int_{\mathbb{R}^d} F(u_0^0)(x) dx + \frac{T}{2} |\partial\Sigma^0| \int_{\mathbb{R}^d} (f(u_0^0))^2(x) dx. \tag{4.134}
\end{aligned}$$

The right hand side in (4.133) and (4.134) are equal precisely when (4.123) holds true. Together with the definition (4.122) of the initial condition of the homogenized problem (4.112), it is equivalent to our assumption (4.124). In such a case, the inequality (4.133) is actually an equality, meaning that the lower semi continuous convergences leading to (4.133) were exact convergences. Then, applying Lemma 4.9.3 for the convex functionals and Proposition 2.7.4 for the sequences on periodic surfaces gives the result (4.125). \square

Next, we prove a result giving the solvability of the nonlinear relation (4.124).

Lemma 4.9.4. *For any given $u^{in} \geq 0$ there always exists a unique solution $v^{in} \geq 0$ of the nonlinear equation (4.124), $\mathcal{H}(u^{init}, v^{init}) = 0$.*

Proof. Define $\eta = |\partial\Sigma^0|/|Y^0|$. Since $0 \leq f(u) \leq \alpha u$, the function $u \rightarrow u + \eta f(u)$ is monotone and invertible on \mathbb{R}^+ . Therefore, (4.122) uniquely defines the homogenized initial data as

$$u_0^0 = (I + \eta f)^{-1} (u^{in} + \eta v^{in}). \quad (4.135)$$

To satisfy the additional relation (4.123) is equivalent to solve the nonlinear equation (4.124) where \mathcal{H} is defined by

$$\mathcal{H}(u^{in}, v^{in}) = F(u^{in}) + \frac{1}{2}\eta(v^{in})^2 - \left(F + \frac{1}{2}\eta f^2\right)(u_0^0), \quad (4.136)$$

where u_0^0 is defined by (4.135). For a given $u^{in} \geq 0$, let us differentiate \mathcal{H} with respect to v^{in}

$$\partial_{v^{in}} \mathcal{H}(u^{in}, v^{in}) = \eta v^{in} - (f(u_0^0) + \eta f(u_0^0)f'(u_0^0))\partial_{v^{in}} u_0^0. \quad (4.137)$$

Differentiating (4.122) with respect to v^{in} leads to

$$(1 + \eta f'(u_0^0))\partial_{v^{in}} u_0^0 = \eta, \quad (4.138)$$

implying that $\partial_{v^{in}} u_0^0 > 0$. Using (4.138) in (4.137) simplifies the derivative of \mathcal{H} with respect to v^{in} as

$$\partial_{v^{in}} \mathcal{H}(u^{in}, v^{in}) = \eta v^{in} - \eta f(u_0^0). \quad (4.139)$$

Since $f \geq 0$, we have

$$\partial_{v^{in}} \mathcal{H}(u^{in}, 0) = -\eta f(u_0^0) \leq 0.$$

Also since $f \leq \alpha/\beta$, we have

$$\lim_{v^{in} \rightarrow +\infty} \partial_{v^{in}} \mathcal{H}(u^{in}, v^{in}) = +\infty.$$

Let us differentiate (4.139) with respect to v^{in}

$$\partial_{v^{in}}^2 \mathcal{H}(u^{in}, v^{in}) = \eta - \eta f'(u_0^0)\partial_{v^{in}} u_0^0. \quad (4.140)$$

Using (4.138) in (4.140) leads to

$$\partial_{v^{in}}^2 \mathcal{H}(u^{in}, v^{in}) = \partial_{v^{in}} u_0^0 > 0.$$

Thus, for a fixed u^{in} , $v^{in} \rightarrow \partial_{v^{in}} \mathcal{H}(u^{in}, v^{in})$ is continuous monotone increasing function so there exists a unique v_*^{in} such that $\partial_{v^{in}} \mathcal{H}(u^{in}, v_*^{in}) = 0$. By (4.139) we have $v_*^{in} = f(u_0^0)$ and from (4.122) we deduce $u^{in} = u_0^0$. Plugging these values in (4.135) implies that $\mathcal{H}(u^{in}, v_*^{in}) = 0$. Since the function $v^{in} \rightarrow \mathcal{H}(u^{in}, v^{in})$ is decreasing from 0 to v_*^{in} and then increasing, v_*^{in} is the only possible root for \mathcal{H} . \square

4.10 Numerical study

This section is devoted to the numerical computations of the cell problem and the effective dispersion, given in Theorem 4.8.1. All our numerical tests are done in two dimensions. The unit periodicity cell is the unit square $]0, 1[\times]0, 1[$ and the solid obstacle is a disk of radius 0.2 centered at $(0.5, 0.5)$. The periodic porous medium that we have considered is again $]0, 1[\times]0, 1[$ with periodically arranged circular disks of radius 0.05 with period $\varepsilon = 0.25$. The periodic porous medium is just the unit periodicity cell scaled by 0.25 and repeated in $]0, 1[\times]0, 1[$ with period 0.25. FreeFem++ package [141] is used to perform all the numerical simulations. We have used Lagrange P1 finite elements with 21416 vertices (degrees of freedom). We have taken the reaction parameters α, β to be unity.

In all our computations, we have taken a zero drift velocity

$$b^* = 0. \quad (4.141)$$

This is actually a necessary condition for the present geometrical setting of isolated solid obstacles. Indeed, recall our assumption (4.1) on the velocity fields b, b^s :

$$b^* = \frac{1}{|Y^0|} \int_{Y^0} b(y) dy = \frac{1}{|\partial\Sigma^0|} \int_{\partial\Sigma^0} b^s(y) d\sigma(y).$$

Since the surface velocity field b^s is divergence free, an integration by parts shows that

$$\int_{\partial\Sigma^0} e_k \cdot b^s(y) d\sigma(y) = - \int_{\partial\Sigma^0} y_k \operatorname{div}^s b^s(y) d\sigma(y) = 0.$$

(It is only in the case of a connected solid part, which can happen only in dimension $d \geq 3$, that one can have $b^* \neq 0$.) For simplicity we have taken $b^s = 0$ on $\partial\Sigma^0$. We have computed the mean zero velocity field b in Y^0 by taking $b = \operatorname{curl} \psi = (-\partial_{x_2} \psi, \partial_{x_1} \psi)$, with

$$\begin{cases} -\operatorname{div}(\mathcal{M}(y)\nabla\psi) = 1 & \text{in } Y^0, \\ \psi = 0 & \text{on } \partial\Sigma^0, \\ \psi & Y - \text{periodic.} \end{cases} \quad (4.142)$$

where \mathcal{M} is a 2×2 matrix. We can choose the velocity field b to be either symmetric or non-symmetric. For example, taking \mathcal{M} to be an identity matrix we obtain a symmetric matrix. On the other hand, taking \mathcal{M} to be a variable diagonal matrix with the following diagonal elements we obtain a non-symmetric velocity field.

$$\mathcal{M}_{11} = \begin{cases} 0.01 + (0.5 * y_1) & \text{if } y_1 < 0.5 \\ 0.26 + (y_1 - 0.5) & \text{otherwise} \end{cases}$$

$$\mathcal{M}_{22} = \cos(y_1)$$

Thus obtained velocity fields are shown in Figure 4.1.

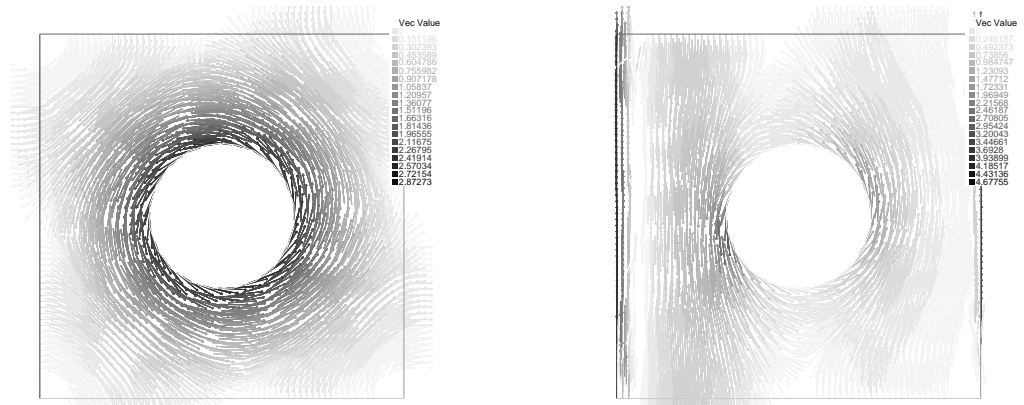


Figure 4.1: Left: Symmetric velocity field in the unit cell, Right: Non-symmetric velocity field in the unit cell.

The expression for the dispersion matrix given in (4.113) implies that the dispersion tensor depends on the homogenized solution. In a first experiment, we study the behaviour of \mathcal{D}_{11} and \mathcal{D}_{22} with respect to the magnitude of u_0 when the velocity field b is symmetric. Figure 4.2 shows the results obtained

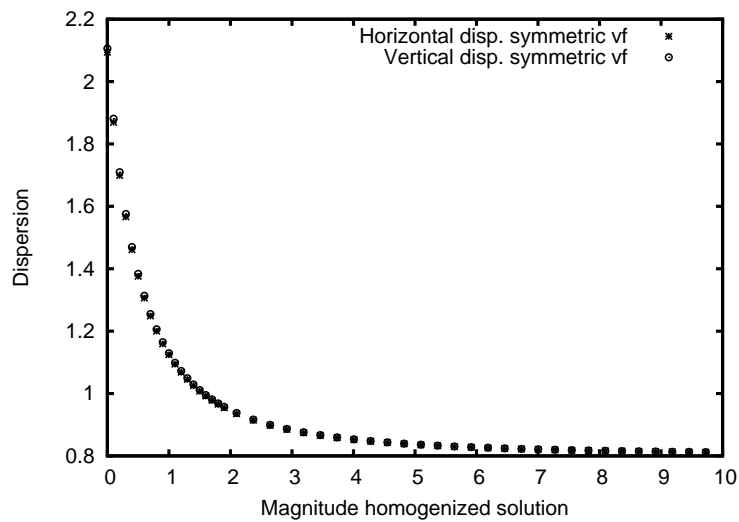


Figure 4.2: Dispersion w.r.t the magnitude of u_0 .

In our second experiment, we take the velocity field b to be non-symmetric and study the behaviour of \mathcal{D}_{11} and \mathcal{D}_{22} with respect to the magnitude of u_0 . Figure 4.3 shows the results obtained.

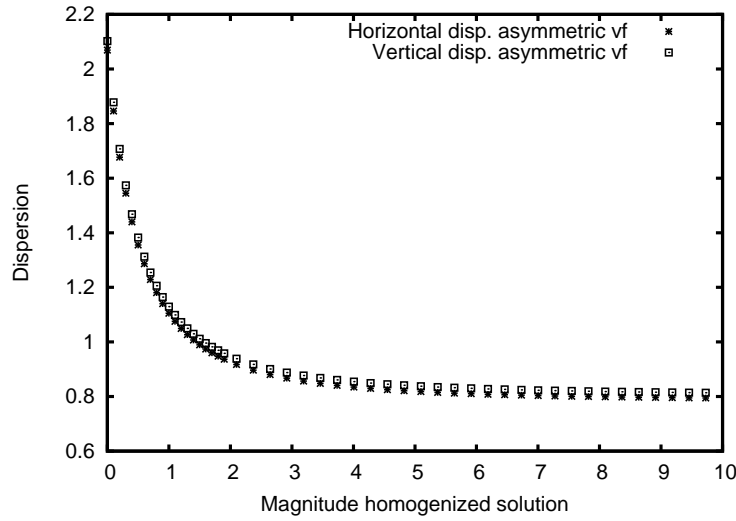


Figure 4.3: Dispersion w.r.t the magnitude of u_0 .

As seen in Figures 4.2 and 4.3, in the limit $u_0 \rightarrow \infty$, both horizontal and vertical dispersions attain a limit. In this limit, the cell problem (4.114) gets decoupled. The equation for χ_i is given by

$$\begin{cases} -b^* \cdot e_i + b(y) \cdot (e_i + \nabla_y \chi_i) - \operatorname{div}_y(D(e_i + \nabla_y \chi_i)) = 0 & \text{in } Y^0, \\ -D(e_i + \nabla_y \chi_i) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \chi_i(y) & Y\text{-periodic.} \end{cases} \quad (4.143)$$

The cell solution χ_i from (4.143) acts as a source term for the cell solution on the surface governed by the following equation.

$$-b^* \cdot e_i + b^s(y) \cdot (e_i + \nabla_y^s \omega_i) - \operatorname{div}_y^s(D^s(e_i + \nabla_y^s \omega_i)) + \kappa \omega_i = \kappa \chi_i \quad \text{on } \partial \Sigma^0$$

In our case, we have taken the velocity field b^s to be zero and also the drift b^* is zero. Thus, the above equation for ω_i is a simple elliptic equation.

In Figure 4.4 we plot the horizontal dispersion with respect to D^s .

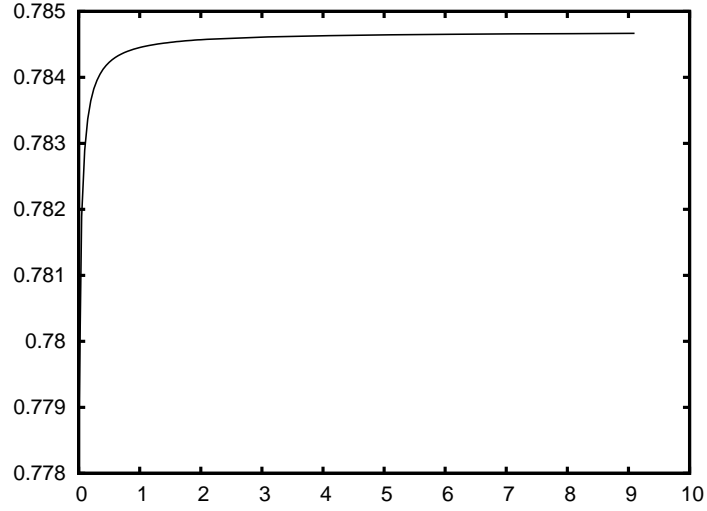


Figure 4.4: Horizontal Dispersion w.r.t surface molecular diffusion.

Clearly the dispersion increases with D^s . However, as shown by Figure 4.4, the dispersion reaches a limit as D^s goes to infinity. This can be explained formally by the fact that, in such a case, the cell solution satisfies in the limit that $(\omega_i + y_i)$ is constant on the pore surface $\partial\Sigma^0$. In this limit, the bulk correctors χ_i satisfy the following limit problem

$$\left\{ \begin{array}{ll} b(y) \cdot \nabla_y \chi_i - \operatorname{div}_y (D(\nabla_y \chi_i + e_i)) = (b^* - b) \cdot e_i & \text{in } Y^0, \\ -D(\nabla_y \chi_i + e_i) \cdot n + b_i^* = \\ \frac{\alpha \kappa}{(1 + \beta u_0)^2} \left(\chi_i + y_i - |\partial\Sigma^0|^{-1} \int_{\partial\Sigma^0} (\chi_i + y_i) d\sigma(y) \right) & \text{on } \partial\Sigma^0, \\ y \rightarrow \chi_i(y) & Y\text{-periodic.} \end{array} \right. \quad (4.144)$$

In Figure 4.5 we plot the horizontal dispersion with respect to κ .

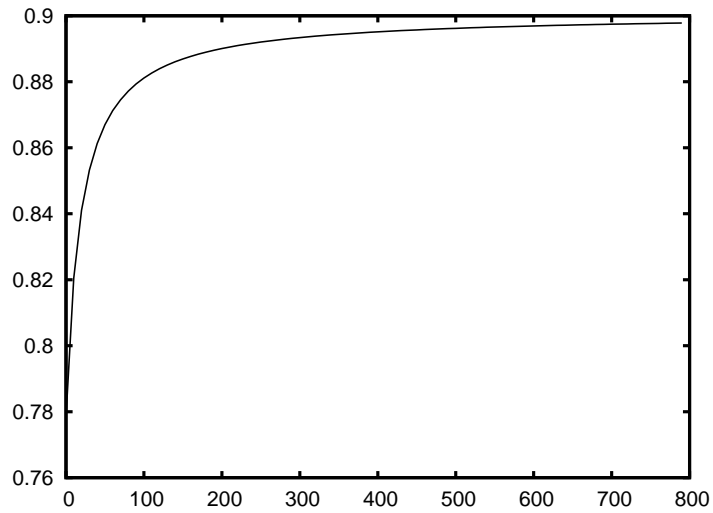


Figure 4.5: Horizontal Dispersion w.r.t reaction rate.

In the limit $\kappa \rightarrow \infty$, we get an asymptote for the dispersion, corresponding to a limit cell problem

where $\chi_i = \omega_i$. In this limit, the corresponding system satisfied by the bulk correctors χ_i is

$$\begin{cases} b(y) \cdot \nabla_y \chi_i - \operatorname{div}_y (D(\nabla_y \chi_i + e_i)) = (b^* - b) \cdot e_i & \text{in } Y^0, \\ -D(\nabla_y \chi_i + e_i) \cdot n + (b^* - b^S) \cdot e_i = \\ \quad b^S(y) \cdot \nabla_y^S \chi_i - \operatorname{div}_y^S (D^S(\nabla_y^S \chi_i + e_i)) & \text{on } \partial \Sigma^0, \\ y \rightarrow \chi_i(y) & Y\text{-periodic.} \end{cases} \quad (4.145)$$

Unlike (4.144), the limit cell problem corresponding to the infinite reaction limit is no longer dependent on the homogenized solution u_0 .

In the final experiment, we wish to compare the homogenized solution $u_0(t, x)$ and the reconstructed solution $\tilde{u}_\varepsilon(t, x)$ in the periodic porous medium of period $\varepsilon = 0.25$ where the reconstructed solution $\tilde{u}_\varepsilon(t, x)$ is given by

$$\tilde{u}_\varepsilon(t, x) = u_0(t, x) + \varepsilon \left(\chi_1(x/\varepsilon) \partial_{x_1} u_0(t, x) + \chi_2(x/\varepsilon) \partial_{x_2} u_0(t, x) \right) \quad (4.146)$$

The solutions to the cell problem (χ_1, χ_2) are computed in the unit cell. Figure 4.6 depicts the cell solutions χ_1 and χ_2 . Then, they are copied to each cell in the periodic domain where the cells are of size $(0.25)^2$.

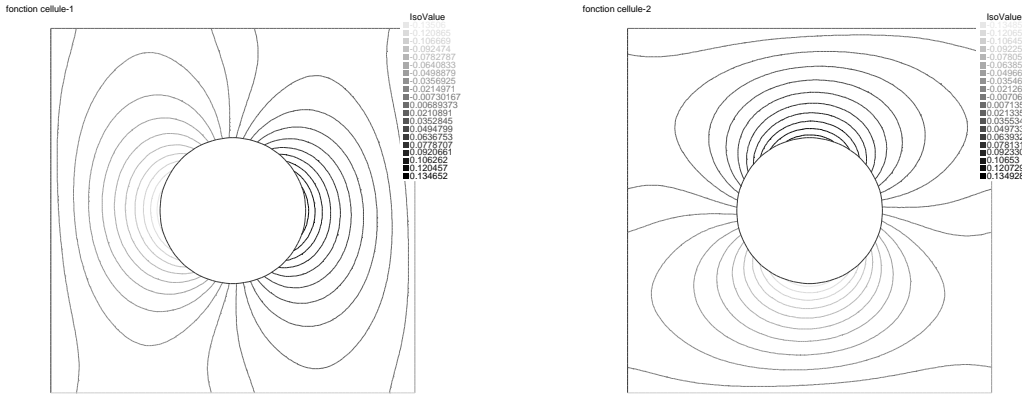


Figure 4.6: Left: Cell solution χ_1 in the unit cell, Right: Cell solution χ_2 in the unit cell.

The next task is to compute the homogenized solution to the effective equation (4.112). We have taken the initial data, (u^{in}, v^{in}) , such that the initial data to the homogenized equation has a compact support in the periodic domain. The well-prepared initial data that we have considered are

$$u^{in} = 10^3 * \max(0.0, x_1 - 0.2) * (-\min(0.0, x_1 - 0.8)) * \max(0.0, x_2 - 0.2) * (-\min(0.0, x_2 - 0.8))$$

$$\text{and } v^{in} = \alpha u^{in}.$$

We employ Rothe's method where we discretize the time derivative in the effective diffusion equation followed by Newton's method to solve the resulting elliptic equation. Since we are working with bounded domain, we need to provide boundary conditions on the exterior boundary of $]0, 1[\times]0, 1[$. As working with Dirichlet boundary data may lead to boundary layers, we have taken periodic boundary conditions. Once we have computed the homogenized solution, we can calculate the reconstructed solution using (4.146). Figures 4.7, 4.8, 4.9 refer to the evolution of the exact solution, homogenized solution and reconstructed solution respectively in the periodic porous domain.

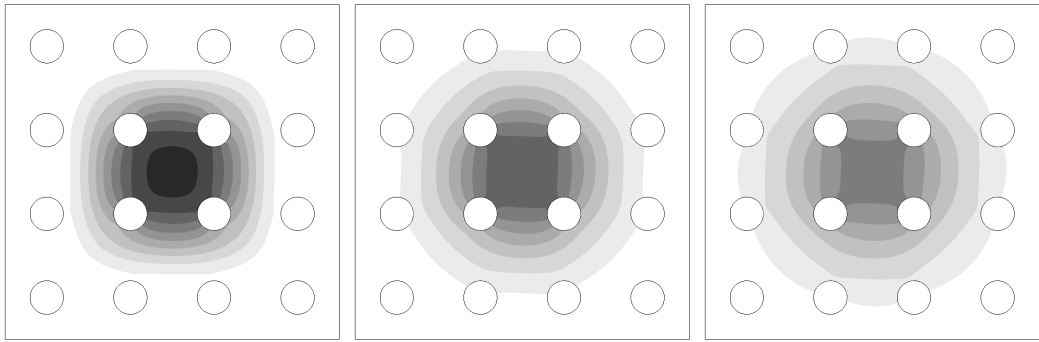


Figure 4.7: Exact Solutions: Left, Time instant 0.001; Middle, Time instant 0.005; Right, Time instant 0.01.

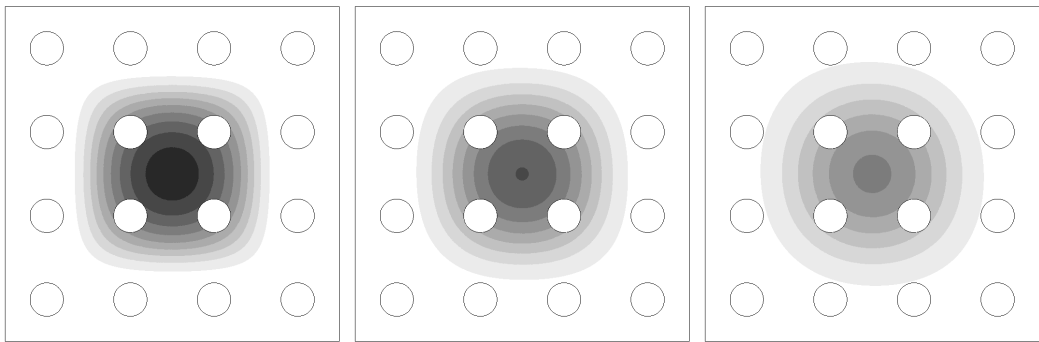


Figure 4.8: Homogenized Solutions: Left, Time instant 0.001; Middle, Time instant 0.005; Right, Time instant 0.01.

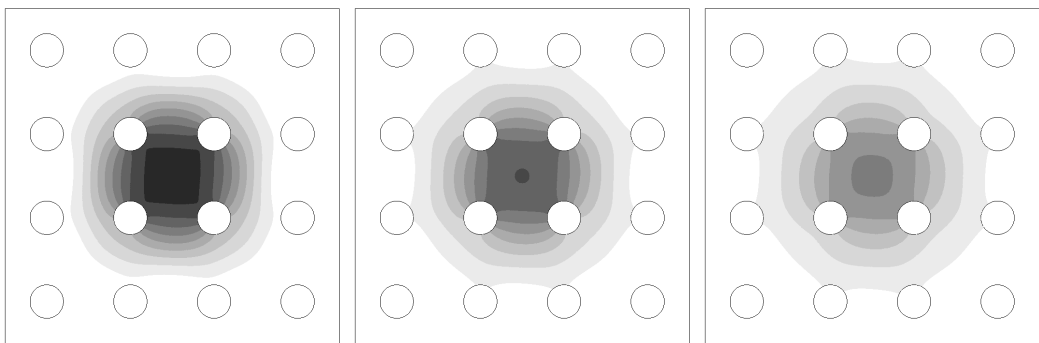


Figure 4.9: Reconstructed Solutions: Left, Time instant 0.001; Middle, Time instant 0.005; Right, Time instant 0.01.

We remark that there isn't a very good agreement between the exact solution (Figure 4.7) and with the reconstructed solution (4.9). We believe it is due to the fact that we have taken the periodicity to be 0.25 which might be too big to appreciate the homogenization results.

4.11 Comments

The comments on the locally periodic coefficients in Section 3.14 of Chapter 3 do hold true for the nonlinear model considered in this chapter.

Constraints on the velocity fields

The presence of the nonlinear term in (4.12)-(4.14) forced us to impose a constraint that the bulk and surface drifts are the same i.e.,

$$\frac{1}{|Y^0|} \int_{Y^0} b(y) dy = \frac{1}{|\partial\Sigma^0|} \int_{\partial\Sigma^0} b^s(y) d\sigma(y) = b^*. \quad (4.147)$$

We are unable to upscale, even formally, the microscopic equations (4.12)-(4.14) unless the constraint (4.147) holds true. The main reason for imposing this equal drift constraint is the inability of the method of two-scale convergence with drift to handle non constant drifts. We remarked in Section 4.10 that, in two dimensions, the constraint (4.147) translates as $b^* = 0$. Only for $d \geq 3$ we can have a non zero drift under the assumption (4.147). This difficulty in handling, at least purely periodic velocity fields, in presence of nonlinear isotherms emphasize the need for generalizing the method of two-scale convergence with drift to non constant drift scenarios.

Let us consider the following two-scale asymptotic expansions with drift.

$$u_\varepsilon(t, x) = \sum_{i \geq 0} \varepsilon^i u_i \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right). \quad (4.148)$$

The above ansatz (4.148) can be rewritten in the following manner

$$u_\varepsilon(t, x) = \sum_{i \geq 0} \varepsilon^i u_i \left(t, X(-\tau, x), \frac{x}{\varepsilon} \right) \quad (4.149)$$

where $X(\tau, x)$ with $\tau = \varepsilon^{-1}t$ is the solution of

$$\begin{cases} \frac{dX}{d\tau} = b^* \\ X(0) = x. \end{cases} \quad (4.150)$$

In [87], the following singularly perturbed convection equation is studied.

$$\frac{\partial u_\varepsilon}{\partial t} + a \cdot \nabla u_\varepsilon + \frac{1}{\varepsilon} b \cdot \nabla u_\varepsilon = 0. \quad (4.151)$$

There are no fast oscillating coefficients in (4.151) i.e., $a = a(t, x)$ and $b = b(t, x)$. It is shown in [87] that u_ε admits the following asymptotic expansion.

$$u_\varepsilon(t, x) = \sum_{i \geq 0} \varepsilon^i u_i \left(t, \tau, x \right) \quad (4.152)$$

where $u_i(t, \tau, x)$ are 2π periodic in $\tau = \varepsilon^{-1}t$. The authors of [87] consider

$$\begin{cases} \frac{dX}{d\tau} = b(t, X) \\ X(0) = x. \end{cases} \quad (4.153)$$

An assumption is made on the velocity b such that $\tau \rightarrow X(\tau; t, x)$ is 2π periodic in τ . Denote the Jacobian matrix of $x \rightarrow X(\tau; t, x)$ by $\nabla X(\tau; t, x)$. It is proved in [87] that the first term of (4.152) is given by

$$u_0(t, \tau, x) = v_0(t, X(-\tau; t, x)) \quad (4.154)$$

where v_0 satisfies

$$\frac{\partial v_0}{\partial t} + \tilde{a}^0 \cdot \nabla v_0 = 0 \quad \text{in } (0, T) \times \mathbb{R}^d. \quad (4.155)$$

and u_0 satisfies

$$\frac{\partial u_0}{\partial t} + a^0 \cdot \nabla v_0 = 0 \quad \text{in } (0, T) \times \mathbb{R}^d. \quad (4.156)$$

with a^0 and \tilde{a}^0 given by the following expressions

$$a^0(t, x) = \frac{1}{2\pi} \int_0^{2\pi} \nabla X(\tau; t, x)^{-1} a(t, X(\tau; t, x)) d\tau, \quad (4.157)$$

$$\tilde{a}^0(t, x) = \frac{1}{2\pi} \int_0^{2\pi} \alpha(t, \tau, x) d\tau, \quad (4.158)$$

with

$$\alpha(t, \tau, x) = \nabla X(\tau; t, x)^{-1} \left(a(t, X(\tau; t, x)) - \frac{\partial X}{\partial t}(\tau; t, x) \right). \quad (4.159)$$

Remark the similarities between (4.149) and (4.154). Once again, it should be noted that the problem studied in [87] has no fast oscillating coefficients in (4.151). We hope that a careful adaptation of some of the results from [87] can result in a generalization of the method of two-scale asymptotic with drift by replacing the constant drift b^* in (4.150) by a variable. Of course, the approach of [87] makes certain assumptions on the velocity field b (please refer to [87] for details) in order to guarantee 2π periodic solutions for (4.153). Asymptotic expansions similar to the ones used in [87] had appeared earlier in [123] in the context of Euler equations with rapidly varying initial data.

Conclusions

This Chapter considered the upscaling of reactive flow equations with Langmuir isotherm in periodic porous media. The lack of technical tools in the theory of homogenization has restricted the analysis as can be gathered by the equal drifts assumption (4.147). In Section 3.12 of Chapter 3, we considered compressible flows. We had used Factorization principle to homogenize the model. The presence of the nonlinear term in the present chapter has restricted us from relaxing the incompressibility condition on the velocity fields as is not clear as to the approach of the principle of Factorization adapted to the nonlinear setting. So, there is a lot of room for improvement with regard to the homogenization of the current nonlinear adsorption model. Even though we have demonstrated the calculations for the Langmuir isotherm, the result of homogenization holds to in case of Freundlich isotherm too. However, the technical details get more involved in the latter case. In the previous and the current chapters, we studied single component flows. The next Chapter aims at generalizing the results to the multicomponent flows.

Chapter 5

Multicomponent flows

5.1 Introduction

Chapters 3 and 4 were dedicated to the study of reactive transport of a single dissolved solute in a fluid filling the porous medium, the type of reaction considered being the adsorption/desorption type. In Section 3.12 of Chapter 3, we even remarked that the presence of a compressible fluid is equivalent to the study of convection diffusion reaction equation in the fluid bulk. This Chapter tries to generalize the results obtained previously to the transport of multiple solutes in porous media. In presence of multiple components, one approach would be to consider transport equations for each of the scalar quantities with no coupling terms. The approach of decoupled system is simple. In the present work, we study a system of convection-diffusion equations coupled through a zero order term. As in all homogenization problems, we scale the adimensionalized system. The scaling considered is parabolic i.e., $(\tau, y) \rightarrow (\varepsilon^{-2}t, \varepsilon^{-1}x)$. Homogenization of parabolically scaled scalar parabolic equation with a zero order term was studied in [76] where they showed the induction of a large drift in the concentration profiles of the homogenized solution. In [25] the results of [76] are adopted in the case of transport phenomena in porous media. In [25], reactions are considered both in the bulk (zero order term) and on the surface of the porous skeleton (non-homogeneous Neumann boundary condition). This Chapter generalizes the results in [76] to a multicomponent flow in porous media. The reaction among multiple solutes can be modelled mathematically via a coupling matrix (linear model). In [98], a coupled system of convection-diffusion-reaction systems are considered. The problem addressed in [98] is in a porous medium with semi-permeable porous skeleton using the double-porosity model [29]. The system they study, however, is under different scaling (Diffusion dominated regime) which avoids the phenomena of drift in the concentration profiles.

The motivation for the choice of scaling to be parabolic is to study the long term behaviour of the system. It is to be noted that there are other scaling techniques available. One such among them is the hyperbolic scaling where the space variable is scaled as in the parabolic scaling whereas the time variable is scaled as $\tau \rightarrow \varepsilon^{-1}t$. In other words, for shorter times. In [139] and [128] hyperbolic scaling is considered in connection to the study of motor proteins.

Starting with a Cauchy problem for a coupled convection-diffusion-reaction system of which u_α^ε are solutions, we show in Proposition 5.4.1 that they admit a representation, for $1 \leq \alpha \leq N$,

$$u_\alpha^\varepsilon(t, x) \approx \exp(-\lambda t/\varepsilon^2) \varphi_\alpha\left(\frac{x}{\varepsilon}\right) \left(v\left(t, x - \frac{b^*}{\varepsilon}t\right) + \varepsilon \sum_{i=1}^d \frac{\partial v}{\partial x_i}\left(t, x - \frac{b^*}{\varepsilon}t\right) \omega_{i,\alpha}\left(\frac{x}{\varepsilon}\right) \right)$$

where $(\lambda, \varphi_\alpha)$ is the first eigenpair associated with an eigen cell problem. The drift velocity b^* is

given in term of the microscopic velocity fields, diffusion matrices and the eigenfunctions of the same eigen cell problem and its adjoint. v is the solution of the following scalar homogenized diffusion equation.

$$\rho^* \frac{\partial v}{\partial t} - \operatorname{div}(\mathcal{D}\nabla v) = 0.$$

Making the change of functions: $\tilde{v}(t, x) = \exp(-\lambda t/\varepsilon^2)v(t, x - \frac{b^*}{\varepsilon}t)$, we remark that \tilde{v} indeed satisfies the following scalar convection-diffusion-reaction equation.

$$\rho^* \frac{\partial \tilde{v}}{\partial t} + \rho^* \frac{b^*}{\varepsilon} \cdot \nabla \tilde{v} - \operatorname{div}(\mathcal{D}\nabla \tilde{v}) + \rho^* \frac{\lambda}{\varepsilon^2} \tilde{v} = 0.$$

Proposition 5.4.1 has close resemblance with the results obtained in [139], [128]. Their approach is to use the classical exponential transformation $u_\alpha^\varepsilon = \exp(-R_\alpha/\varepsilon)$ and to study an averaged Hamilton-Jacobi equation satisfied by the common limit R of R_α in the Crandall-Lions viscosity sense. The result of the non-stationary problem studied in [128] is that

$$u_\alpha^\varepsilon(t, x) \approx \phi_\alpha\left(\frac{x}{\varepsilon}\right)\delta(x - b^*t)$$

where a Dirac mass appears instead of our homogenized solution v . The drift velocity $b^* = \nabla H(0)$ with H being the effective Hamiltonian. The absence of the exponential term in their results is because 0 happens to be the first eigenvalue of the associated cell eigen problem.

Proposition 5.4.1 uses a formal approach to upscale the system. We use two-scale asymptotic expansions with drift where we assume that u_α^ε has an the asymptotic expansion in ε where we insert the large drift b^*/ε only in the macroscopic variable of the coefficients. This formal method of two-scale asymptotics with drift has been recalled in Section 2.6 of Chapter 2. Also, we multiply the asymptotic expression with $\exp(-\lambda t/\varepsilon^2)$ to get rid of any exponential growth. This method of Factorization is detailed in Section 2.8 of Chapter 2. This formal method of obtaining the homogenized equation will be made rigorous in Sections 5.5 and 5.6 where we derive compactness of the solution sequences $(u_\alpha^\varepsilon)_{1 \leq \alpha \leq N}$ in the moving coordinates $x + \frac{b^*}{\varepsilon}t$. Then, using the compactness results of Chapter 2, we can pass to the limit in the variational formulation of the original problem to arrive at the homogenization result. This concept of drift has been used in the asymptotic analysis literature for some time now. In case of a stationary elliptic eigenvalue problem, the concept of drift was used in [51], [53] via θ -exponential eigenvalue problems. This approach via θ -exponential eigenvalue problems has also been applied in the context of multigroup neutronic diffusion models of evolution type in [52]. The drift in the non stationary parabolic equations was used in [76].

In Section 5.7, we consider a multicomponent flow model where the zero order coupling term appears as a Neumann condition on the pore boundaries. The homogenization result concerning this boundary reaction model is given in Section 5.8. Adsorption isotherm that we studied in Chapter 3 is also incorporated into a multicomponent flow model in Section 5.9 where each component is allowed to adsorb/desorb on to the porous skeleton followed by a diffusive reaction among the adsorbed quantities on the boundary.

5.2 Mathematical model

Let us consider N components dissolved in a fluid filling a porous medium. Denote by u_α , the concentration of the α^{th} component. Consider a system of weakly coupled linear convection diffusion reaction equations. The weak coupling is in the sense that the coupling is via zero order terms.

$$\rho_\alpha \frac{\partial u_\alpha}{\partial \tau} + b_\alpha \cdot \nabla u_\alpha - \operatorname{div}(D_\alpha \nabla u_\alpha) + \sum_{\beta=1}^N \Pi_{\alpha\beta} u_\beta = 0 \text{ in } (0, \zeta) \times \Omega_f \quad \text{for each } 1 \leq \alpha \leq N, \quad (5.1)$$

where ρ_α is the porosity, b_α is the fluid velocity, D_α for each $1 \leq \alpha \leq N$ are the diffusion matrices associated with the solutes and the coupling matrix Π models the possible bulk reactions. In reality there is only one velocity field, $b_\alpha = b$ present in (5.1) as part of a convection term. As our analysis works for N velocity fields, one for each of the components, we have considered N velocity fields $(b_\alpha)_{1 \leq \alpha \leq N}$. To complete (5.1), we have to supplement it with initial and boundary data. The boundary data we consider is of Neumann type, i.e., zero flux condition on the surface of the pores.

$$D_\alpha \nabla u_\alpha \cdot n = 0 \quad \text{on } (0, \zeta) \times \partial\Omega_s \quad \text{for each } 1 \leq \alpha \leq N. \quad (5.2)$$

We assume that the coefficients in (5.1) are all Y -periodic. The porosity coefficients $\rho_\alpha(y)$, for every $1 \leq \alpha \leq N$, are assumed to be strictly positive. The velocity fields are assumed to be independent of time and given. We don't impose any constraint of incompressibility. In the linear single solute case studied in Chapter 3 we observed, in Section 3.12, that the condition of incompressibility on the fluid field can be relaxed. However, this wasn't the case in Chapter 4 where a convection diffusion reaction equation was studied with a zero order nonlinear term. Of course, some regularity is required for the fluid velocity and we assume that

$$b_\alpha(y) \in L^\infty(Y^0; \mathbb{R}^d). \quad (5.3)$$

Associated with N solutes, we have N diffusion matrices $D_\alpha(y)$, each of which are assumed to be in $L^\infty(Y^0)$, symmetric and uniformly coercive. That is, there exists a positive constant C such that, for any $\xi \in \mathbb{R}^d$,

$$D_\alpha(y)\xi \cdot \xi \geq C|\xi|^2 \text{ a.e. in } Y^0. \quad (5.4)$$

Now, the assumptions on the constant coupling matrix $(\Pi_{\alpha\beta})_{1 \leq \alpha, \beta \leq N}$. For the wellposedness of the system (5.1)-(5.2), we make the following assumption on the coupling matrix:

$$\Pi_{\alpha\beta} \leq 0 \text{ for } \alpha \neq \beta, \quad (5.5)$$

we also assume that the coupling matrix Π is irreducible i.e.,

$$\{1, \dots, N\} \neq \mathcal{B} \cup \mathcal{B}', \mathcal{B} \cap \mathcal{B}' = \emptyset \text{ such that } \Pi_{\alpha\beta} = 0 \text{ for } \alpha \in \mathcal{B}, \beta \in \mathcal{B}'. \quad (5.6)$$

The hypothesis (5.5)-(5.6) are borrowed from [152], [11], [53] where systems of elliptic and parabolic equations are studied. A matrix satisfying (5.5) is sometimes referred to as ‘‘cooperative matrix’’ or ‘‘essentially positive matrix’’.

In order to study the system (5.1)-(5.2) in an ε -periodic porous medium, we need to scale it on to the underlying microstructure. As the system under consideration is of evolution type, we need to scale the time variable too. The scaling that we employ shall be ‘‘parabolic scaling’’ in order to study the long time behavior of the considered transport phenomena. Upon parabolic scaling $(\tau, y) \rightarrow (\varepsilon^{-2}t, \varepsilon^{-1}x)$, (5.1)-(5.2) yields, for each $1 \leq \alpha \leq N$,

$$\rho_\alpha^\varepsilon \frac{\partial u_\alpha^\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\alpha^\varepsilon \cdot \nabla u_\alpha^\varepsilon - \operatorname{div}(D_\alpha^\varepsilon \nabla u_\alpha^\varepsilon) + \frac{1}{\varepsilon^2} \sum_{\beta=1}^N \Pi_{\alpha\beta} u_\beta^\varepsilon = 0 \text{ in } (0, T) \times \Omega_\varepsilon, \quad (5.7)$$

$$D_\alpha^\varepsilon \nabla u_\alpha^\varepsilon \cdot n = 0 \quad \text{on} \quad (0, T) \times \partial\Omega_\varepsilon, \quad (5.8)$$

$$u_\alpha^\varepsilon(0, x) = u_\alpha^{in}(x) \quad x \in \mathbb{R}^d. \quad (5.9)$$

As usual upon rescaling, the Y -periodic coefficients of the adimensionalized system turn out to be ε -periodic in the dimensionalized system. So, $\rho_\alpha^\varepsilon(x) = \rho_\alpha\left(\frac{x}{\varepsilon}\right)$, $b^\varepsilon(x) = b\left(\frac{x}{\varepsilon}\right)$, $D_\alpha^\varepsilon(x) = D_\alpha\left(\frac{x}{\varepsilon}\right)$ are all ε -periodic coefficients.

5.3 Qualitative analysis

The microscopic model (5.7)-(5.9) models the transport of dissolved solutes in presence of convection diffusion and reaction. In Section 2.8 of Chapter 2, while recapping the Factorization principle, we illustrated the method via a parabolically scaled scalar convection diffusion reaction equation (2.95). The present model (5.7)-(5.9) is a generalization to the transport of N solutes. The assumption (5.5) on the coefficients $\Pi_{\alpha\beta}$ in the zero order term doesn't help us obtain a priori estimates on $(u_\alpha^\varepsilon)_{1 \leq \alpha \leq N}$. In the absence of a priori estimates, it would be impossible to apply the compactness results from Homogenization theory of Chapter 2. This difficulty with partial differential equations with large lower order terms has been long recognized [100], [106], [76], [25]. The idea is to pass through spectral cell problems associated with (5.7)-(5.8).

$$\left\{ \begin{array}{ll} b_\alpha(y) \cdot \nabla_y \varphi_\alpha - \operatorname{div}_y (D_\alpha \nabla_y \varphi_\alpha) + \sum_{\beta=1}^N \Pi_{\alpha\beta} \varphi_\beta = \lambda \rho_\alpha \varphi_\alpha & \text{in } Y^0, \\ D_\alpha \nabla_y \varphi_\alpha \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \varphi_\alpha(y) & Y \text{ - periodic.} \end{array} \right. \quad (5.10)$$

In general we have no maximum principles for systems, thus making Krein-Rutman theorem [108] inapplicable. However in [152] it is shown that the first eigenvalue λ for systems similar in structure to (5.10) is positive, real and simple. And the first eigenfunction can be chosen positive. Let us denote the first eigenpair for (5.10) by $(\lambda, \varphi_\alpha)$. The first eigenvalue λ measures the balance between convection-diffusion and reaction. The spectral cell problem (5.10) isn't self-adjoint. The associated adjoint problem is

$$\left\{ \begin{array}{ll} -\operatorname{div}_y (b_\alpha \varphi_\alpha^*) - \operatorname{div}_y (D_\alpha \nabla_y \varphi_\alpha^*) + \sum_{\beta=1}^N \Pi_{\alpha\beta}^* \varphi_\beta^* = \lambda \rho_\alpha \varphi_\alpha^* & \text{in } Y^0, \\ D_\alpha \nabla_y \varphi_\alpha^* \cdot n + b_\alpha(y) \cdot n \varphi_\alpha^* = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \varphi_\alpha^*(y) & Y \text{-periodic,} \end{array} \right. \quad (5.11)$$

where Π^* is the transpose of Π . Again by [152] it follows that the first eigenvalue λ for (5.11) is the same as that for (5.10). And the first eigenfunction for (5.11) can be chosen positive. The uniqueness of the eigenfunction of (5.11) is up to a chosen normalization. The normalization that we consider is the following

$$\sum_{\alpha=1}^N \int_{Y^0} \varphi_\alpha \varphi_\alpha^* dy = 1. \quad (5.12)$$

Let us denote the first eigenpair for (5.11) by $(\lambda, \varphi_\alpha^*)$. As explained in [12, 76, 25] the first eigenvalue of the spectral cell problem λ governs the time decay of the solution u_α^ε . So, as is done in the references cited, we perform time renormalization in the spirit of the factorization principle. Also the first eigenfunction φ_α is factored out of u_α^ε . The idea is to make the following change of unknowns

$$v_\alpha^\varepsilon(t, x) = \exp(\lambda t / \varepsilon^2) \frac{u_\alpha^\varepsilon(t, x)}{\varphi_\alpha\left(\frac{x}{\varepsilon}\right)}. \quad (5.13)$$

With the above change of unknowns, we will be able to overcome the inability we had with the derivation of a priori estimates. Now we state a result that gives the system satisfied by the new unknown $(v_\alpha^\varepsilon)_{1 \leq \alpha \leq N}$.

Lemma 5.3.1. *The system (5.7)-(5.9) is equivalent to*

$$\varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon \frac{\partial v_\alpha^\varepsilon}{\partial t} + \frac{1}{\varepsilon} \tilde{b}_\alpha^\varepsilon \cdot \nabla v_\alpha^\varepsilon - \operatorname{div} \left(\tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \right) + \frac{1}{\varepsilon^2} \sum_{\beta=1}^N \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\beta^\varepsilon - v_\alpha^\varepsilon) = 0 \text{ in } (0, T) \times \Omega_\varepsilon, \quad (5.14)$$

$$\tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot n = 0 \quad \text{on } (0, T) \times \partial\Omega_\varepsilon, \quad (5.15)$$

$$v_\alpha^\varepsilon(0, x) = \frac{u_\alpha^{\text{in}}(x)}{\varphi_\alpha\left(\frac{x}{\varepsilon}\right)} \quad x \in \mathbb{R}^d, \quad (5.16)$$

for each $1 \leq \alpha \leq N$, where the components of $(v_\alpha^\varepsilon)_{1 \leq \alpha \leq N}$ are defined by (5.13). The convective velocity, $\tilde{b}_\alpha^\varepsilon(x) = \tilde{b}_\alpha\left(\frac{x}{\varepsilon}\right)$, in (5.14) is given by

$$\tilde{b}_\alpha(y) = \varphi_\alpha \varphi_\alpha^* b_\alpha + \varphi_\alpha D_\alpha \nabla_y \varphi_\alpha^* - \varphi_\alpha^* D_\alpha \nabla_y \varphi_\alpha \quad \text{for every } 1 \leq \alpha \leq N \quad (5.17)$$

and the diffusion matrix, $\tilde{D}_\alpha^\varepsilon(x) = \tilde{D}_\alpha\left(\frac{x}{\varepsilon}\right)$, in (5.14)-(5.15) is given by

$$\tilde{D}_\alpha(y) = \varphi_\alpha \varphi_\alpha^* D_\alpha \quad \text{for every } 1 \leq \alpha \leq N. \quad (5.18)$$

Proof. We shall plug the expression (5.13) in (5.7)-(5.9) while keeping in mind the following chain rule formulae

$$\begin{cases} \frac{\partial u_\alpha^\varepsilon}{\partial t}(t, x) = \frac{-\lambda}{\varepsilon^2} \exp(-\lambda t/\varepsilon^2) \varphi_\alpha\left(\frac{x}{\varepsilon}\right) v_\alpha^\varepsilon(t, x) + \exp(-\lambda t/\varepsilon^2) \varphi_\alpha\left(\frac{x}{\varepsilon}\right) \frac{\partial v_\alpha^\varepsilon}{\partial t}(t, x), \\ \nabla\left(u_\alpha^\varepsilon(t, x)\right) = \frac{1}{\varepsilon} \exp(-\lambda t/\varepsilon^2) v_\alpha^\varepsilon(t, x) \left(\nabla_y \varphi_\alpha\right)\left(\frac{x}{\varepsilon}\right) + \exp(-\lambda t/\varepsilon^2) \varphi_\alpha\left(\frac{x}{\varepsilon}\right) \nabla_x v_\alpha^\varepsilon(t, x). \end{cases} \quad (5.19)$$

Using the spectral cell problem (5.10) and its adjoint (5.11) and identifying the expressions (5.17) and (5.18), the calculations simplify to yield the system of equations (5.14)-(5.16) satisfied by $(v_\alpha^\varepsilon)_{1 \leq \alpha \leq N}$. \square

Lemma 5.3.2. *The divergence of the convective fields \tilde{b}_α satisfy*

$$\operatorname{div}_y \tilde{b}_\alpha = \sum_{\beta=1}^N \Pi_{\alpha\beta}^* \varphi_\alpha \varphi_\beta^* - \sum_{\beta=1}^N \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta \quad (5.20)$$

Proof. Let us take the divergence of the convective fields \tilde{b}_α given in (5.17), we arrive at

$$\operatorname{div}_y \tilde{b}_\alpha = \varphi_\alpha \left(\operatorname{div}_y (b_\alpha \varphi_\alpha^*) + \operatorname{div}_y (D_\alpha \nabla_y \varphi_\alpha^*) \right) + \varphi_\alpha^* \left(b_\alpha \cdot \nabla_y \varphi_\alpha - \operatorname{div}_y (D_\alpha \nabla_y \varphi_\alpha) \right) \quad (5.21)$$

Using information from the spectral cell problem (5.10) and its adjoint (5.11), we have

$$\operatorname{div}_y \tilde{b}_\alpha = -\lambda \varphi_\alpha \varphi_\alpha^* + \sum_{\beta=1}^N \Pi_{\alpha\beta}^* \varphi_\alpha \varphi_\beta^* + \lambda \varphi_\alpha \varphi_\alpha^* - \sum_{\beta=1}^N \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta$$

Thus we arrive at the result (5.20). \square

From the expression for the divergence derived in (5.20), it follows that

$$\sum_{\alpha=1}^N \operatorname{div}_y \tilde{b}_\alpha = 0. \quad (5.22)$$

By the definition (5.17) of \tilde{b}_α , it follows that

$$\tilde{b}_\alpha \cdot n = 0 \text{ on } \partial\Sigma^0. \quad (5.23)$$

Lemma 5.3.3. *Let (v_α^ε) be a weak solution of (5.14)-(5.16). There exists a constant C , independent of ε , such that*

$$\begin{aligned} & \sum_{\alpha=1}^N \left\| v_\alpha^\varepsilon \right\|_{L^\infty((0,T);L^2(\Omega_\varepsilon))} + \sum_{\alpha=1}^N \left\| \nabla v_\alpha^\varepsilon \right\|_{L^2((0,T)\times\Omega_\varepsilon)} \\ & + \frac{1}{\varepsilon} \sum_{\alpha=1}^N \sum_{\beta=1}^N \left\| v_\alpha^\varepsilon - v_\beta^\varepsilon \right\|_{L^2((0,T)\times\Omega_\varepsilon)} \leq C \sum_{\alpha=1}^N \|v_\alpha^{in}\|_{L^2(\mathbb{R}^d)} \end{aligned} \quad (5.24)$$

Proof. To derive the a priori estimates, we shall multiply (5.14) by v_α^ε and add the thus obtained expressions followed by integrating over Ω_ε .

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon |v_\alpha^\varepsilon|^2 dx - \frac{1}{2\varepsilon} \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \operatorname{div}(\tilde{b}_\alpha^\varepsilon) |v_\alpha^\varepsilon|^2 dx \\ & + \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot \nabla v_\alpha^\varepsilon dx + \frac{1}{\varepsilon^2} \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_{\Omega_\varepsilon} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\beta^\varepsilon - v_\alpha^\varepsilon) v_\alpha^\varepsilon = 0 \end{aligned} \quad (5.25)$$

To derive the energy estimate for (5.14)-(5.16), the spectral cell problem (5.10) and its adjoint (5.11) come in handy. Let us consider the bulk equation in (5.10) and multiply it by $\varphi_\alpha^*(v_\alpha^\varepsilon)^2$ followed by integration over the fluid part Y^0 .

$$\begin{aligned} & \int_{Y^0} b_\alpha \cdot \nabla_y \varphi_\alpha \varphi_\alpha^* (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \operatorname{div}_y (D_\alpha \nabla_y \varphi_\alpha) \varphi_\alpha^* (v_\alpha^\varepsilon)^2 dy + \sum_{\beta=1}^N \int_{Y^0} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \lambda \rho_\alpha \varphi_\alpha \varphi_\alpha^* (v_\alpha^\varepsilon)^2 dy \end{aligned} \quad (5.26)$$

$$= - \int_{Y^0} \operatorname{div}_y (b_\alpha \varphi_\alpha^*) \varphi_\alpha (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \varphi_\alpha \varphi_\alpha^* b_\alpha \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy + \int_{Y^0} \varphi_\alpha^* D_\alpha \nabla_y \varphi_\alpha \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy$$

$$+ \int_{Y^0} (v_\alpha^\varepsilon)^2 D_\alpha \nabla_y \varphi_\alpha \cdot \nabla_y \varphi_\alpha^* dy + \sum_{\beta=1}^N \int_{Y^0} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \lambda \rho_\alpha \varphi_\alpha \varphi_\alpha^* (v_\alpha^\varepsilon)^2 dy$$

$$= - \int_{Y^0} \operatorname{div}_y (b_\alpha \varphi_\alpha^*) \varphi_\alpha (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \varphi_\alpha \varphi_\alpha^* b_\alpha \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy + \int_{Y^0} \varphi_\alpha^* D_\alpha \nabla_y \varphi_\alpha \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy$$

$$- \int_{Y^0} \varphi_\alpha D_\alpha \nabla_y \varphi_\alpha^* \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy + \int_{Y^0} \varphi_\alpha D_\alpha \nabla_y \varphi_\alpha^* \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy$$

$$+ \int_{Y^0} (v_\alpha^\varepsilon)^2 D_\alpha \nabla_y \varphi_\alpha \cdot \nabla_y \varphi_\alpha^* dy + \sum_{\beta=1}^N \int_{Y^0} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \lambda \rho_\alpha \varphi_\alpha \varphi_\alpha^* (v_\alpha^\varepsilon)^2 dy$$

$$= - \int_{Y^0} \operatorname{div}_y (b_\alpha \varphi_\alpha^*) \varphi_\alpha (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \operatorname{div}_y (D_\alpha \nabla_y \varphi_\alpha^*) \varphi_\alpha (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \lambda \rho_\alpha \varphi_\alpha \varphi_\alpha^* (v_\alpha^\varepsilon)^2 dy \quad (5.27)$$

$$- \int_{Y^0} \varphi_\alpha \varphi_\alpha^* b_\alpha \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy + \int_{Y^0} \varphi_\alpha^* D_\alpha \nabla_y \varphi_\alpha \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \varphi_\alpha D_\alpha \nabla_y \varphi_\alpha^* \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy \quad (5.28)$$

$$+ \sum_{\beta=1}^N \int_{Y^0} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\alpha^\varepsilon)^2 dy = 0. \quad (5.29)$$

In the above simplified form, we recognize the adjoint cell problem (5.11) in (5.27). We also recognize the expression for \tilde{b}_α in (5.28). Taking all these contributions into account, (5.27)-(5.28)-(5.29) result in

$$-\sum_{\beta=1}^N \int_{Y^0} \Pi_{\alpha\beta}^* \varphi_\beta^* \varphi_\alpha (v_\alpha^\varepsilon)^2 d\sigma(y) - \int_{Y^0} \tilde{b}_\alpha \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy + \sum_{\beta=1}^N \int_{Y^0} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\alpha^\varepsilon)^2 d\sigma(y) = 0 \quad (5.30)$$

Summing (5.30) over α leads to

$$\sum_{\alpha=1}^N \int_{Y^0} \operatorname{div}_y \tilde{b}_\alpha (v_\alpha^\varepsilon)^2 dy = 0. \quad (5.31)$$

Using the above observation (5.31) in the expression (5.25) results in the following energy estimate.

$$\frac{1}{2} \frac{d}{dt} \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon |v_\alpha^\varepsilon|^2 dx + \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot \nabla v_\alpha^\varepsilon dx + \frac{1}{\varepsilon^2} \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_{\Omega_\varepsilon} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta |v_\alpha^\varepsilon - v_\beta^\varepsilon|^2 = 0 \quad (5.32)$$

Integrating the energy estimate (5.32) over $(0, T)$ yields the a priori estimates (5.24). \square

In the above Lemma 5.3.3, we have derived a priori estimates for the solution sequences of (5.14)-(5.16) obtained upon performing a change of unknowns (5.13). Now we state a result asserting the well-posedness of the system of equations (5.7)-(5.9).

Proposition 5.3.4. *Assume that the initial data u_α^{in} belongs to $L^2(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ for every $1 \leq \alpha \leq N$. For any given $\varepsilon > 0$, there exists a unique solution u_α^ε of (5.7)-(5.9) in the following energy space*

$$u_\alpha^\varepsilon \in L^\infty((0, T); L^2(\Omega_\varepsilon)); \quad \nabla u_\alpha^\varepsilon \in L^2((0, T) \times \Omega_\varepsilon) \quad \text{for every } 1 \leq \alpha \leq N. \quad (5.33)$$

Further if the initial data $u_\alpha^{in} \geq 0$ in Ω_ε , then the solution $u_\alpha^\varepsilon(t, x) \geq 0$ in $(0, T) \times \Omega_\varepsilon$.

We avoid the proof of the Proposition 5.3.4. The arguments of the proof are similar to the existence results and maximum principles proved in [152], [129], [43].

5.4 Formal asymptotics

This section is concerned with finding the effective behaviour of (5.7)-(5.9). We shall be employing a formal method of asymptotic expansions. We consider the following time renormalized asymptotic ansatz for the solution u_α^ε .

$$u_\alpha^\varepsilon(t, x) = \exp(-\lambda t/\varepsilon^2) \sum_{i \geq 0} \varepsilon^i u_{i,\alpha} \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \quad \text{for every } 1 \leq \alpha \leq N. \quad (5.34)$$

Proposition 5.4.1. *If the ansatz for the solution (u_α^ε) of (5.7)-(5.9) given in (5.34) is true, then the solution formally satisfies*

$$u_\alpha^\varepsilon(t, x) \approx \exp(-\lambda t/\varepsilon^2) \varphi_\alpha \left(\frac{x}{\varepsilon} \right) \left(v \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon \sum_{i=1}^d \frac{\partial v}{\partial x_i} \left(t, x - \frac{b^* t}{\varepsilon} \right) \omega_{i,\alpha} \left(\frac{x}{\varepsilon} \right) \right), \quad (5.35)$$

with $(\lambda, \varphi_\alpha)$ being the first eigenpair associated with (5.10). The components $(\omega_{i,\alpha})_{1 \leq \alpha \leq N}$, for every $1 \leq i \leq d$, satisfy a so called cell problem.

$$\begin{cases} \tilde{b}_\alpha(y) \cdot (\nabla_y \omega_{i,\alpha} + e_i) - \operatorname{div}_y (\tilde{D}_\alpha (\nabla_y \omega_{i,\alpha} + e_i)) \\ + \sum_{\beta=1}^N \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (\omega_{i,\beta} - \omega_{i,\alpha}) = \varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* \cdot e_i & \text{in } Y^0, \\ \tilde{D}_\alpha (\nabla_y \omega_{i,\alpha} + e_i) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \omega_{i,\alpha} & Y\text{-periodic,} \end{cases} \quad (5.36)$$

where the drift velocity b^* is given by

$$b^* = \frac{1}{\rho^*} \sum_{\alpha=1}^N \int_{Y^0} \tilde{b}_\alpha(y) dy \quad (5.37)$$

where ρ^* is the effective porosity given by

$$\rho^* = \sum_{\alpha=1}^N \int_{Y^0} \varphi_\alpha \varphi_\alpha^* \rho_\alpha(y) dy \quad (5.38)$$

with φ_α^* the first eigenfunction associated with the adjoint spectral cell problem (5.11).

Further, v in (5.35) satisfies the following scalar homogenized equation:

$$\begin{cases} \rho^* \frac{\partial v}{\partial t} - \operatorname{div}(\mathcal{D} \nabla v) = 0 & \text{in } (0, T) \times \mathbb{R}^d, \\ v(0, x) = \sum_{\alpha=1}^N u_\alpha^{in}(x) \int_{Y^0} \varphi_\alpha^*(y) dy & \text{in } \mathbb{R}^d. \end{cases} \quad (5.39)$$

where \mathcal{D} is defined by

$$\begin{aligned} \mathcal{D}_{ij} &= \sum_{\alpha=1}^N \int_{Y^0} \tilde{D}_\alpha (\nabla_y \omega_{i,\alpha} + e_i) \cdot (\nabla_y \omega_{j,\alpha} + e_j) dy \\ &\quad - \frac{1}{2} \sum_{\alpha,\beta=1}^N \int_{Y^0} \varphi_\alpha^* \varphi_\beta \Pi_{\alpha\beta} (\omega_{i,\alpha} - \omega_{i,\beta}) (\omega_{j,\alpha} - \omega_{j,\beta}) dy. \end{aligned} \quad (5.40)$$

In the expression (5.37) for the effective drift, remark the possibility of having a non zero drift even in the absence of microscopic convective velocity field. This is sometimes referred to as ‘‘Reaction induced convection’’ in the literature. Before we give the proof of Proposition 5.4.1, we shall state and prove some results that fill in the calculations for the formal asymptotic analysis with the assumed ansatz (5.34).

Lemma 5.4.2. *Each of the zero-order terms in the postulated ansatz (5.34), $u_{0,\alpha}(t, x, y)$, can be expressed as a product of a purely periodic function and a macroscopic function not depending on the fast variable y . The purely periodic function turns out to be the first eigenfunction associated with the spectral cell problem (5.10).*

Proof. Upon plugging (5.34) into (5.7)-(5.9), we identify the system at order ε^{-2} , for each $1 \leq \alpha \leq N$,

$$\begin{cases} b_\alpha(y) \cdot \nabla_y u_{0,\alpha} - \operatorname{div}_y \left(D_\alpha \nabla_y u_{0,\alpha} \right) + \sum_{\beta=1}^N \Pi_{\alpha\beta} u_{0,\beta} = \lambda \rho_\alpha u_{0,\alpha} & \text{in } Y^0, \\ D_\alpha \nabla_y u_{0,\alpha} \cdot n = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow u_{0,\alpha} & Y\text{-periodic.} \end{cases} \quad (5.41)$$

The above system is a spectral problem same as (5.10) of which λ is the first eigenvalue and φ_α is the first positive eigenfunction. Thus, we deduce that there exists a function v independent of y such that

$$u_{0,\alpha}(t, x, y) = \varphi_\alpha(y)v(t, x) \quad \text{for every } 1 \leq \alpha \leq N. \quad (5.42)$$

□

Lemma 5.4.3. *The first order correctors in the postulated ansatz (5.34), $u_{1,\alpha}(t, x, y)$, can be decomposed as a product of the derivatives of the zero order term and periodic functions satisfying a system of stationary convection-diffusion-reaction equations in a unit cell which we call the cell problem.*

$$\begin{cases} \tilde{b}_\alpha(y) \cdot \left(\nabla_y \omega_{i,\alpha} + e_i \right) - \operatorname{div}_y \left(\tilde{D}_\alpha \left(\nabla_y \omega_{i,\alpha} + e_i \right) \right) \\ + \sum_{\beta=1}^N \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta \left(\omega_{i,\beta} - \omega_{i,\alpha} \right) = \varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* \cdot e_i & \text{in } Y^0, \\ \tilde{D}_\alpha \left(\nabla_y \omega_{i,\alpha} + e_i \right) \cdot n = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow \omega_{i,\alpha} & Y\text{-periodic,} \end{cases} \quad (5.43)$$

for every $1 \leq i \leq d$ and for every $1 \leq \alpha \leq N$. The unknown drift velocity b^* in the ansatz (5.34) is given by (5.37).

Proof. As with the analysis of asymptotic analysis, we identify the coefficients at different orders of ε upon substituting (5.34) in (5.7)-(5.9). In the proof of Lemma 5.4.2, we identified the system at order ε^{-2} . In the current proof, we shall identify the system that we obtain at order ε^{-1} .

$$\begin{cases} b_\alpha \cdot \nabla_y u_{1,\alpha} - \operatorname{div}_y \left(D_\alpha \nabla_y u_{1,\alpha} \right) + \sum_{\alpha=1}^N \Pi_{\alpha\beta} u_{1,\beta} - \lambda \rho_\alpha u_{1,\alpha} \\ = \left(\rho_\alpha b^* - b_\alpha \right) \cdot \nabla_x u_{0,\alpha} + \operatorname{div}_y \left(D_\alpha \nabla_x u_{0,\alpha} \right) + \operatorname{div}_x \left(D_\alpha \nabla_y u_{0,\alpha} \right) & \text{in } Y^0, \\ D_\alpha \left(\nabla_y u_{1,\alpha} + \nabla_x u_{0,\alpha} \right) \cdot n = 0 & \text{on } \partial\Sigma^0, \\ y \rightarrow u_{1,\alpha} & Y\text{-periodic.} \end{cases} \quad (5.44)$$

Since we know the form of $u_{0,\alpha}$ from (5.42), the linearity of (5.44) help us deduce that

$$u_{1,\alpha}(t, x, y) = \sum_{i=1}^d \frac{\partial v}{\partial x_i}(t, x) \varphi_\alpha(y) \omega_{i,\alpha}(y) \quad \text{for every } 1 \leq \alpha \leq N. \quad (5.45)$$

By taking $\varphi_\alpha(y) \omega_{i,\alpha}(y) = \zeta_{i,\alpha}(y)$, for every $1 \leq \alpha \leq N$, we shall write the following system for

$(\zeta_{i,\alpha})_{1 \leq i \leq d}$:

$$\begin{cases} b_\alpha(y) \cdot \nabla_y \zeta_{i,\alpha} - \operatorname{div}_y (D_\alpha \nabla_y \zeta_{i,\alpha}) + \sum_{\beta=1}^N \Pi_{\alpha\beta} \zeta_{i,\beta} - \lambda \rho_\alpha \zeta_{i,\alpha} \\ = \varphi_\alpha (\rho_\alpha b^* - b_\alpha) \cdot e_i + \operatorname{div}_y (\varphi_\alpha D_\alpha e_i) + D_\alpha \nabla_y \varphi_\alpha \cdot e_i & \text{in } Y^0, \\ D_\alpha (\nabla_y \zeta_{i,\alpha} + \varphi_\alpha e_i) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \zeta_{i,\alpha} & Y\text{-periodic.} \end{cases} \quad (5.46)$$

Invoking Fredholm alternative we know that the compatibility condition for the existence of first eigenpair for the above system is that the right hand side of (5.46) is orthogonal to $(\varphi_\alpha^*)_{1 \leq \alpha \leq N}$, i.e.,

$$\begin{aligned} & \sum_{\alpha=1}^N \left(\int_{Y^0} \varphi_\alpha^* \varphi_\alpha (\rho_\alpha b^* - b_\alpha) \cdot e_i \, dy + \int_{Y^0} \operatorname{div}_y (\varphi_\alpha D_\alpha e_i) \varphi_\alpha^* \, dy \right. \\ & \left. + \int_{Y^0} \varphi_\alpha^* D_\alpha \nabla_y \varphi_\alpha \cdot e_i \, dy - \int_{\partial \Sigma^0} \varphi_\alpha^* \varphi_\alpha D_\alpha e_i \cdot n \, d\sigma(y) \right) = 0 \end{aligned}$$

which is nothing but

$$\begin{aligned} & \sum_{\alpha=1}^N \left(\int_{Y^0} \varphi_\alpha^* \varphi_\alpha (\rho_\alpha b^* - b_\alpha) \cdot e_i \, dy + \int_{Y^0} \operatorname{div}_y (\varphi_\alpha \varphi_\alpha^* D_\alpha e_i) \, dy - \int_{Y^0} \varphi_\alpha D_\alpha \nabla_y \varphi_\alpha^* \cdot e_i \, dy \right. \\ & \left. + \int_{Y^0} \varphi_\alpha^* D_\alpha \nabla_y \varphi_\alpha \cdot e_i \, dy - \int_{\partial \Sigma^0} \varphi_\alpha^* \varphi_\alpha D_\alpha e_i \cdot n \, d\sigma(y) \right) = 0 \end{aligned}$$

Using the divergence theorem and identifying the expression for \tilde{b}_α from (5.17), we have

$$b^* = \frac{1}{\rho^*} \sum_{\alpha=1}^N \int_{Y^0} \tilde{b}_\alpha(y) \, dy.$$

Thus the expression for the drift velocity coincides with (5.37). Now to derive the cell problem (5.43), we shall substitute for $(\zeta_{i,\alpha})$ in (5.46) in terms of the eigenfunction (φ_α) and the cell solutions $(\omega_{i,\alpha})$.

$$\begin{cases} \varphi_\alpha b_\alpha \cdot \nabla_y \omega_{i,\alpha} - \operatorname{div}_y (\varphi_\alpha D_\alpha \nabla_y \omega_{i,\alpha}) - D_\alpha \nabla_y \varphi_\alpha \cdot \nabla_y \omega_{i,\alpha} + \sum_{\beta=1}^N \Pi_{\alpha\beta} \varphi_\beta (\omega_{i,\beta} - \omega_{i,\alpha}) \\ = \varphi_\alpha (\rho_\alpha b^* - b_\alpha) \cdot e_i + \operatorname{div}_y (\varphi_\alpha D_\alpha e_i) + D_\alpha \nabla_y \varphi_\alpha \cdot e_i & \text{in } Y^0 \\ \varphi_\alpha D_\alpha (\nabla_y \omega_{i,\alpha} + e_i) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \omega_{i,\alpha} & Y\text{-periodic.} \end{cases} \quad (5.47)$$

The simplifications to arrive at (5.47) are possible because of the spectral problem (5.10). Now, let us multiply (5.47) by (φ_α^*) both in the fluid and on the solid part. A little algebra will thus yield (5.43). \square

Before we proceed with the proof of Proposition 5.4.1 let us consider the variational formulation for the cell problem (5.36) with $(\phi_\alpha)_{1 \leq \alpha \leq N}$ as test functions.

$$\begin{aligned} & \sum_{\alpha=1}^N \int_{Y^0} (\tilde{b}_\alpha \cdot \nabla_y \omega_{i,\alpha}) \phi_\alpha dy + \sum_{\alpha=1}^N \int_{Y^0} \tilde{D}_\alpha (\nabla_y \omega_{i,\alpha} + e_i) \cdot \nabla_y \phi_\alpha dy \\ & + \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_{Y^0} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (\omega_{i,\beta} - \omega_{i,\alpha}) \phi_\alpha dy = \sum_{\alpha=1}^N \int_{Y^0} (\varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* - \tilde{b}_\alpha) \cdot e_i \phi_\alpha dy. \end{aligned} \quad (5.48)$$

Proof of Proposition 5.4.1. From Lemma 5.4.2 we have found the structure (5.42) of the zero order term in (5.34) and from Lemma 5.4.3 we have the structure of the cell problem (5.43). Continuing the identification of the coefficients, the system corresponding to the coefficients of ε^0 among the cascade is

$$\left\{ \begin{array}{l} b_\alpha \cdot \nabla_y u_{2,\alpha} - \operatorname{div}_y (D_\alpha \nabla_y u_{2,\alpha}) + \sum_{\beta=1}^N \Pi_{\alpha\beta} u_{2,\beta} - \lambda \rho_\alpha u_{2,\alpha} = -\rho_\alpha \frac{\partial u_{0,\alpha}}{\partial t} \\ + (\rho_\alpha b^* - b_\alpha) \cdot \nabla_x u_{1,\alpha} + \operatorname{div}_x (D_\alpha (\nabla_x u_{0,\alpha} + \nabla_y u_{1,\alpha})) + \operatorname{div}_y (D_\alpha \nabla_x u_{1,\alpha}) \quad \text{in } Y^0, \\ D_\alpha (\nabla_y u_{2,\alpha} + \nabla_x u_{1,\alpha}) \cdot n = 0 \quad \text{on } \partial \Sigma^0, \\ y \rightarrow u_{2,\alpha} \quad \text{Y-periodic.} \end{array} \right. \quad (5.49)$$

The solvability of the above eigenvalue problem follows from the Fredholm alternative. The compatibility condition being that the right hand side of (5.44) is orthogonal to $(\varphi_\alpha^*)_{1 \leq \alpha \leq N}$. We shall compute term by term.

$$-\sum_{\alpha=1}^N \int_{Y^0} \rho_\alpha \varphi_\alpha^* \frac{\partial u_{0,\alpha}}{\partial t} dy = -\frac{\partial v}{\partial t} \sum_{\alpha=1}^N \int_{Y^0} \varphi_\alpha \varphi_\alpha^* \rho_\alpha dy = -\rho^* \frac{\partial v}{\partial t}, \quad (5.50)$$

$$\sum_{\alpha=1}^N \int_{Y^0} \varphi_\alpha^* (\rho_\alpha b^* - b_\alpha) \cdot \nabla_x u_{1,\alpha} dy = \frac{\partial}{\partial x_i} \left\{ \sum_{\alpha=1}^N \int_{Y^0} \varphi_\alpha \varphi_\alpha^* \omega_{j,\alpha} (\rho_\alpha b^* - b_\alpha) \cdot e_i dy \right\} \frac{\partial v}{\partial x_j}, \quad (5.51)$$

$$\sum_{\alpha=1}^N \operatorname{div}_x \int_{Y^0} \varphi_\alpha^* D_\alpha \nabla_x u_{0,\alpha} dy = \frac{\partial}{\partial x_i} \left\{ \sum_{\alpha=1}^N \int_{Y^0} \tilde{D}_\alpha e_j \cdot e_i dy \right\} \frac{\partial v}{\partial x_j}, \quad (5.52)$$

$$\begin{aligned} \sum_{\alpha=1}^N \operatorname{div}_x \int_{Y^0} \varphi_\alpha^* D_\alpha \nabla_y u_{1,\alpha} dy &= \frac{\partial}{\partial x_i} \left\{ \sum_{\alpha=1}^N \int_{Y^0} \tilde{D}_\alpha \nabla_y \omega_{j,\alpha} \cdot e_i dy \right\} \frac{\partial v}{\partial x_j} \\ &+ \frac{\partial}{\partial x_i} \left\{ \sum_{\alpha=1}^N \int_{Y^0} (\omega_{j,\alpha} \varphi_\alpha^* D_\alpha \nabla_y \varphi_\alpha \cdot e_i dy \right\} \frac{\partial v}{\partial x_j}, \end{aligned} \quad (5.53)$$

$$\sum_{\alpha=1}^N \int_{Y^0} \operatorname{div}_y (D_\alpha \nabla_x u_{1,\alpha}) \varphi_\alpha^* dy = -\sum_{\alpha=1}^N \int_{Y^0} D_\alpha \nabla_x u_{1,\alpha} \cdot \nabla_y \varphi_\alpha^* dy + \sum_{\alpha=1}^N \int_{\partial \Sigma^0} \varphi_\alpha^* D_\alpha \nabla_x u_{1,\alpha} \cdot n d\sigma(y)$$

$$= -\frac{\partial}{\partial x_i} \left\{ \sum_{\alpha=1}^N \int_{Y_0} \omega_{j,\alpha} \varphi_\alpha D_\alpha \nabla_y \varphi_\alpha^* \cdot e_i dy \right\} \frac{\partial v}{\partial x_j}. \quad (5.54)$$

The boundary integrals disappear in (5.54) as they cancel off with the terms due to the Neumann condition in (5.49). Adding the terms (5.50) through (5.54), we arrive at an equation of the form

$$\rho^* \frac{\partial v}{\partial t} - \operatorname{div}(\mathcal{D} \nabla v) = 0 \quad (5.55)$$

with the elements of \mathcal{D} given by

$$\begin{aligned} \mathcal{D}_{ij} = & \sum_{\alpha=1}^N \int_{Y_0} \tilde{D}_\alpha e_j \cdot e_i dy + \frac{1}{2} \left\{ \sum_{\alpha=1}^N \int_{Y_0} \left(\tilde{D}_\alpha \nabla_y \omega_{i,\alpha} \cdot e_j + \tilde{D}_\alpha \nabla_y \omega_{j,\alpha} \cdot e_i \right) dy \right\} \\ & + \frac{1}{2} \left\{ \sum_{\alpha=1}^N \int_{Y_0} \left(\omega_{i,\alpha} (\varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* - \tilde{b}_\alpha) \cdot e_j + \omega_{j,\alpha} (\varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* - \tilde{b}_\alpha) \cdot e_i \right) dy \right\} \end{aligned} \quad (5.56)$$

In the expression (5.56) for \mathcal{D} , the dispersion tensor is symmetrized. The observation (2.51) that we made in Chapter 2 implies that the non symmetric part of the dispersion matrix \mathcal{D} doesn't contribute to the homogenized equation (5.55) as the Hessian matrix $\nabla \nabla v$ is symmetric. The expression (5.56) for \mathcal{D} is given in terms of the cell solutions $(\omega_{i,\alpha})_{1 \leq i \leq d; 1 \leq \alpha \leq N}$. To obtain the expression for the elements of \mathcal{D} given in (5.40), we shall use information from the cell problem (5.36). Let us consider the variational formulation (5.48) for $(\omega_{i,\alpha})$ in (5.36) with test function $(\phi_\alpha)_{1 \leq \alpha \leq N} = (\omega_{j,\alpha})_{1 \leq \alpha \leq N}$. Then the one for $(\omega_{j,\alpha})$ in (5.36) with test function $(\phi_\alpha)_{1 \leq \alpha \leq N} = (\omega_{i,\alpha})_{1 \leq \alpha \leq N}$. This leads to

$$\begin{aligned} & \frac{1}{2} \left\{ \sum_{\alpha=1}^N \int_{Y_0} \left(\omega_{i,\alpha} (\varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* - \tilde{b}_\alpha) \cdot e_j + \omega_{j,\alpha} (\varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* - \tilde{b}_\alpha) \cdot e_i \right) dy \right\} \\ = & \sum_{\alpha=1}^N \int_{Y_0} \tilde{D}_\alpha \nabla_y \omega_{i,\alpha} \cdot \nabla_y \omega_{j,\alpha} dy + \frac{1}{2} \left\{ \sum_{\alpha=1}^N \int_{Y_0} \left(\tilde{D}_\alpha \nabla_y \omega_{i,\alpha} \cdot e_j + \tilde{D}_\alpha \nabla_y \omega_{j,\alpha} \cdot e_i \right) dy \right\} \\ & - \frac{1}{2} \left\{ \sum_{\alpha=1}^N \int_{Y_0} \omega_{i,\alpha} \omega_{j,\alpha} \operatorname{div}_y \tilde{b}_\alpha dy \right\} \\ + & \frac{1}{2} \left\{ \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_{Y_0} \left(\Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (\omega_{i,\beta} - \omega_{i,\alpha}) \omega_{j,\alpha} + \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (\omega_{j,\beta} - \omega_{j,\alpha}) \omega_{i,\alpha} \right) dy \right\}. \end{aligned} \quad (5.57)$$

Lemma 5.3.2 gives an expression for the divergence of the convective field \tilde{b}_α in (5.20) which will lead us to conclude that the right hand side of (5.57) is same as

$$\begin{aligned} & \sum_{\alpha=1}^N \int_{Y_0} \tilde{D}_\alpha \nabla_y \omega_{i,\alpha} \cdot \nabla_y \omega_{j,\alpha} dy + \frac{1}{2} \left\{ \sum_{\alpha=1}^N \int_{Y_0} \left(\tilde{D}_\alpha \nabla_y \omega_{i,\alpha} \cdot e_j + \tilde{D}_\alpha \nabla_y \omega_{j,\alpha} \cdot e_i \right) dy \right\} \\ & - \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_{Y_0} \varphi_\alpha^* \varphi_\beta \Pi_{\alpha\beta} (\omega_{i,\alpha} - \omega_{i,\beta}) (\omega_{j,\alpha} - \omega_{j,\beta}) dy \end{aligned} \quad (5.58)$$

Using information from (5.57) and (5.58) in the expression for \mathcal{D} in (5.56) leads to a compact expression for the dispersion matrix.

$$\begin{aligned} \mathcal{D}_{ij} &= \sum_{\alpha=1}^N \int_{Y^0} \tilde{D}_\alpha \left(\nabla_y \omega_{i,\alpha} + e_i \right) \cdot \left(\nabla_y \omega_{j,\alpha} + e_j \right) dy \\ &\quad - \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_{Y^0} \varphi_\alpha^* \varphi_\beta \Pi_{\alpha\beta} \left(\omega_{i,\alpha} - \omega_{i,\beta} \right) \left(\omega_{j,\alpha} - \omega_{j,\beta} \right) dy \end{aligned}$$

□

Lemma 5.4.4. *The dispersion matrix \mathcal{D} given by (5.40) is symmetric positive definite.*

Proof. The symmetric part is obvious because of the way we derived the expression for \mathcal{D} . By the hypothesis on the coupling matrix and the positivity of the first eigenvector functions, the factor $\Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta$ is always negative. We have also chosen the diffusion matrices D_α to be coercive. For $\xi \in \mathbb{R}^d$, we shall define

$$\omega_{\alpha\xi} = \sum_{i=1}^d \omega_{i,\alpha} \xi_i$$

Then,

$$\mathcal{D}\xi \cdot \xi \geq \sum_{\alpha=1}^N c_\alpha \int_{Y^0} \left| \nabla_y \omega_{\alpha\xi} + \xi \right|^2 dy + \sum_{\alpha=1}^N \sum_{\beta=1}^N c_{\alpha\beta} \int_{Y^0} \left| \omega_{\alpha\xi} - \omega_{\beta\xi} \right|^2 dy \geq 0.$$

Now, we need to show that $\mathcal{D}\xi \cdot \xi > 0$ for all $\xi \neq 0$. Suppose that $\mathcal{D}\xi \cdot \xi = 0$ which in turn implies that

$$\omega_{\alpha\xi} + \xi \cdot y \equiv C_\alpha, \quad \omega_{\alpha\xi} - \omega_{\beta\xi} \equiv C_{\alpha\beta}$$

for some constants $C_\alpha, C_{\alpha\beta}$. As the cell solutions $(\omega_{i,\alpha})$ are Y -periodic, it cannot be affine. Thus the above equalities are possible only when $\xi = 0$. Thus implying the positive definiteness of \mathcal{D} . □

5.5 Two-scale compactness

This section is devoted to finding two-scale limits with drift for the sequence of solutions for the microscopic model (5.7)-(5.9). We prove a theorem which is in the same spirit as Theorem 3.8.2 of Chapter 3 and Theorem 4.7.2 of Chapter 4. As before, the a priori estimates on the solutions come in handy.

Theorem 5.5.1. *Let $b^* \in \mathbb{R}^d$ be given by (5.37). There exists $v \in L^2((0, T); H^1(\mathbb{R}^d))$ and $(v_{1,\alpha}) \in L^2((0, T) \times \mathbb{R}^d; H^1(Y^0))$, for each $1 \leq \alpha \leq N$, such that the sequence of concentrations $(v_\alpha^\varepsilon)_{1 \leq \alpha \leq N} \in L^2((0, T); H^1(\Omega_\varepsilon))^N$, solutions of system (5.14)-(5.16), two-scale converge with drift b^* , up to a subsequence, as $\varepsilon \rightarrow 0$, in the following sense*

$$v_\alpha^\varepsilon \xrightarrow{2\text{-drift}} v, \quad \nabla v_\alpha^\varepsilon \xrightarrow{2\text{-drift}} \nabla_x v + \nabla_y v_{1,\alpha}, \quad \frac{1}{\varepsilon} \left(v_\alpha^\varepsilon - v_\beta^\varepsilon \right) \xrightarrow{2\text{-drift}} v_{1,\alpha} - v_{1,\beta}, \tag{5.59}$$

for every $1 \leq \alpha, \beta \leq N$.

Proof. Consider the a priori bounds (5.24) on v_α^ε obtained in Lemma 5.3.3. It follows from Proposition 2.6.4 of Chapter 2 that there exist two-scale limits, say $v_\alpha \in L^2(0, T; L^2(\mathbb{R}^d))$ such that

$$v_\alpha^\varepsilon \xrightarrow{2\text{-drift}} v_\alpha \quad (5.60)$$

for every $1 \leq \alpha \leq N$. Also from the a priori estimates (5.24) we have

$$\sum_{\alpha=1}^N \sum_{\beta=1}^N \int_0^T \int_{\Omega_\varepsilon} (v_\alpha^\varepsilon - v_\beta^\varepsilon)^2 dx dt \leq C\varepsilon^2. \quad (5.61)$$

The estimate (5.61) implies that the limits obtained in (5.60) do match i.e., $v_\alpha = v$ for every $1 \leq \alpha \leq N$. The H^1 a priori estimate in space as in (5.24) does imply that $v \in L^2(0, T; H^1(\mathbb{R}^d))$ and that there exist limits $v_{1,\alpha} \in L^2(0, T \times \mathbb{R}^d; H^1(Y^0))$ such that

$$\nabla v_\alpha^\varepsilon \xrightarrow{2\text{-drift}} \nabla_x v + \nabla_y v_{1,\alpha} \quad (5.62)$$

for every $1 \leq \alpha \leq N$. However, the limit of the coupled term isn't straightforward. Since $\frac{1}{\varepsilon}(v_\alpha^\varepsilon - v_\beta^\varepsilon)$ is bounded in $L^2((0, T) \times \Omega_\varepsilon)$, we have the existence of $q(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times Y^0)$ such that

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \int_{\Omega_\varepsilon} \frac{1}{\varepsilon} (v_\alpha^\varepsilon - v_\beta^\varepsilon) \phi\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) dx dt = \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} q(t, x, y) \phi(t, x, y) dy dx dt \quad (5.63)$$

Taking $\Psi \in L^2((0, T) \times \mathbb{R}^d \times Y^0)^d$, let us consider

$$\begin{aligned} & \int_0^T \int_{\Omega_\varepsilon} (\nabla v_\alpha^\varepsilon - \nabla v_\beta^\varepsilon) \cdot \Psi\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) dx dt = \\ & - \int_0^T \int_{\Omega_\varepsilon} (v_\alpha^\varepsilon - v_\beta^\varepsilon) \operatorname{div}_x \Psi\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) dx dt - \int_0^T \int_{\Omega_\varepsilon} \frac{1}{\varepsilon} (v_\alpha^\varepsilon - v_\beta^\varepsilon) \operatorname{div}_y \Psi\left(t, x - \frac{b^*}{\varepsilon}t, \frac{x}{\varepsilon}\right) dx dt \end{aligned} \quad (5.64)$$

Upon passing to the limit in (5.64) as $\varepsilon \rightarrow 0$, the first term on the right hand side vanishes as the limits of v_α^ε and v_β^ε match and the second term on the right hand side as in (5.63). Considering the limit (5.62), upon passing to the limit as $\varepsilon \rightarrow 0$ in (5.64) we have

$$\int_0^T \int_{\mathbb{R}^d} \int_{Y^0} \nabla_y (v_{1,\alpha} - v_{1,\beta}) \cdot \Psi(t, x, y) dy dx dt = - \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} q(t, x, y) \operatorname{div}_y \Psi(t, x, y) dy dx dt \quad (5.65)$$

From (5.65) we deduce that $(v_{1,\alpha} - v_{1,\beta})$ and $q(t, x, y)$ differ by a function of (t, x) , say $l(t, x)$. As $v_{1,\alpha}$ and $v_{1,\beta}$ are also defined up to the addition of a function solely dependent on (t, x) , we can get rid of $l(t, x)$ and we recover indeed the following limit

$$\frac{1}{\varepsilon} (v_\alpha^\varepsilon - v_\beta^\varepsilon) \xrightarrow{2\text{-drift}} v_{1,\alpha} - v_{1,\beta}.$$

□

5.6 Proof of homogenization result

This section is dedicated to the rigorous justification of the formal result, Proposition 5.4.1, that we have obtained in Section 5.4. The following theorem characterizes the two-scale limits found in Theorem 5.5.1.

Theorem 5.6.1. *Let $v \in L^2((0, T); H^1(\mathbb{R}^d))$ and $v_{1,\alpha} \in L^2((0, T) \times \mathbb{R}^d; H^1(Y^0))$ for every $1 \leq \alpha \leq N$ be the limits obtained in (5.59). The two-scale limits $v_{1,\alpha}$ admit an explicit representation given by*

$$v_{1,\alpha}(t, x, y) = \sum_{i=1}^d \frac{\partial v}{\partial x_i}(t, x) \omega_{i,\alpha}(y) \quad \text{for every } 1 \leq \alpha \leq N \quad (5.66)$$

where $(\omega_{i,\alpha})_{1 \leq i \leq d}$ satisfy the cell problem (5.36). Further, the two-scale limit $v(t, x)$ is the unique solution of the homogenized problem (5.39) with the elements of the dispersion matrix \mathcal{D} given by (5.40).

Proof. The idea is to test the bulk equation (5.14) in the factorized system (5.14)-(5.16) with

$$\phi_\alpha^\varepsilon = \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon \phi_{1,\alpha} \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right). \quad (5.67)$$

Here $\phi(t, x)$ and $\phi_{1,\alpha}(t, x, y)$ are smooth compactly supported functions which vanish at the final time T .

$$\begin{aligned} & \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon \frac{\partial v_\alpha^\varepsilon}{\partial t} \phi_\alpha^\varepsilon dx dt + \frac{1}{\varepsilon} \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \tilde{b}_\alpha^\varepsilon \cdot \nabla v_\alpha^\varepsilon \phi_\alpha^\varepsilon dx dt + \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot \nabla \phi_\alpha^\varepsilon dx dt \\ & + \frac{1}{\varepsilon^2} \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_0^T \int_{\Omega_\varepsilon} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\beta^\varepsilon - v_\alpha^\varepsilon) \phi_\alpha^\varepsilon = 0. \end{aligned} \quad (5.68)$$

Substituting for ϕ_α^ε from (5.67) in the variational formulation (5.68) and integrating by parts lead to

$$\begin{aligned} & - \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon v_\alpha^\varepsilon \frac{\partial \phi}{\partial t} \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt + \frac{1}{\varepsilon} \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon v_\alpha^\varepsilon b^* \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt \\ & - \frac{1}{\varepsilon} \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \operatorname{div}(\tilde{b}_\alpha^\varepsilon) v_\alpha^\varepsilon \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt - \frac{1}{\varepsilon} \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} v_\alpha^\varepsilon \tilde{b}_\alpha^\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt \\ & + \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt + \frac{1}{\varepsilon^2} \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_0^T \int_{\Omega_\varepsilon} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\beta^\varepsilon - v_\alpha^\varepsilon) \phi \left(t, x - \frac{b^* t}{\varepsilon} \right) dx dt \\ & + \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon v_\alpha^\varepsilon b^* \cdot \nabla \phi_{1,\alpha} \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt + \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} (\tilde{b}_\alpha^\varepsilon \cdot \nabla v_\alpha^\varepsilon) \phi_{1,\alpha} \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt \\ & + \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot \nabla_y \phi_{1,\alpha} \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) dx dt \end{aligned}$$

$$+\frac{1}{\varepsilon} \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_0^T \int_{\Omega_\varepsilon} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\beta^\varepsilon - v_\alpha^\varepsilon) \phi_{1,\alpha} \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) dx dt + \mathcal{O}(\varepsilon) = 0. \quad (5.69)$$

Taking $\phi \equiv 0$ in (5.69), we arrive at a variational formulation involving only $\phi_{1,\alpha}$.

$$\begin{aligned} \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* v_\alpha^\varepsilon \rho_\alpha^\varepsilon b^* \cdot \nabla \phi_{1,\alpha} \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) dx dt + \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \left(\tilde{b}_\alpha^\varepsilon \cdot \nabla v_\alpha^\varepsilon \right) \phi_{1,\alpha} \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) dx dt \\ + \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot \nabla_y \phi_{1,\alpha} \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) dx dt \\ + \frac{1}{\varepsilon} \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_0^T \int_{\Omega_\varepsilon} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\beta^\varepsilon - v_\alpha^\varepsilon) \phi_{1,\alpha} \left(t, x - \frac{b^*}{\varepsilon} t, \frac{x}{\varepsilon} \right) dx dt = 0. \end{aligned} \quad (5.70)$$

Passing to the limit in (5.70) as $\varepsilon \rightarrow 0$ yields

$$\begin{aligned} - \sum_{\alpha=1}^N \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} \varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* \cdot \nabla_x v(t, x) \phi_{1,\alpha}(t, x, y) dy dx dt \\ + \sum_{\alpha=1}^N \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} \tilde{b}_\alpha \cdot \left(\nabla_x v(t, x) + \nabla_y v_{1,\alpha}(t, x, y) \right) \phi_{1,\alpha}(t, x, y) dy dx dt \\ - \sum_{\alpha=1}^N \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} \operatorname{div}_y \left(\tilde{D}_\alpha \left(\nabla_x v(t, x) + \nabla_y v_{1,\alpha}(t, x, y) \right) \right) \phi_{1,\alpha}(t, x, y) dy dx dt \\ + \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta \left(v_{1,\beta}(t, x, y) - v_{1,\alpha}(t, x, y) \right) \phi_{1,\alpha}(t, x, y) dy dx dt = 0. \end{aligned} \quad (5.71)$$

The above expression (5.71) is the variational formulation for

$$\left\{ \begin{array}{ll} \tilde{b}_\alpha \cdot \left(\nabla_y v_{1,\alpha} + \nabla_x v \right) - \operatorname{div}_y \left(\tilde{D}_\alpha \left(\nabla_y v_{1,\alpha} + \nabla_x v \right) \right) \\ + \sum_{\beta=1}^N \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_{1,\beta} - v_{1,\alpha}) = \varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* \cdot \nabla_x v & \text{in } Y^0, \\ \tilde{D}_\alpha \left(\nabla_y v_{1,\alpha} + \nabla_x v \right) \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow v_{1,\alpha} & Y\text{-periodic.} \end{array} \right. \quad (5.72)$$

for every $1 \leq \alpha \leq N$. By Fredholm alternative we have the existence and uniqueness of $v_{1,\alpha} \in L^2(0, T \times \mathbb{R}^d; H^1(Y^0)/\mathbb{R})$ if and only if the drift velocity b^* satisfies (5.37) which is indeed the value we chose for the drift velocity in Theorem 5.5.1. Also by linearity of (5.72), we deduce that we can separate the slow and fast variables in $v_{1,\alpha}$ as in (5.66) with $\omega_{i,\alpha}$ satisfying the coupled cell problem (5.36).

As a next step, we shall choose $\phi_{1,\alpha} \equiv (0, 0)$ in the variational expression (5.69). This gives us a variational formulation involving only ϕ .

$$\begin{aligned}
& - \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon v_\alpha^\varepsilon \frac{\partial \phi}{\partial t} \left(t, x - \frac{b^*}{\varepsilon} t \right) dx dt + \frac{1}{\varepsilon} \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* v_\alpha^\varepsilon \rho_\alpha^\varepsilon b^* \cdot \nabla_x \phi \left(t, x - \frac{b^*}{\varepsilon} t \right) dx dt \\
& - \frac{1}{\varepsilon} \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \operatorname{div}(\tilde{b}_\alpha^\varepsilon) v_\alpha^\varepsilon \phi \left(t, x - \frac{b^*}{\varepsilon} t \right) dx dt - \frac{1}{\varepsilon} \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} v_\alpha^\varepsilon \tilde{b}_\alpha^\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^*}{\varepsilon} t \right) dx dt \\
& + \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^*}{\varepsilon} t \right) dx dt + \frac{1}{\varepsilon^2} \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_0^T \int_{\Omega_\varepsilon} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\beta^\varepsilon - v_\alpha^\varepsilon) \phi \left(t, x - \frac{b^*}{\varepsilon} t \right) dx dt = 0.
\end{aligned} \tag{5.73}$$

Thanks to the expressions for the divergence of \tilde{b}_α in (5.20) as they help us get rid of the terms of order ε^{-2} in the variational formulation (5.73). There are still some problematic terms of order ε^{-1} in the variational formulation (5.73). To simplify them we shall introduce an auxiliary problem which is well-posed, thanks to the expression for the drift velocity b^* from (5.37).

$$\begin{cases} -\Delta \Xi = \sum_{\alpha=1}^N \varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* - \tilde{b}_\alpha & \text{in } Y^0, \\ -\nabla \Xi \cdot n = 0 & \text{on } \partial \Sigma^0, \\ y \rightarrow \Xi(y) & \text{is } Y\text{-periodic.} \end{cases} \tag{5.74}$$

The scaled auxiliary problem associated with (5.74) shall be

$$\begin{cases} -\varepsilon^2 \Delta \Xi^\varepsilon(x/\varepsilon) = \sum_{\alpha=1}^N \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon b^* - \tilde{b}_\alpha^\varepsilon & \text{in } \Omega_\varepsilon, \\ -\varepsilon \nabla \Xi^\varepsilon(x/\varepsilon) \cdot n = 0 & \text{on } \partial \Omega_\varepsilon, \\ x \rightarrow \Xi^\varepsilon & \text{is } \varepsilon\text{-periodic.} \end{cases} \tag{5.75}$$

Now, let us regroup the problematic terms from (5.73) as we are equipped to handle them.

$$\begin{aligned}
& \frac{1}{\varepsilon} \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon v_\alpha^\varepsilon b^* \cdot \nabla_x \phi \left(t, x - \frac{b^*}{\varepsilon} t \right) dx dt - \frac{1}{\varepsilon} \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} v_\alpha^\varepsilon \tilde{b}_\alpha^\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^*}{\varepsilon} t \right) dx dt \\
& = -\frac{\varepsilon^2}{\varepsilon} \int_0^T \int_{\Omega_\varepsilon} \Delta \Xi_i^\varepsilon \frac{\partial \phi}{\partial x_i} v_\alpha^\varepsilon dx dt + \frac{1}{\varepsilon} \sum_{\beta=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\beta \varphi_\beta^* \rho_\beta^\varepsilon (v_\beta^\varepsilon - v_\alpha^\varepsilon) b^* \cdot \nabla_x \phi dx dt \\
& \quad + \frac{1}{\varepsilon} \sum_{\beta=1}^N \int_0^T \int_{\Omega_\varepsilon} (v_\alpha^\varepsilon - v_\beta^\varepsilon) \tilde{b}_\beta^\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^*}{\varepsilon} t \right) dx dt \\
& = \varepsilon \int_0^T \int_{\Omega_\varepsilon} \nabla \Xi_i^\varepsilon \cdot \nabla \left(\frac{\partial \phi}{\partial x_i} \right) v_\alpha^\varepsilon dx dt + \varepsilon \int_0^T \int_{\Omega_\varepsilon} \nabla \Xi_i^\varepsilon \cdot \nabla v_\alpha^\varepsilon \left(\frac{\partial \phi}{\partial x_i} \right) dx dt
\end{aligned}$$

$$+\frac{1}{\varepsilon} \sum_{\beta=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\beta \varphi_\beta^* \rho_\beta^\varepsilon (v_\beta^\varepsilon - v_\alpha^\varepsilon) b^* \cdot \nabla_x \phi \, dx \, dt + \frac{1}{\varepsilon} \sum_{\beta=1}^N \int_0^T \int_{\Omega_\varepsilon} (v_\alpha^\varepsilon - v_\beta^\varepsilon) \tilde{b}_\beta^\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^*}{\varepsilon} t \right) \, dx \, dt \quad (5.76)$$

Using (5.76) in (5.73) we write down the final variational formulation where we can pass to the limit as we know the two-scale limits of all the sequences involved.

$$\begin{aligned} & - \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon v_\alpha^\varepsilon \frac{\partial \phi}{\partial t} \left(t, x - \frac{b^*}{\varepsilon} t \right) \, dx \, dt + \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^*}{\varepsilon} t \right) \, dx \, dt \\ & + \varepsilon \int_0^T \int_{\Omega_\varepsilon} \nabla \Xi_i^\varepsilon \cdot \nabla \left(\frac{\partial \phi}{\partial x_i} \right) v_\alpha^\varepsilon \, dx \, dt + \varepsilon \int_0^T \int_{\Omega_\varepsilon} \nabla \Xi_i^\varepsilon \cdot \nabla v_\alpha^\varepsilon \left(\frac{\partial \phi}{\partial x_i} \right) \, dx \, dt \\ & + \frac{1}{\varepsilon} \sum_{\beta=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\beta \varphi_\beta^* \rho_\beta^\varepsilon (v_\beta^\varepsilon - v_\alpha^\varepsilon) b^* \cdot \nabla_x \phi \, dx \, dt + \frac{1}{\varepsilon} \sum_{\beta=1}^N \int_0^T \int_{\Omega_\varepsilon} (v_\alpha^\varepsilon - v_\beta^\varepsilon) \tilde{b}_\beta^\varepsilon \cdot \nabla_x \phi \left(t, x - \frac{b^*}{\varepsilon} t \right) \, dx \, dt = 0. \end{aligned} \quad (5.77)$$

Passing to the limit as $\varepsilon \rightarrow 0$ in (5.77) we have

$$\begin{aligned} & \int_0^T \int_{\mathbb{R}^d} \rho^* \frac{\partial v}{\partial t} \phi \, dx \, dt + \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} \nabla_y \Xi_i \cdot \nabla_y v_{1,\alpha} \frac{\partial \phi}{\partial x_i} \, dy \, dx \, dt + \sum_{\alpha=1}^N \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} \tilde{D}_\alpha (\nabla v + \nabla_y v_{1,\alpha}) \cdot \nabla_x \phi \, dx \, dt \\ & + \sum_{\beta=1}^N \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} \varphi_\beta \varphi_\beta^* \rho_\beta (v_{1,\beta} - v_{1,\alpha}) b^* \cdot \nabla_x \phi \, dy \, dx \, dt + \sum_{\beta=1}^N \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} (v_{1,\alpha} - v_{1,\beta}) \tilde{b}_\beta \cdot \nabla_x \phi \, dy \, dx \, dt = 0. \end{aligned} \quad (5.78)$$

We know the representations for $v_{1,\alpha}$ from (5.66) in terms of the cell solutions. We shall substitute them in the limit equation (5.78).

$$\begin{aligned} & \int_0^T \int_{\mathbb{R}^d} \frac{\partial v}{\partial t} \phi \, dx \, dt - \sum_{i,j} \int_0^T \int_{\mathbb{R}^d} \frac{\partial v}{\partial x_j} \frac{\partial \phi}{\partial x_i} \int_{Y^0} (\Delta_y \Xi_i) \omega_{j,\alpha} \, dy \, dx \, dt \\ & + \sum_{\alpha=1}^N \sum_{i,j} \int_0^T \int_{\mathbb{R}^d} \frac{\partial v}{\partial x_j} \frac{\partial \phi}{\partial x_i} \int_{Y^0} \tilde{D}_\alpha (\nabla_y y_j + \nabla_y \omega_{j,\alpha}) \cdot \nabla_y y_i \, dy \, dx \, dt \\ & + \sum_{\beta=1}^N \sum_{i,j} \int_0^T \int_{\mathbb{R}^d} \frac{\partial v}{\partial x_j} \frac{\partial \phi}{\partial x_i} \int_{Y^0} \varphi_\beta \varphi_\beta^* \rho_\beta (\omega_{j,\beta} - \omega_{j,\alpha}) b^* \cdot \nabla_y y_i \, dy \, dx \, dt \\ & + \sum_{\beta=1}^N \sum_{i,j} \int_0^T \int_{\mathbb{R}^d} \frac{\partial v}{\partial x_j} \frac{\partial \phi}{\partial x_i} \int_{Y^0} (\omega_{j,\alpha} - \omega_{j,\beta}) \tilde{b}_\beta \cdot \nabla_y y_i \, dy \, dx \, dt = 0. \end{aligned} \quad (5.79)$$

The expression (5.79) is a variational formulation of the homogenized equation (5.39). Using the auxiliary problem (5.74) we shall give the elements of \mathcal{D}

$$\mathcal{D}_{ij} = \sum_{\alpha=1}^N \int_{Y^0} \tilde{D}_\alpha (\nabla_y y_j + \nabla_y \omega_{j,\alpha}) \cdot \nabla_y y_i \, dy + \sum_{\alpha=1}^N \int \varphi_\alpha \varphi_\alpha^* \rho_\alpha \omega_{j,\alpha} b^* \cdot e_i \, dy - \sum_{\alpha=1}^N \int \omega_{j,\alpha} \tilde{b}_\alpha \cdot e_i \, dy. \quad (5.80)$$

The non symmetric part of \mathcal{D} doesn't play the role in the homogenized equation (5.39) as explained in Section 5.4. The dispersion matrix \mathcal{D} in (5.80) upon symmetrizing leads to

$$\begin{aligned} \mathcal{D}_{ij} &= \sum_{\alpha=1}^N \int_{Y_0} \tilde{D}_\alpha e_j \cdot e_i dy + \frac{1}{2} \left\{ \sum_{\alpha=1}^N \int_{Y_0} \left(\tilde{D}_\alpha \nabla_y \omega_{i,\alpha} \cdot e_j + \tilde{D}_\alpha \nabla_y \omega_{j,\alpha} \cdot e_i \right) dy \right\} \\ &+ \frac{1}{2} \left\{ \sum_{\alpha=1}^N \int_{Y_0} \left(\omega_{i,\alpha} (\varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* - \tilde{b}_\alpha) \cdot e_j + \omega_{j,\alpha} (\varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* - \tilde{b}_\alpha) \cdot e_i \right) dy \right\}. \end{aligned} \quad (5.81)$$

The symmetric expression in (5.81) is the same as the one obtained in (5.56) via the formal method in Section 5.4. We can redo the calculations that followed (5.56) using the cell problem (5.36) to arrive at

$$\begin{aligned} \mathcal{D}_{ij} &= \sum_{\alpha=1}^N \int_{Y_0} \tilde{D}_\alpha \left(\nabla_y \omega_{i,\alpha} + e_i \right) \cdot \left(\nabla_y \omega_{j,\alpha} + e_j \right) dy \\ &- \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_{Y_0} \varphi_\alpha^* \varphi_\beta \Pi_{\alpha\beta} \left(\omega_{i,\alpha} - \omega_{i,\beta} \right) \left(\omega_{j,\alpha} - \omega_{j,\beta} \right) dy. \end{aligned}$$

□

Remark 5.6.2. *The irreducibility assumption (5.6) on the coupling matrix Π ensures microscopic equilibrium among solutes resulting in a single homogenized concentration $v(t, x)$ i.e., if the coupling matrix $\Pi \equiv 0$ (say), we get N different homogenized concentrations.*

5.7 Boundary reaction: Model and qualitative analysis

In this Chapter, so far we have studied a system of convection diffusion reaction equations (5.7)-(5.9) where the bulk reactions are considered and the reaction terms appear as a zero order term in (5.7). Now, we shall slightly modify the reaction model. Let us consider surface reaction terms, similar to the bulk reaction term in (5.7). This model is very close to (5.7)-(5.9) except for the reactions on the boundary and absence of bulk reactions, for each $1 \leq \alpha \leq N$,

$$\rho_\alpha \frac{\partial u_\alpha}{\partial \tau} + b_\alpha(y) \cdot \nabla u_\alpha - \operatorname{div}(D_\alpha \nabla u_\alpha) = 0 \text{ in } (0, \zeta) \times \Omega_f, \quad (5.82)$$

$$-D_\alpha \nabla u_\alpha \cdot n = \sum_{\beta=1}^N \Pi_{\alpha\beta} u_\beta \quad \text{on } (0, \zeta) \times \Omega_s. \quad (5.83)$$

We will be working with the same hypothesis on all the coefficients as before. Upon parabolic scaling, (5.82)-(5.83) yields

$$\rho_\alpha^\varepsilon \frac{\partial u_\alpha^\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\alpha^\varepsilon \cdot \nabla u_\alpha^\varepsilon - \operatorname{div}(D_\alpha^\varepsilon \nabla u_\alpha^\varepsilon) = 0 \text{ in } (0, T) \times \Omega_\varepsilon, \quad (5.84)$$

$$-D_\alpha^\varepsilon \nabla u_\alpha^\varepsilon \cdot n = \frac{1}{\varepsilon} \sum_{\beta=1}^N \Pi_{\alpha\beta} u_\beta^\varepsilon \quad \text{on } (0, T) \times \partial\Omega_\varepsilon, \quad (5.85)$$

$$u_\alpha^\varepsilon(0, x) = u_\alpha^{\text{in}}(x) \quad x \in \mathbb{R}^d. \quad (5.86)$$

In Section 5.3 we remarked that the difficulty in arriving at the a priori estimates for (5.7)-(5.9) could be overcome by spectral cell problems associated with (5.7)-(5.9) followed by a factorization

principle. We shall employ the same approach to treat the current model too. Let us consider the spectral and its adjoint cell problems, for each $1 \leq \alpha \leq N$,

$$\begin{cases} b_\alpha(y) \cdot \nabla_y \varphi_\alpha - \operatorname{div}_y (D_\alpha \nabla_y \varphi_\alpha) = \lambda \rho_\alpha \varphi_\alpha & \text{in } Y^0, \\ -D_\alpha \nabla_y \varphi_\alpha \cdot n = \sum_{\beta=1}^N \Pi_{\alpha\beta} \varphi_\beta & \text{on } \partial\Sigma^0, \\ y \rightarrow \varphi_\alpha(y) & Y\text{-periodic.} \end{cases} \quad (5.87)$$

$$\begin{cases} -\operatorname{div}_y (b_\alpha \varphi_\alpha^*) - \operatorname{div}_y (D_\alpha \nabla_y \varphi_\alpha^*) = \lambda \rho_\alpha \varphi_\alpha^* & \text{in } Y^0, \\ -D_\alpha \nabla_y \varphi_\alpha^* \cdot n - b_\alpha(y) \cdot n \varphi_\alpha^* = \sum_{\beta=1}^N \Pi_{\alpha\beta}^* \varphi_\beta^* & \text{on } \partial\Sigma^0, \\ y \rightarrow \varphi_\alpha^*(y) & Y\text{-periodic.} \end{cases} \quad (5.88)$$

Proposition 5.7.1. *The system (5.84)-(5.86) is equivalent to*

$$\varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon \frac{\partial v_\alpha^\varepsilon}{\partial t} + \frac{1}{\varepsilon} \tilde{b}_\alpha^\varepsilon \cdot \nabla v_\alpha^\varepsilon - \operatorname{div} \left(\tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \right) = 0 \text{ in } (0, T) \times \Omega_\varepsilon, \quad (5.89)$$

$$-\tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot n = \frac{1}{\varepsilon} \sum_{\beta=1}^N \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\beta^\varepsilon - v_\alpha^\varepsilon) \text{ on } (0, T) \times \partial\Omega_\varepsilon, \quad (5.90)$$

$$v_\alpha^\varepsilon(0, x) = \frac{u_\alpha^{in}(x)}{\varphi_\alpha\left(\frac{x}{\varepsilon}\right)} \quad x \in \Omega_\varepsilon, \quad (5.91)$$

for each $1 \leq \alpha \leq N$. The components of $(v_\alpha^\varepsilon)_{1 \leq \alpha \leq N}$ are defined by

$$v_\alpha^\varepsilon(t, x) = \exp(-\lambda t / \varepsilon^2) \varphi_\alpha\left(\frac{x}{\varepsilon}\right) v_\alpha^\varepsilon(t, x) \quad (5.92)$$

The convective velocity, $\tilde{b}_\alpha^\varepsilon(x) = \tilde{b}_\alpha\left(\frac{x}{\varepsilon}\right)$, in (5.89) is given by

$$\tilde{b}_\alpha(y) = \varphi_\alpha \varphi_\alpha^* b_\alpha + \varphi_\alpha D_\alpha \nabla_y \varphi_\alpha^* - \varphi_\alpha^* D_\alpha \nabla_y \varphi_\alpha \quad \text{for every } 1 \leq \alpha \leq N \quad (5.93)$$

and the diffusion matrix, $\tilde{D}_\alpha^\varepsilon(x) = \tilde{D}_\alpha\left(\frac{x}{\varepsilon}\right)$, in (5.89)-(5.90) is given by

$$\tilde{D}_\alpha(y) = \varphi_\alpha \varphi_\alpha^* D_\alpha \quad \text{for every } 1 \leq \alpha \leq N, \quad (5.94)$$

where $(\lambda, \varphi_\alpha)$ is the first eigenpair for the spectral cell problem (5.87) and $(\lambda, \varphi_\alpha^*)$ is the first eigenpair for the adjoint spectral cell problem (5.88).

The proof of Proposition 5.7.1 is straightforward upon using the chain rule for differentiation (5.19).

Lemma 5.7.2. *Let (v_α^ε) be a weak solution of (5.89)-(5.91). There exists a constant C such that*

$$\begin{aligned} & \sum_{\alpha=1}^N \left\| v_\alpha^\varepsilon \right\|_{L^\infty((0, T); L^2(\Omega_\varepsilon))} + \sum_{\alpha=1}^N \left\| \nabla v_\alpha^\varepsilon \right\|_{L^2((0, T) \times \Omega_\varepsilon)} \\ & + \sum_{\alpha=1}^N \sum_{\beta=1}^N \sqrt{\varepsilon} \left\| \frac{1}{\varepsilon} (v_\alpha^\varepsilon - v_\beta^\varepsilon) \right\|_{L^2((0, T) \times \partial\Omega_\varepsilon)} \leq C \sum_{\alpha=1}^N \|v_\alpha^{in}\|_{L^2(\mathbb{R}^d)} \end{aligned} \quad (5.95)$$

Proof. To derive the a priori estimates, as is done with parabolic equations, we shall multiply (5.89) by v_α^ε and add the thus obtained expressions followed by integrating over Ω_ε .

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon |v_\alpha^\varepsilon|^2 dx - \frac{1}{2\varepsilon} \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \operatorname{div}(\tilde{b}_\alpha^\varepsilon) |v_\alpha^\varepsilon|^2 dx \\ & + \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot \nabla v_\alpha^\varepsilon dx + \frac{1}{\varepsilon} \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_{\partial\Omega_\varepsilon} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\beta^\varepsilon - v_\alpha^\varepsilon) v_\alpha^\varepsilon = 0 \end{aligned}$$

which is the same as

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon |v_\alpha^\varepsilon|^2 dx - \frac{1}{2\varepsilon} \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \operatorname{div}(\tilde{b}_\alpha^\varepsilon) |v_\alpha^\varepsilon|^2 dx \\ & + \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot \nabla v_\alpha^\varepsilon dx - \sum_{\alpha=1}^N \sum_{\beta=1}^N \varepsilon \int_{\partial\Omega_\varepsilon} \frac{1}{\varepsilon^2} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\alpha^\varepsilon - v_\beta^\varepsilon)^2 = 0 \end{aligned} \quad (5.96)$$

To arrive at the energy estimate, we shall make use of the spectral cell problem (5.87) and its adjoint (5.88). To begin with, let us test the bulk equation in (5.87) by $\varphi_\alpha^*(v_\alpha^\varepsilon)^2$ and integrate over Y^0 . We shall compute term by term.

$$\begin{aligned} & \int_{Y^0} b_\alpha \cdot \nabla_y \varphi_\alpha \varphi_\alpha^* (v_\alpha^\varepsilon)^2 dy = - \int_{Y^0} \operatorname{div}_y (b_\alpha \varphi_\alpha^*) \varphi_\alpha (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \varphi_\alpha \varphi_\alpha^* b_\alpha \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy, \quad (5.97) \\ & - \int_{Y^0} \operatorname{div}_y (D_\alpha \nabla_y \varphi_\alpha) \varphi_\alpha^* (v_\alpha^\varepsilon)^2 dy = \int_{Y^0} \varphi_\alpha^* D_\alpha \nabla_y \varphi_\alpha \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy + \int_{Y^0} (v_\alpha^\varepsilon)^2 D_\alpha \nabla_y \varphi_\alpha \cdot \nabla_y \varphi_\alpha^* dy \\ & \quad + \sum_{\beta=1}^N \int_{\partial\Sigma^0} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\alpha^\varepsilon)^2 d\sigma(y) \\ & = \int_{Y^0} \varphi_\alpha^* D_\alpha \nabla_y \varphi_\alpha \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \varphi_\alpha D_\alpha \nabla_y \varphi_\alpha^* \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy + \int_{Y^0} \varphi_\alpha D_\alpha \nabla_y \varphi_\alpha^* \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy \\ & \quad + \int_{Y^0} (v_\alpha^\varepsilon)^2 D_\alpha \nabla_y \varphi_\alpha \cdot \nabla_y \varphi_\alpha^* dy + \sum_{\beta=1}^N \int_{\partial\Sigma^0} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\alpha^\varepsilon)^2 d\sigma(y) \end{aligned}$$

which implies

$$\begin{aligned} & - \int_{Y^0} \operatorname{div}_y (D_\alpha \nabla_y \varphi_\alpha) \varphi_\alpha^* (v_\alpha^\varepsilon)^2 dy = \int_{Y^0} \varphi_\alpha^* D_\alpha \nabla_y \varphi_\alpha \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \varphi_\alpha D_\alpha \nabla_y \varphi_\alpha^* \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy \\ & - \int_{Y^0} \operatorname{div}_y (D_\alpha \nabla_y \varphi_\alpha^*) \varphi_\alpha (v_\alpha^\varepsilon)^2 dy - \sum_{\beta=1}^N \int_{\partial\Sigma^0} \Pi_{\beta\alpha} \varphi_\alpha \varphi_\beta^* (v_\alpha^\varepsilon)^2 d\sigma(y) + \sum_{\beta=1}^N \int_{\partial\Sigma^0} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\alpha^\varepsilon)^2 d\sigma(y), \end{aligned} \quad (5.98)$$

$$- \int_{Y^0} \lambda \varphi_\alpha \varphi_\alpha^* \rho_\alpha (v_\alpha^\varepsilon)^2 dy, \quad (5.99)$$

Adding (5.97), (5.98) and (5.99) we arrive at

$$\begin{aligned}
& - \int_{Y^0} \operatorname{div}_y (b_\alpha \varphi_\alpha^*) \varphi_\alpha (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \operatorname{div}_y (D_\alpha \nabla_y \varphi_\alpha^*) \varphi_\alpha (v_\alpha^\varepsilon)^2 dy - \int_{Y^0} \lambda \varphi_\alpha^* \varphi_\alpha \rho_\alpha (v_\alpha^\varepsilon)^2 dy \\
& - \int_{Y^0} \left(\varphi_\alpha \varphi_\alpha^* b_\alpha + \varphi_\alpha D_\alpha \nabla_y \varphi_\alpha^* - \varphi_\alpha^* D_\alpha \nabla_y \varphi_\alpha \right) \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy \\
& - \sum_{\beta=1}^N \int_{\partial \Sigma^0} \Pi_{\beta\alpha} \varphi_\alpha \varphi_\beta^* (v_\alpha^\varepsilon)^2 d\sigma(y) + \sum_{\beta=1}^N \int_{\partial \Sigma^0} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\alpha^\varepsilon)^2 d\sigma(y) = 0 \quad (5.100)
\end{aligned}$$

Identifying the expression for \tilde{b}_α from (5.93) in (5.100) and the information from the adjoint spectral cell problem (5.88), we simplify (5.100) as

$$- \int_{Y^0} \tilde{b}_\alpha \cdot \nabla_y (v_\alpha^\varepsilon)^2 dy - \sum_{\beta=1}^N \int_{\partial \Sigma^0} \Pi_{\beta\alpha} \varphi_\alpha \varphi_\beta^* (v_\alpha^\varepsilon)^2 d\sigma(y) + \sum_{\beta=1}^N \int_{\partial \Sigma^0} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\alpha^\varepsilon)^2 d\sigma(y) = 0 \quad (5.101)$$

Summing (5.101) over α leads to

$$\sum_{\alpha=1}^N \int_{Y^0} \operatorname{div}_y \tilde{b}_\alpha (v_\alpha^\varepsilon)^2 dy = 0. \quad (5.102)$$

Scaling (5.102) and using it in (5.96) results in

$$\frac{1}{2} \frac{d}{dt} \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon |v_\alpha^\varepsilon|^2 dx + \sum_{\alpha=1}^N \int_{\Omega_\varepsilon} \tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot \nabla v_\alpha^\varepsilon dx - \sum_{\alpha=1}^N \sum_{\beta=1}^N \varepsilon \int_{\partial \Omega_\varepsilon} \frac{1}{\varepsilon^2} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\alpha^\varepsilon - v_\beta^\varepsilon)^2 = 0 \quad (5.103)$$

which is the needed energy equality for (5.89)-(5.91) as $\Pi_{\alpha\beta} \leq 0$ for $\alpha \neq \beta$. Integrating (5.103) over $(0, T)$ will lead to the a priori estimates (5.95). \square

Now we shall state a result on the well-posedness of the system. This result is similar to Proposition 5.3.4 of Section 5.3.

Proposition 5.7.3. *Assume that the initial data u_α^{in} belongs to $L^2(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ for every $1 \leq \alpha \leq N$. For any given $\varepsilon > 0$, there exists a unique solution u_α^ε of (5.84)-(5.86) in the following energy space*

$$u_\alpha^\varepsilon \in L^\infty((0, T); L^2(\Omega_\varepsilon)); \quad \nabla u_\alpha^\varepsilon \in L^2((0, T) \times \Omega_\varepsilon) \quad \text{for every } 1 \leq \alpha \leq N. \quad (5.104)$$

Further if the initial data $u_\alpha^{\text{in}} \geq 0$ in Ω_ε , then the solution $u_\alpha^\varepsilon(t, x) \geq 0$ in $(0, T) \times \Omega_\varepsilon$.

Here too we shall avoid the proof of the Proposition 5.7.3. The arguments of the proof can be adapted from the existence results and maximum principles proved in [152], [129], [43].

5.8 Boundary reaction: Homogenization

Let us define drift velocity $b^* \in \mathbb{R}^d$ as

$$b^* = \frac{1}{\rho^*} \sum_{\alpha=1}^N \int_{Y^0} \tilde{b}_\alpha(y) dy \quad (5.105)$$

where the convective velocity \tilde{b}_α is given by (5.93) in terms of the first eigenfunctions associated with the spectral cell problem (5.87) and its adjoint (5.88). In Chapters 3 and 4 we had a priori estimates on the boundary similar to the ones in (5.95). The two-scale limits of the coupled term

Theorem 5.8.1. *Let $b^* \in \mathbb{R}^d$ be given by (5.105). There exists $v \in L^2((0, T); H^1(\mathbb{R}^d))$ and $\omega_{i,\alpha} \in H^1_{\#}(Y^0)$, for each $1 \leq \alpha \leq N$ and for each $1 \leq i \leq d$, such that the sequence of concentrations $(v_\alpha^\varepsilon)_{1 \leq \alpha \leq N} \in L^2((0, T); H^1(\Omega_\varepsilon))^N$, solutions of system (5.89)-(5.91), two-scale converge with drift b^* , up to a subsequence, as $\varepsilon \rightarrow 0$, in the following sense*

$$\left\{ \begin{array}{l} v_\alpha^\varepsilon \xrightarrow{2\text{-drift}} v, \\ \nabla v_\alpha^\varepsilon \xrightarrow{2\text{-drift}} \nabla_x v + \nabla_y \left(\sum_{i=1}^d \omega_{i,\alpha} \frac{\partial v}{\partial x_i} \right), \\ \frac{1}{\varepsilon} (v_\alpha^\varepsilon - v_\beta^\varepsilon) \xrightarrow{2s\text{-drift}} \sum_{i=1}^d (\omega_{i,\alpha} - \omega_{i,\beta}) \frac{\partial v}{\partial x_i}, \end{array} \right. \quad (5.106)$$

for every $1 \leq \alpha, \beta \leq N$. The two-scale limit $v(t, x)$ in (5.106) satisfies the following homogenized equation

$$\left\{ \begin{array}{l} \rho^* \frac{\partial v}{\partial t} - \operatorname{div}(\mathcal{D} \nabla v) = 0 \quad \text{in } (0, T) \times \mathbb{R}^d, \\ v(0, x) = \sum_{\alpha=1}^N u_\alpha^{\text{in}}(x) \int_{Y^0} \varphi_\alpha^*(y) dy \quad \text{in } \mathbb{R}^d. \end{array} \right. \quad (5.107)$$

where the dispersion tensor \mathcal{D} is given by

$$\begin{aligned} \mathcal{D}_{ij} &= \sum_{\alpha=1}^N \int_{Y^0} \tilde{D}_\alpha (\nabla_y \omega_{i,\alpha} + e_i) \cdot (\nabla_y \omega_{j,\alpha} + e_j) dy \\ &\quad - \frac{1}{2} \sum_{\alpha,\beta=1}^N \int_{\partial Y^0} \varphi_\alpha^* \varphi_\beta \Pi_{\alpha\beta} (\omega_{i,\alpha} - \omega_{i,\beta}) (\omega_{j,\alpha} - \omega_{j,\beta}) dy \end{aligned} \quad (5.108)$$

and the components $(\omega_{i,\alpha})_{1 \leq \alpha \leq N}$, for every $1 \leq i \leq d$, satisfy a so called cell problem.

$$\left\{ \begin{array}{l} \tilde{b}_\alpha(y) \cdot (\nabla_y \omega_{i,\alpha} + e_i) - \operatorname{div}_y (\tilde{D}_\alpha (\nabla_y \omega_{i,\alpha} + e_i)) = \varphi_\alpha \varphi_\alpha^* \rho_\alpha b^* \cdot e_i \quad \text{in } Y^0, \\ \tilde{D}_\alpha (\nabla_y \omega_{i,\alpha} + e_i) \cdot n = \sum_{\beta=1}^N \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (\omega_{i,\beta} - \omega_{i,\alpha}) \quad \text{on } \partial Y^0, \\ y \rightarrow \omega_{i,\alpha} \quad \text{Y-periodic.} \end{array} \right. \quad (5.109)$$

Further the effective porosity in (5.107) is given by

$$\rho^* = \sum_{\alpha=1}^N \int_{Y^0} \varphi_\alpha \varphi_\alpha^* \rho_\alpha(y) dy. \quad (5.110)$$

Proof. The relative compactness results from Section 2.6 of Chapter 2 are of importance in arriving at the two-scale limits (5.106). Let us consider the a priori estimates (5.95). It follows from Proposition 2.6.4 of Chapter 2 that there exist two-scale limits, say $(v_\alpha)_{1 \leq \alpha \leq N} \in L^2(0, T; L^2(\mathbb{R}^d))^N$ such that

$$v_\alpha^\varepsilon \xrightarrow{2\text{-drift}} v_\alpha \quad (5.111)$$

for every $1 \leq \alpha \leq N$. For $w \in H^1(\Omega_\varepsilon)$, consider the following Poincaré type inequality derived in [67].

$$\|w\|_{L^2(\Omega_\varepsilon)}^2 \leq C \left(\varepsilon^2 \|\nabla w\|_{L^2(\Omega_\varepsilon)}^2 + \varepsilon \|w\|_{L^2(\partial\Omega_\varepsilon)} \right) \quad (5.112)$$

Taking $w = \frac{1}{\varepsilon} (v_\alpha^\varepsilon - v_\beta^\varepsilon)$, we deduce from (5.112) and a priori estimates (5.95) that

$$\sum_{\alpha=1}^d \sum_{\beta=1}^d \|v_\alpha^\varepsilon - v_\beta^\varepsilon\|_{L^2((0,T) \times \Omega_\varepsilon)} \leq C \varepsilon. \quad (5.113)$$

The estimate (5.113) implies that the limits obtained in (5.111) do match i.e., $v_\alpha = v$ for every $1 \leq \alpha \leq N$. The H^1 a priori estimate in space as in (5.95) does imply that $v \in L^2(0, T; H^1(\mathbb{R}^d))$ and that there exist limits $v_{1,\alpha} \in L^2(0, T \times \mathbb{R}^d; H^1(Y^0))$ such that

$$\nabla v_\alpha^\varepsilon \xrightarrow{2\text{-drift}} \nabla_x v + \nabla_y v_{1,\alpha} \quad (5.114)$$

for every $1 \leq \alpha \leq N$.

To handle the two-scale limit of the coupled term in (5.106), we shall be using the technical Lemma 3.8.1 that we used in Section 3.8 of Chapter 3. Lemma 3.8.1 states that for a function $\phi(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times \partial\Sigma^0)$ be such that

$$\int_{\partial\Sigma^0} \phi(t, x, y) d\sigma(y) = 0 \quad \forall (t, x) \in (0, T) \times \mathbb{R}^d. \quad (5.115)$$

There exists a vector field $\theta(t, x, y) \in L^2((0, T) \times \mathbb{R}^d \times \mathbb{T}^d)^d$ such that

$$\begin{cases} \operatorname{div}_y \theta = 0 & \text{in } Y^0, \\ \theta \cdot n = \phi & \text{on } \partial\Sigma^0, \\ y \rightarrow \theta & Y\text{-periodic.} \end{cases} \quad (5.116)$$

Taking ϕ from (5.115) as the test function, consider the following expression with the coupled term.

$$\begin{aligned} \varepsilon \int_0^T \int_{\partial\Omega_\varepsilon} \frac{1}{\varepsilon} (v_\alpha^\varepsilon - v_\beta^\varepsilon) \phi \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) d\sigma_\varepsilon(x) dt &= \int_0^T \int_{\Omega_\varepsilon} \operatorname{div} \left((v_\alpha^\varepsilon - v_\beta^\varepsilon) \theta \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) \right) dx dt \\ &= \int_0^T \int_{\Omega_\varepsilon} \left[(\nabla v_\alpha^\varepsilon - \nabla v_\beta^\varepsilon) \cdot \theta \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) + (v_\alpha^\varepsilon - v_\beta^\varepsilon) (\operatorname{div}_x \theta) \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right) \right] dx dt \\ &\quad \xrightarrow{2\text{-drift}} \int_0^T \int_{\mathbb{R}^d} \int_{Y^0} (\nabla_y v_{1,\alpha} - \nabla_y v_{1,\beta}) \cdot \theta dy dx dt \\ &= \int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} (v_{1,\alpha} - v_{1,\beta}) \theta \cdot n d\sigma(y) dx dt = \int_0^T \int_{\mathbb{R}^d} \int_{\partial\Sigma^0} (v_{1,\alpha} - v_{1,\beta}) \phi d\sigma(y) dx dt. \end{aligned}$$

The idea is to test the bulk equation (5.89) in the factorized system (5.89)-(5.91) with

$$\phi_\alpha^\varepsilon = \phi \left(t, x - \frac{b^*t}{\varepsilon} \right) + \varepsilon \phi_{1,\alpha} \left(t, x - \frac{b^*t}{\varepsilon}, \frac{x}{\varepsilon} \right). \quad (5.117)$$

Here $\phi(t, x)$ and $\phi_{1,\alpha}(t, x, y)$ are smooth compactly supported functions which vanish at the final time T .

$$\begin{aligned} \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \varphi_\alpha \varphi_\alpha^* \rho_\alpha^\varepsilon \frac{\partial v_\alpha^\varepsilon}{\partial t} \phi_\alpha^\varepsilon dx dt + \frac{1}{\varepsilon} \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \tilde{b}_\alpha^\varepsilon \cdot \nabla v_\alpha^\varepsilon \phi_\alpha^\varepsilon dx dt + \sum_{\alpha=1}^N \int_0^T \int_{\Omega_\varepsilon} \tilde{D}_\alpha^\varepsilon \nabla v_\alpha^\varepsilon \cdot \nabla \phi_\alpha^\varepsilon dx dt \\ + \frac{1}{\varepsilon} \sum_{\alpha=1}^N \sum_{\beta=1}^N \int_0^T \int_{\partial\Omega_\varepsilon} \Pi_{\alpha\beta} \varphi_\alpha^* \varphi_\beta (v_\beta^\varepsilon - v_\alpha^\varepsilon) \phi_\alpha^\varepsilon = 0. \end{aligned} \quad (5.118)$$

As the rest of the proof proceeds as in Theorem 5.6.1 using the two-scale limits found in the beginning of this proof, we shall avoid the details on passing to the limit as $\varepsilon \rightarrow 0$ in the variational formulation (5.118). \square

5.9 Adsorption: Model and qualitative analysis

In this section we would like to incorporate the adsorption models that we studied in Chapters 3 and 4 into the multiple component models that we have been working on in this chapter. Let u_α be the bulk concentration of the α^{th} component and v_α be its adsorbed surface concentration.

$$\frac{\partial u_\alpha}{\partial \tau} + b_\alpha \cdot \nabla u_\alpha - \operatorname{div}(D_\alpha \nabla u_\alpha) = 0 \text{ in } (0, \zeta) \times \Omega_f, \quad (5.119)$$

$$-D_\alpha \nabla u_\alpha \cdot n = \frac{\partial v_\alpha}{\partial \tau} - \operatorname{div}(D_\alpha \nabla v_\alpha) + \sum_{\beta=1}^N \Pi_{\alpha\beta} v_\beta = \kappa_\alpha (u_\alpha - v_\alpha) \quad \text{on } (0, \zeta) \times \Omega_s. \quad (5.120)$$

As we wish to work in the strong convection regime, we shall perform parabolic scaling. That leads to

$$\frac{\partial u_\alpha^\varepsilon}{\partial t} + \frac{1}{\varepsilon} b_\alpha^\varepsilon \cdot \nabla u_\alpha^\varepsilon - \operatorname{div}(D_\alpha^\varepsilon \nabla u_\alpha^\varepsilon) = 0 \text{ in } (0, T) \times \Omega_\varepsilon, \quad (5.121)$$

$$-\frac{1}{\varepsilon} D_\alpha^\varepsilon \nabla u_\alpha^\varepsilon \cdot n = \frac{\partial v_\alpha^\varepsilon}{\partial t} - \operatorname{div}(D_\alpha^\varepsilon \nabla v_\alpha^\varepsilon) + \frac{1}{\varepsilon^2} \sum_{\beta=1}^N \Pi_{\alpha\beta} v_\beta^\varepsilon = \frac{\kappa_\alpha}{\varepsilon^2} (u_\alpha^\varepsilon - v_\alpha^\varepsilon) \quad \text{on } (0, T) \times \partial\Omega_\varepsilon. \quad (5.122)$$

For simplicity, let us work with two component model. Let $u_\varepsilon^{(1)}$, $u_\varepsilon^{(2)}$ denote the bulk concentrations of the solutes and $v_\varepsilon^{(1)}$, $v_\varepsilon^{(2)}$ denote the adsorbed surface concentrations.

$$\frac{\partial u_\varepsilon^{(1)}}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^{(1)} \cdot \nabla u_\varepsilon^{(1)} - \operatorname{div}(D_\varepsilon^{(1)} \nabla u_\varepsilon^{(1)}) = 0 \quad \text{in } (0, T) \times \Omega_\varepsilon \quad (5.123)$$

$$\frac{\partial u_\varepsilon^{(2)}}{\partial t} + \frac{1}{\varepsilon} b_\varepsilon^{(2)} \cdot \nabla u_\varepsilon^{(2)} - \operatorname{div}(D_\varepsilon^{(2)} \nabla u_\varepsilon^{(2)}) = 0 \quad \text{in } (0, T) \times \Omega_\varepsilon \quad (5.124)$$

$$\frac{\partial v_\varepsilon^{(1)}}{\partial t} + \frac{1}{\varepsilon^2} (m_{11} v_\varepsilon^{(1)} - m_{12} v_\varepsilon^{(2)}) = -\frac{1}{\varepsilon} D_\varepsilon^{(1)} \nabla u_\varepsilon^{(1)} \cdot n = \frac{\kappa_1}{\varepsilon^2} (u_\varepsilon^{(1)} - v_\varepsilon^{(1)}) \quad \text{on } (0, T) \times \partial\Omega_\varepsilon \quad (5.125)$$

$$\frac{\partial v_\varepsilon^{(2)}}{\partial t} + \frac{1}{\varepsilon^2} (m_{22} v_\varepsilon^{(2)} - m_{21} v_\varepsilon^{(1)}) = -\frac{1}{\varepsilon} D_\varepsilon^{(2)} \nabla u_\varepsilon^{(2)} \cdot n = \frac{\kappa_2}{\varepsilon^2} (u_\varepsilon^{(2)} - v_\varepsilon^{(2)}) \quad \text{on } (0, T) \times \partial\Omega_\varepsilon \quad (5.126)$$

$$u_\varepsilon^{(1)}(0, x) = u_{init}^{(1)}(x), \quad u_\varepsilon^{(2)}(0, x) = u_{init}^{(2)}(x) \quad x \in \Omega_\varepsilon. \quad (5.127)$$

$$v_\varepsilon^{(1)}(0, x) = v_{init}^{(1)}(x), \quad v_\varepsilon^{(2)}(0, x) = v_{init}^{(2)}(x) \quad x \in \partial\Omega_\varepsilon. \quad (5.128)$$

where $b_\varepsilon^{(1)}$, $b_\varepsilon^{(2)}$ are ε -periodic velocity fields. In the previous sections we remarked that there is no need to make any further assumptions on the velocity fields (like incompressibility or no penetration conditions on the obstacles). $D_\varepsilon^{(1)}$, $D_\varepsilon^{(2)}$ are ε -periodic symmetric coercive diffusion matrices. The coupling matrix

$$\begin{pmatrix} m_{11} & -m_{12} \\ -m_{21} & m_{22} \end{pmatrix}$$

is such that $m_{ij} \geq 0$ for $i \neq j$. This assumption on the coupling matrix m_{ij} is the same as the one on Π that we have been using all through this chapter. In order to obtain a priori estimates, we need to factorize possible oscillations from the solutions of (5.123)-(5.128) as suggested by the Factorization principle. So, we shall introduce the following spectral cell problem associated with (5.123)-(5.128).

$$\left\{ \begin{array}{ll} b^{(1)}(y) \cdot \nabla_y \psi^{(1)} - \operatorname{div}_y \left(D^{(1)} \nabla_y \psi^{(1)} \right) = \lambda \psi^{(1)} & \text{in } Y^0, \\ -D^{(1)} \nabla_y \psi^{(1)} \cdot n = \kappa_1(\psi^{(1)} - \phi^{(1)}) = m_{11}\phi^{(1)} - m_{12}\phi^{(2)} - \lambda\phi^{(1)} & \text{on } \partial\Sigma^0, \\ b^{(2)}(y) \cdot \nabla_y \psi^{(2)} - \operatorname{div}_y \left(D^{(2)} \nabla_y \psi^{(2)} \right) = \lambda \psi^{(2)} & \text{in } Y^0, \\ -D^{(2)} \nabla_y \psi^{(2)} \cdot n = \kappa_2(\psi^{(2)} - \phi^{(2)}) = m_{22}\phi^{(2)} - m_{21}\phi^{(1)} - \lambda\phi^{(2)} & \text{on } \partial\Sigma^0, \\ y \rightarrow \left(\psi^{(1)}, \psi^{(2)}, \phi^{(1)}, \phi^{(2)} \right) & Y\text{-periodic.} \end{array} \right. \quad (5.129)$$

The adjoint of the eigenvalue problem (5.129) is the following

$$\left\{ \begin{array}{ll} -\operatorname{div}_y (b^{(1)} \psi^{(1)*}) - \operatorname{div}_y \left(D^{(1)} \nabla_y \psi^{(1)*} \right) = \lambda \psi^{(1)*} & \text{in } Y^0, \\ -D^{(1)} \nabla_y \psi^{(1)*} \cdot n - b^{(1)} \cdot n \psi^{(1)*} = \kappa_1(\psi^{(1)*} - \phi^{(1)*}) = m_{11}\phi^{(1)*} - m_{21}\phi^{(2)*} - \lambda\phi^{(1)*} & \text{on } \partial\Sigma^0, \\ -\operatorname{div}_y (b^{(2)} \psi^{(2)*}) - \operatorname{div}_y \left(D^{(2)} \nabla_y \psi^{(2)*} \right) = \lambda \psi^{(2)*} & \text{in } Y^0, \\ -D^{(2)} \nabla_y \psi^{(2)*} \cdot n - b^{(2)} \cdot n \psi^{(2)*} = \kappa_2(\psi^{(2)*} - \phi^{(2)*}) = m_{22}\phi^{(2)*} - m_{12}\phi^{(1)*} - \lambda\phi^{(2)*} & \text{on } \partial\Sigma^0, \\ y \rightarrow \left(\psi^{(1)*}, \psi^{(2)*} \right) \text{ and } y \rightarrow \left(\phi^{(1)*}, \phi^{(2)*} \right) & Y\text{-periodic.} \end{array} \right. \quad (5.130)$$

The existence of the first simple positive eigenvalue λ for (5.129) and (5.130) follow from the results in [152]. Using the first eigenfunctions $\psi^{(1)}$, $\psi^{(2)}$, $\phi^{(1)}$, $\phi^{(2)}$, we shall make the following change of unknowns

$$u_\varepsilon^{(1)}(t, x) = e^{-\lambda t/\varepsilon^2} \psi^{(1)}\left(\frac{x}{\varepsilon}\right) U_\varepsilon^{(1)}(t, x); \quad u_\varepsilon^{(2)}(t, x) = e^{-\lambda t/\varepsilon^2} \psi^{(2)}\left(\frac{x}{\varepsilon}\right) U_\varepsilon^{(2)}(t, x) \quad (5.131)$$

$$v_\varepsilon^{(1)}(t, x) = e^{-\lambda t/\varepsilon^2} \phi^{(1)}\left(\frac{x}{\varepsilon}\right) V_\varepsilon^{(1)}(t, x); \quad v_\varepsilon^{(2)}(t, x) = e^{-\lambda t/\varepsilon^2} \phi^{(2)}\left(\frac{x}{\varepsilon}\right) V_\varepsilon^{(2)}(t, x), \quad (5.132)$$

Now we state a result that gives the system of equations satisfied by $\left(U_\varepsilon^{(1)}, U_\varepsilon^{(2)}, V_\varepsilon^{(1)}, V_\varepsilon^{(2)} \right)$

Lemma 5.9.1. *Upon making the change of unknowns as in (5.131) and (5.132), we arrive at the following coupled system for $\left(U_\varepsilon^{(1)}, U_\varepsilon^{(2)}, V_\varepsilon^{(1)}, V_\varepsilon^{(2)} \right)$.*

$$\psi^{(1)} \psi^{(1)*} \frac{\partial U_\varepsilon^{(1)}}{\partial t} + \frac{1}{\varepsilon} \tilde{b}_\varepsilon^{(1)} \cdot \nabla U_\varepsilon^{(1)} - \operatorname{div} \left(\tilde{D}_\varepsilon^{(1)} \nabla U_\varepsilon^{(1)} \right) = 0 \quad \text{in } (0, T) \times \Omega_\varepsilon \quad (5.133)$$

$$\psi^{(2)}\psi^{(2)*}\frac{\partial U_\varepsilon^{(2)}}{\partial t} + \frac{1}{\varepsilon}\tilde{b}_\varepsilon^{(2)} \cdot \nabla U_\varepsilon^{(2)} - \operatorname{div} \left(\tilde{D}_\varepsilon^{(2)} \nabla U_\varepsilon^{(2)} \right) = 0 \quad \text{in } (0, T) \times \Omega_\varepsilon \quad (5.134)$$

$$-\frac{1}{\varepsilon}\tilde{D}_\varepsilon^{(1)} \nabla U_\varepsilon^{(1)} \cdot n = \psi^{(1)*}\phi^{(1)}\frac{\kappa_1}{\varepsilon^2} \left(U_\varepsilon^{(1)} - V_\varepsilon^{(1)} \right) \quad \text{on } (0, T) \times \partial\Omega_\varepsilon \quad (5.135)$$

$$-\frac{1}{\varepsilon}\tilde{D}_\varepsilon^{(2)} \nabla U_\varepsilon^{(2)} \cdot n = \psi^{(2)*}\phi^{(2)}\frac{\kappa_2}{\varepsilon^2} \left(U_\varepsilon^{(2)} - V_\varepsilon^{(2)} \right) \quad \text{on } (0, T) \times \partial\Omega_\varepsilon \quad (5.136)$$

$$\phi^{(1)}\phi^{(1)*}\frac{\partial V_\varepsilon^{(1)}}{\partial t} + \frac{1}{\varepsilon^2}m_{12}\phi^{(1)*}\phi^{(2)} \left(V_\varepsilon^{(1)} - V_\varepsilon^{(2)} \right) = \phi^{(1)*}\psi^{(1)}\frac{\kappa_1}{\varepsilon^2} \left(U_\varepsilon^{(1)} - V_\varepsilon^{(1)} \right) \quad \text{on } (0, T) \times \partial\Omega_\varepsilon \quad (5.137)$$

$$\phi^{(2)}\phi^{(2)*}\frac{\partial V_\varepsilon^{(2)}}{\partial t} + \frac{1}{\varepsilon^2}m_{21}\phi^{(1)}\phi^{(2)*} \left(V_\varepsilon^{(2)} - V_\varepsilon^{(1)} \right) = \phi^{(2)*}\psi^{(2)}\frac{\kappa_2}{\varepsilon^2} \left(U_\varepsilon^{(2)} - V_\varepsilon^{(2)} \right) \quad \text{on } (0, T) \times \partial\Omega_\varepsilon \quad (5.138)$$

where $\tilde{b}^{(1)}$ is given by an expression similar to that of \tilde{b}_α in (5.17) in terms of the bulk eigenfunction $\psi^{(1)}$, the velocity field $b^{(1)}$ and the diffusion matrix $D^{(1)}$. Similar expression for $\tilde{b}^{(2)}$ too. The $\tilde{D}^{(1)}$ is given by an expression similar to that of \tilde{D}_α in (5.18) in terms of the bulk eigenfunction $\psi^{(1)}$ and the diffusion matrix $D^{(1)}$. Similar expression for $\tilde{D}^{(2)}$ too.

The proof of Lemma 5.9.1 is straightforward upon using the chain rule for differentiation (5.19). Our next task is to derive a priori estimates for the solutions of (5.133)-(5.138).

Lemma 5.9.2. *Let $(U_\varepsilon^{(1)}, U_\varepsilon^{(2)}, V_\varepsilon^{(1)}, V_\varepsilon^{(2)})$ be a weak solution of (5.133)-(5.138). Then we have the following a priori estimates.*

$$\left\{ \begin{array}{l} \left\| U_\varepsilon^{(1)} \right\|_{L^\infty((0,T);L^2(\Omega_\varepsilon))} + \left\| U_\varepsilon^{(2)} \right\|_{L^\infty((0,T);L^2(\Omega_\varepsilon))} + \sqrt{\varepsilon} \left\| V_\varepsilon^{(1)} \right\|_{L^\infty((0,T);L^2(\partial\Omega_\varepsilon))} \\ + \sqrt{\varepsilon} \left\| V_\varepsilon^{(2)} \right\|_{L^\infty((0,T);L^2(\partial\Omega_\varepsilon))} + \left\| \nabla U_\varepsilon^{(1)} \right\|_{L^2((0,T)\times\Omega_\varepsilon)} + \left\| \nabla U_\varepsilon^{(2)} \right\|_{L^2((0,T)\times\Omega_\varepsilon)} \\ + \sqrt{\varepsilon} \left\| \frac{1}{\varepsilon} \left(U_\varepsilon^{(1)} - V_\varepsilon^{(1)} \right) \right\|_{L^2((0,T)\times\partial\Omega_\varepsilon)} + \sqrt{\varepsilon} \left\| \frac{1}{\varepsilon} \left(U_\varepsilon^{(2)} - V_\varepsilon^{(2)} \right) \right\|_{L^2((0,T)\times\partial\Omega_\varepsilon)} \\ + \sqrt{\varepsilon} \left\| \frac{1}{\varepsilon} \left(V_\varepsilon^{(1)} - V_\varepsilon^{(2)} \right) \right\|_{L^2((0,T)\times\partial\Omega_\varepsilon)} \leq C. \end{array} \right. \quad (5.139)$$

Proof. We shall follow the standard approach of deriving a priori estimates for parabolic systems. Let us multiply (5.133) by $U_\varepsilon^{(1)}$ and (5.134) by $U_\varepsilon^{(2)}$ followed by integration over Ω_ε . Let us then multiply (5.137) by $V_\varepsilon^{(1)}$ and (5.138) by $V_\varepsilon^{(2)}$ followed by integration over $\partial\Omega_\varepsilon$. Adding the thus obtained expressions lead to

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_{\Omega_\varepsilon} \psi^{(1)}\psi^{(1)*} |U_\varepsilon^{(1)}|^2 dx + \frac{1}{2} \frac{1}{\varepsilon} \int_{\Omega_\varepsilon} \tilde{b}_\varepsilon^{(1)} \cdot \nabla |U_\varepsilon^{(1)}|^2 dx + \int_{\Omega_\varepsilon} \tilde{D}_\varepsilon^{(1)} \nabla U_\varepsilon^{(1)} \cdot \nabla U_\varepsilon^{(1)} dx \\ & + \frac{1}{2} \frac{d}{dt} \int_{\Omega_\varepsilon} \psi^{(2)}\psi^{(2)*} |U_\varepsilon^{(2)}|^2 dx + \frac{1}{2} \frac{1}{\varepsilon} \int_{\Omega_\varepsilon} \tilde{b}_\varepsilon^{(2)} \cdot \nabla |U_\varepsilon^{(2)}|^2 dx + \int_{\Omega_\varepsilon} \tilde{D}_\varepsilon^{(2)} \nabla U_\varepsilon^{(2)} \cdot \nabla U_\varepsilon^{(2)} dx \\ & + \frac{1}{2} \frac{d}{dt} \varepsilon \int_{\partial\Omega_\varepsilon} \phi^{(1)}\phi^{(1)*} |V_\varepsilon^{(1)}|^2 d\sigma(x) + \frac{1}{2} \frac{d}{dt} \varepsilon \int_{\partial\Omega_\varepsilon} \phi^{(2)}\phi^{(2)*} |V_\varepsilon^{(2)}|^2 d\sigma(x) \\ & + \frac{\kappa_1}{\varepsilon} \int_{\partial\Omega_\varepsilon} \left(\psi^{(1)*}\phi^{(1)}U_\varepsilon^{(1)} - \phi^{(1)*}\psi^{(1)}V_\varepsilon^{(1)} \right) \left(U_\varepsilon^{(1)} - V_\varepsilon^{(1)} \right) d\sigma(x) \end{aligned}$$

$$\begin{aligned}
& + \frac{\kappa_2}{\varepsilon} \int_{\partial\Omega_\varepsilon} \left(\psi^{(2)*} \phi^{(2)} U_\varepsilon^{(2)} - \phi^{(2)*} \psi^{(2)} V_\varepsilon^{(2)} \right) \left(U_\varepsilon^{(2)} - V_\varepsilon^{(2)} \right) d\sigma(x) \\
& + \frac{1}{\varepsilon} \int_{\partial\Omega_\varepsilon} \left(m_{12} \phi^{(1)*} \phi^{(2)} V_\varepsilon^{(1)} - m_{21} \phi^{(1)} \phi^{(2)*} V_\varepsilon^{(2)} \right) \left(V_\varepsilon^{(1)} - V_\varepsilon^{(2)} \right) d\sigma(x) = 0. \tag{5.140}
\end{aligned}$$

To obtain energy estimates, we need to first show that the terms on the left hand side of (5.140) are positive. Here the cell eigenvalue problems (5.129) and (5.130) come to our rescue. To better understand the difficulties at hand, let us regroup the problematic terms from (5.140).

$$-\frac{1}{2} \frac{1}{\varepsilon} \int_{\Omega_\varepsilon} \operatorname{div} \left(\tilde{b}_\varepsilon^{(1)} \right) |U_\varepsilon^{(1)}|^2 dx - \frac{1}{2} \frac{1}{\varepsilon} \int_{\Omega_\varepsilon} \operatorname{div} \left(\tilde{b}_\varepsilon^{(2)} \right) |U_\varepsilon^{(2)}|^2 dx \tag{5.141}$$

$$+ \frac{\kappa_1}{\varepsilon} \int_{\partial\Omega_\varepsilon} \left(\psi^{(1)*} \phi^{(1)} U_\varepsilon^{(1)} - \phi^{(1)*} \psi^{(1)} V_\varepsilon^{(1)} \right) \left(U_\varepsilon^{(1)} - V_\varepsilon^{(1)} \right) d\sigma(x) \tag{5.142}$$

$$+ \frac{\kappa_2}{\varepsilon} \int_{\partial\Omega_\varepsilon} \left(\psi^{(2)*} \phi^{(2)} U_\varepsilon^{(2)} - \phi^{(2)*} \psi^{(2)} V_\varepsilon^{(2)} \right) \left(U_\varepsilon^{(2)} - V_\varepsilon^{(2)} \right) d\sigma(x) \tag{5.143}$$

$$+ \frac{1}{\varepsilon} \int_{\partial\Omega_\varepsilon} \left(m_{12} \phi^{(1)*} \phi^{(2)} V_\varepsilon^{(1)} - m_{21} \phi^{(1)} \phi^{(2)*} V_\varepsilon^{(2)} \right) \left(V_\varepsilon^{(1)} - V_\varepsilon^{(2)} \right) d\sigma(x) \tag{5.144}$$

Let us test the bulk equations in the spectral cell problem (5.129) by $\left(\psi^{(1)*} \left(U_\varepsilon^{(1)} \right)^2, \psi^{(2)*} \left(U_\varepsilon^{(2)} \right)^2 \right)$ and integrate over Y^0 . Then, test the surface equations in the spectral problem (5.129) by $\left(\phi^{(1)*} \left(V_\varepsilon^{(1)} \right)^2, \phi^{(2)*} \left(V_\varepsilon^{(2)} \right)^2 \right)$ and integrate over $\partial\Sigma^0$.

$$\begin{aligned}
& \int_{Y^0} b^{(1)} \cdot \nabla_y \psi^{(1)} \psi^{(1)*} \left(U_\varepsilon^{(1)} \right)^2 dy - \int_{Y^0} \operatorname{div}_y \left(D^{(1)} \nabla_y \psi^{(1)} \right) \psi^{(1)*} \left(U_\varepsilon^{(1)} \right)^2 dy - \int_{Y^0} \lambda \psi^{(1)} \psi^{(1)*} \left(U_\varepsilon^{(1)} \right)^2 dy \\
& + \int_{Y^0} b^{(2)} \cdot \nabla_y \psi^{(2)} \psi^{(2)*} \left(U_\varepsilon^{(2)} \right)^2 dy - \int_{Y^0} \operatorname{div}_y \left(D^{(2)} \nabla_y \psi^{(2)} \right) \psi^{(2)*} \left(U_\varepsilon^{(2)} \right)^2 dy - \int_{Y^0} \lambda \psi^{(2)} \psi^{(2)*} \left(U_\varepsilon^{(2)} \right)^2 dy \\
& + \int_{\partial\Sigma^0} \left(m_{11} \phi^{(1)} - m_{12} \phi^{(2)} - \lambda \phi^{(1)} - \kappa_1 (\psi^{(1)} - \phi^{(1)}) \right) \phi^{(1)*} \left(V_\varepsilon^{(1)} \right)^2 d\sigma(y) \\
& + \int_{\partial\Sigma^0} \left(m_{22} \phi^{(2)} - m_{21} \phi^{(1)} - \lambda \phi^{(2)} - \kappa_2 (\psi^{(2)} - \phi^{(2)}) \right) \phi^{(2)*} \left(V_\varepsilon^{(2)} \right)^2 d\sigma(y) = 0 \tag{5.145}
\end{aligned}$$

After integration by parts and using information from the spectral cell problem (5.129) and its adjoint (5.130), the above equation (5.145) is equivalent to

$$\begin{aligned}
& \int_{Y^0} \left\{ -\operatorname{div}_y (b^{(1)} \psi^{(1)*}) - \operatorname{div}_y \left(D^{(1)} \nabla_y \psi^{(1)*} \right) - \lambda \psi^{(1)*} \right\} \psi^{(1)} \left(U_\varepsilon^{(1)} \right)^2 dy \\
& - \int_{Y^0} \tilde{b}^{(1)} \cdot \nabla_y \left(U_\varepsilon^{(1)} \right)^2 dy + \kappa_1 \int_{\partial\Sigma^0} \left(U_\varepsilon^{(1)} \right)^2 \left(\psi^{(1)} \phi^{(1)*} - \psi^{(1)*} \phi^{(1)} \right) d\sigma(y) \\
& + \int_{Y^0} \left\{ -\operatorname{div}_y (b^{(2)} \psi^{(2)*}) - \operatorname{div}_y \left(D^{(2)} \nabla_y \psi^{(2)*} \right) - \lambda \psi^{(2)*} \right\} \psi^{(2)} \left(U_\varepsilon^{(2)} \right)^2 dy
\end{aligned}$$

$$\begin{aligned}
& - \int_{Y^0} \tilde{b}^{(2)} \cdot \nabla_y \left(U_\varepsilon^{(2)} \right)^2 dy + \kappa_2 \int_{\partial\Sigma^0} \left(U_\varepsilon^{(2)} \right)^2 \left(\psi^{(2)} \phi^{(2)*} - \psi^{(2)*} \phi^{(2)} \right) d\sigma(y) \\
& + \int_{\partial\Sigma^0} \left\{ m_{11} \phi^{(1)*} - m_{21} \phi^{(2)*} - \lambda \phi^{(1)*} \right\} \phi^{(1)} \left(V_\varepsilon^{(1)} \right)^2 + m_{21} \phi^{(1)} \phi^{(2)*} \left\{ \left(V_\varepsilon^{(1)} \right)^2 - \left(V_\varepsilon^{(2)} \right)^2 \right\} d\sigma(y) \\
& + \int_{\partial\Sigma^0} \left\{ m_{22} \phi^{(2)*} - m_{12} \phi^{(1)*} - \lambda \phi^{(2)*} \right\} \phi^{(2)} \left(V_\varepsilon^{(2)} \right)^2 + m_{12} \phi^{(1)*} \phi^{(2)} \left\{ \left(V_\varepsilon^{(2)} \right)^2 - \left(V_\varepsilon^{(1)} \right)^2 \right\} d\sigma(y) \\
& - \kappa_1 \int_{\partial\Sigma^0} \left(\psi^{(1)} - \phi^{(1)} \right) \phi^{(1)*} \left(V_\varepsilon^{(1)} \right)^2 d\sigma(y) - \kappa_2 \int_{\partial\Sigma^0} \left(\psi^{(2)} - \phi^{(2)} \right) \phi^{(2)*} \left(V_\varepsilon^{(2)} \right)^2 d\sigma(y) = 0. \quad (5.146)
\end{aligned}$$

In (5.146), we recognize the adjoint spectral cell problem (5.130). Upon using information from (5.130), we deduce that (5.146) is equivalent to the following.

$$\begin{aligned}
& - \int_{Y^0} \tilde{b}^{(1)} \cdot \nabla_y \left(U_\varepsilon^{(1)} \right)^2 dy + \kappa_1 \int_{\partial\Sigma^0} \left(U_\varepsilon^{(1)} \right)^2 \left(\psi^{(1)} \phi^{(1)*} - \psi^{(1)*} \phi^{(1)} \right) d\sigma(y) \\
& - \int_{Y^0} \tilde{b}^{(2)} \cdot \nabla_y \left(U_\varepsilon^{(2)} \right)^2 dy + \kappa_2 \int_{\partial\Sigma^0} \left(U_\varepsilon^{(2)} \right)^2 \left(\psi^{(2)} \phi^{(2)*} - \psi^{(2)*} \phi^{(2)} \right) d\sigma(y) \\
& + \kappa_1 \int_{\partial\Sigma^0} \left(\psi^{(1)*} \phi^{(1)} - \psi^{(1)} \phi^{(1)*} \right) \left(V_\varepsilon^{(1)} \right)^2 d\sigma(y) + \kappa_2 \int_{\partial\Sigma^0} \left(\psi^{(2)*} \phi^{(2)} - \psi^{(2)} \phi^{(2)*} \right) \left(V_\varepsilon^{(2)} \right)^2 d\sigma(y) \\
& + \int_{\partial\Sigma^0} m_{21} \phi^{(1)} \phi^{(2)*} \left\{ \left(V_\varepsilon^{(1)} \right)^2 - \left(V_\varepsilon^{(2)} \right)^2 \right\} d\sigma(y) + \int_{\partial\Sigma^0} m_{12} \phi^{(1)*} \phi^{(2)} \left\{ \left(V_\varepsilon^{(2)} \right)^2 - \left(V_\varepsilon^{(1)} \right)^2 \right\} d\sigma(y) = 0. \quad (5.147)
\end{aligned}$$

Rescaling the above equation (5.147) onto Ω_ε and using them in the problematic terms (5.141)-(5.142)-(5.143)-(5.144), we can show that the problematic terms (5.141) through (5.144) contribute as

$$\begin{aligned}
& \frac{\kappa_1}{\varepsilon} \frac{1}{2} \int_{\partial\Omega_\varepsilon} \left(\psi^{(1)} \phi^{(1)*} + \psi^{(1)*} \phi^{(1)} \right) \left(U_\varepsilon^{(1)} - V_\varepsilon^{(1)} \right)^2 \\
& + \frac{\kappa_2}{\varepsilon} \frac{1}{2} \int_{\partial\Omega_\varepsilon} \left(\psi^{(2)} \phi^{(2)*} + \psi^{(2)*} \phi^{(2)} \right) \left(U_\varepsilon^{(2)} - V_\varepsilon^{(2)} \right)^2 \\
& + \frac{1}{\varepsilon} \frac{1}{2} \int_{\partial\Omega_\varepsilon} \left(m_{12} \phi^{(1)*} \phi^{(2)} + m_{21} \phi^{(1)} \phi^{(2)*} \right) \left(V_\varepsilon^{(1)} - V_\varepsilon^{(2)} \right)^2 \quad (5.148)
\end{aligned}$$

Using (5.148) for the problematic terms in (5.140), we arrive at the following energy estimate.

$$\begin{aligned}
& \frac{1}{2} \frac{d}{dt} \int_{\Omega_\varepsilon} \psi^{(1)} \psi^{(1)*} |U_\varepsilon^{(1)}|^2 dx + \int_{\Omega_\varepsilon} \tilde{D}_\varepsilon^{(1)} \nabla U_\varepsilon^{(1)} \cdot \nabla U_\varepsilon^{(1)} dx \\
& + \frac{1}{2} \frac{d}{dt} \int_{\Omega_\varepsilon} \psi^{(2)} \psi^{(2)*} |U_\varepsilon^{(2)}|^2 dx + \int_{\Omega_\varepsilon} \tilde{D}_\varepsilon^{(2)} \nabla U_\varepsilon^{(2)} \cdot \nabla U_\varepsilon^{(2)} dx \\
& + \frac{1}{2} \frac{d}{dt} \varepsilon \int_{\partial\Omega_\varepsilon} \phi^{(1)} \phi^{(1)*} |V_\varepsilon^{(1)}|^2 d\sigma(x) + \frac{1}{2} \frac{d}{dt} \varepsilon \int_{\partial\Omega_\varepsilon} \phi^{(2)} \phi^{(2)*} |V_\varepsilon^{(2)}|^2 d\sigma(x)
\end{aligned}$$

$$\begin{aligned}
& + \frac{\kappa_1}{\varepsilon} \frac{1}{2} \int_{\partial\Omega_\varepsilon} \left(\psi^{(1)} \phi^{(1)*} + \psi^{(1)*} \phi^{(1)} \right) \left(U_\varepsilon^{(1)} - V_\varepsilon^{(1)} \right)^2 \\
& + \frac{\kappa_2}{\varepsilon} \frac{1}{2} \int_{\partial\Omega_\varepsilon} \left(\psi^{(2)} \phi^{(2)*} + \psi^{(2)*} \phi^{(2)} \right) \left(U_\varepsilon^{(2)} - V_\varepsilon^{(2)} \right)^2 \\
& + \frac{1}{\varepsilon} \frac{1}{2} \int_{\partial\Omega_\varepsilon} \left(m_{12} \phi^{(1)*} \phi^{(2)} + m_{21} \phi^{(1)} \phi^{(2)*} \right) \left(V_\varepsilon^{(1)} - V_\varepsilon^{(2)} \right)^2 = 0.
\end{aligned} \tag{5.149}$$

Integrating (5.149) over time interval $(0, T)$ leads to the a priori estimates (5.139). \square

5.10 Adsorption: Homogenization

In this section, we shall give the homogenization result concerning the microscopic model (5.123)-(5.128). Consider the following asymptotic expansions for the solutions of (5.123)-(5.128).

$$u_\varepsilon^{(1)}(t, x) = e^{-\lambda t/\varepsilon^2} \sum_{i \geq 0} \varepsilon^i u_i^{(1)} \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \quad u_\varepsilon^{(2)}(t, x) = e^{-\lambda t/\varepsilon^2} \sum_{i \geq 0} \varepsilon^i u_i^{(2)} \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right). \tag{5.150}$$

$$v_\varepsilon^{(1)}(t, x) = \exp(-\lambda t/\varepsilon^2) \sum_{i \geq 0} \varepsilon^i v_i^{(1)} \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \quad v_\varepsilon^{(2)}(t, x) = \exp(-\lambda t/\varepsilon^2) \sum_{i \geq 0} \varepsilon^i v_i^{(2)} \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right). \tag{5.151}$$

Proposition 5.10.1. *If the asymptotic expansions for the solutions of (5.123)-(5.128) as given in (5.150) and (5.151) hold true, then the solutions can be approximated as*

$$u_\varepsilon^{(1)}(t, x) \approx \exp(-\lambda t/\varepsilon^2) \psi^{(1)} \left(\frac{x}{\varepsilon} \right) \left[v \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon \sum_{i=1}^d \frac{\partial v}{\partial x_i} \left(t, x - \frac{b^* t}{\varepsilon} \right) \omega_i^{(1)} \left(\frac{x}{\varepsilon} \right) \right] \tag{5.152}$$

$$u_\varepsilon^{(2)}(t, x) \approx \exp(-\lambda t/\varepsilon^2) \psi^{(2)} \left(\frac{x}{\varepsilon} \right) \left[v \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon \sum_{i=1}^d \frac{\partial v}{\partial x_i} \left(t, x - \frac{b^* t}{\varepsilon} \right) \omega_i^{(2)} \left(\frac{x}{\varepsilon} \right) \right] \tag{5.153}$$

$$v_\varepsilon^{(1)}(t, x) \approx \exp(-\lambda t/\varepsilon^2) \phi^{(1)} \left(\frac{x}{\varepsilon} \right) \left[v \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon \sum_{i=1}^d \frac{\partial v}{\partial x_i} \left(t, x - \frac{b^* t}{\varepsilon} \right) \chi_i^{(1)} \left(\frac{x}{\varepsilon} \right) \right] \tag{5.154}$$

$$v_\varepsilon^{(2)}(t, x) \approx \exp(-\lambda t/\varepsilon^2) \phi^{(2)} \left(\frac{x}{\varepsilon} \right) \left[v \left(t, x - \frac{b^* t}{\varepsilon} \right) + \varepsilon \sum_{i=1}^d \frac{\partial v}{\partial x_i} \left(t, x - \frac{b^* t}{\varepsilon} \right) \chi_i^{(2)} \left(\frac{x}{\varepsilon} \right) \right] \tag{5.155}$$

with the effective drift b^* given by

$$b^* = \int_{Y^0} \left(\tilde{b}^{(1)} + \tilde{b}^{(2)} \right) dy, \tag{5.156}$$

$\lambda > 0$ is the first eigenvalue of the spectral cell problems (5.129) and (5.130) with $(\psi^{(1)}, \psi^{(2)})$ and $(\phi^{(1)}, \phi^{(2)})$ are the associated first eigenvector functions.

The $(\omega_i^{(1)}, \omega_i^{(2)}, \chi_i^{(1)}, \chi_i^{(2)})$ in the above approximations satisfy the following coupled cell problem.

$$\left\{ \begin{array}{ll} \tilde{b}^{(1)}(y) \cdot (\nabla_y \omega_i^{(1)} + e_i) - \operatorname{div}_y (\tilde{D}^{(1)} (\nabla_y \omega_i^{(1)} + e_i)) = \psi^{(1)*} \psi^{(1)} b^* \cdot e_i & \text{in } Y^0, \\ -\tilde{D}^{(1)} (\nabla_y \omega_i^{(1)} + e_i) \cdot n = \kappa_1 (\psi^{(1)} \psi^{(1)*} \omega_i^{(1)} - \phi^{(1)} \psi^{(1)*} \chi_i^{(1)}) & \text{on } \partial \Sigma^0, \\ \kappa_1 \psi^{(1)} \phi^{(1)*} (\omega_i^{(1)} - \chi_i^{(1)}) = -\phi^{(1)} \phi^{(1)*} b^* \cdot e_i + m_{12} \phi^{(2)} \phi^{(1)*} (\chi_i^{(1)} - \chi_i^{(2)}) & \text{on } \partial \Sigma^0, \\ \tilde{b}^{(2)}(y) \cdot (\nabla_y \omega_i^{(2)} + e_i) - \operatorname{div}_y (\tilde{D}^{(2)} (\nabla_y \omega_i^{(2)} + e_i)) = \psi^{(2)*} \psi^{(2)} b^* \cdot e_i & \text{in } Y^0, \\ -\tilde{D}^{(2)} (\nabla_y \omega_i^{(2)} + e_i) \cdot n = \kappa_2 (\psi^{(2)} \psi^{(2)*} \omega_i^{(2)} - \phi^{(2)} \psi^{(2)*} \chi_i^{(2)}) & \text{on } \partial \Sigma^0, \\ \kappa_2 \psi^{(2)} \phi^{(2)*} (\omega_i^{(2)} - \chi_i^{(2)}) = -\phi^{(2)} \phi^{(2)*} b^* \cdot e_i + m_{21} \phi^{(2)*} \phi^{(1)} (\chi_i^{(2)} - \chi_i^{(1)}) & \text{on } \partial \Sigma^0, \\ y \rightarrow (\omega_i^{(1)}, \omega_i^{(2)}, \chi_i^{(1)}, \chi_i^{(2)}) & Y - \text{periodic.} \end{array} \right. \quad (5.157)$$

Further, the zero order non-oscillating term $v(t, x)$ in the above approximations satisfy the following scalar diffusion equation.

$$\frac{\partial v}{\partial t} = \operatorname{div}(\mathcal{D} \nabla v) \quad \text{in } (0, T) \times \mathbb{R}^d. \quad (5.158)$$

The expression for the effective dispersion \mathcal{D} in (5.158) is given in terms of the solutions to the cell problem (5.157) as follows

$$\left\{ \begin{array}{l} \mathcal{D}_{ij} = \sum_{l=1}^2 \int_{Y^0} \tilde{D}^{(l)} (\nabla_y \omega_i^{(l)} + e_i) \cdot (\nabla_y \omega_j^{(l)} + e_j) \\ + \sum_{l=1}^2 \int_{\partial \Sigma^0} (\phi^{(l)} \psi^{(l)*} + \psi^{(l)} \phi^{(l)*}) (\omega_i^{(l)} - \chi_i^{(l)}) (\omega_j^{(l)} - \chi_j^{(l)}) d\sigma(y) \\ + \sum_{l=1}^2 \sum_{k=1}^2 \int_{\partial \Sigma^0} m_{lk} \phi^{(l)} \phi^{(k)*} (\chi_i^{(l)} - \chi_j^{(k)}) (\chi_j^{(l)} - \chi_i^{(k)}) d\sigma(y). \end{array} \right. \quad (5.159)$$

We shall avoid the proof of Proposition 5.10.1 as the details of the proof are almost similar to the ones found in Section 5.4 where we formally obtained the effective equation using Factorization principle and two-scale asymptotic expansions with drift. We can also justify the above formal result using the notion of two-scale convergence with drift. This approach has been applied to two different models in this chapter alone (Sections 5.5, 5.6, 5.8). Using the a priori estimates from Lemma 5.9.2, we will be able to prove relative compactness property of the solution sequences. These compactness results shall be helpful while passing to the limit as $\varepsilon \rightarrow 0$ in the variational formulation. This being the recipe for all homogenization problems via two-scale convergence, we shall skip the proof.

Conclusions

All the multicomponent models studied in this chapter are linear models. There is a work underway to model nonlinear reactions in multicomponent flows. We are taking cues from [92] to incorporate the aspects of thermodynamics into the reactive transport models. The analysis at this moment are quite formal. We hope to come up with a framework to handle more complex systems and means to upscale them.

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Abstract

Our work is a contribution to the understanding of transport of solutes in a porous medium. It has applications in groundwater contaminant transport, CO₂ sequestration, underground storage of nuclear waste, oil reservoir simulations. We derive expressions for the effective Taylor dispersion taking into account convection, diffusion, heterogeneous geometry of the porous medium and reaction phenomena. Microscopic phenomena at the pore scale are upscaled to obtain effective behaviour at the observation scale. Method of two-scale convergence with drift from the theory of homogenization is employed as an upscaling technique. In the first part of our work, we consider reactions of mass exchange type, adsorption/desorption, at the fluid-solid interface of the porous medium. Starting with coupled convection-diffusion equations for bulk and surface concentrations of a single solute, coupled via adsorption isotherms, at a microscopic scale we derive effective equations at the macroscopic scale. We consider the microscopic system with highly oscillating coefficients in a strong convection regime i.e., large Péclet regime. The presence of strong convection in the microscopic model leads to the induction of a large drift in the concentration profiles. Both linear and nonlinear adsorption isotherms are considered and the results are compared. In the second part of our work we generalize our results on single component flow to multicomponent flow in a linear setting. In the latter case, the effective parameters are obtained using Factorization principle and two-scale convergence with drift. The behaviour of effective parameters with respect to Péclet number and Damköhler number are numerically studied. Freefem++ is used to perform numerical tests in two dimensions.

Keywords: Homogenization, Porous media, Periodic structures, Two-scale convergence, Dispersion Tensor, Reactive flows, Adsorption isotherms, Multicomponent flow.

Résumé

Ce travail est une contribution pour mieux comprendre le transport de solutés dans un milieu poreux. Ce phénomène se rencontre dans de nombreux domaines: transport de contaminants dans les eaux souterraines, séquestration du CO₂, stockage souterrain des déchets nucléaires, simulations de réservoirs pétroliers. On obtient la dispersion effective de Taylor en tenant compte de la convection, de la diffusion, de la géométrie du milieu poreux et des réactions chimiques. Le but de la théorie d'homogénéisation est, à partir d'équations microscopiques, de dériver un modèle effectif à l'échelle macroscopique. Ici, on applique la méthode de convergence à deux échelles avec dérive pour arriver au comportement effectif. Dans un premier temps, on considère les réactions de type adsorption à la surface des pores. À l'échelle microscopique, le phénomène de transport est modélisé par des équations couplées de type advection-diffusion, une pour la concentration dans le fluide et l'autre pour la concentration à la surface de milieu poreux. Le couplage est fait par les isothermes d'adsorption. Le système microscopique avec des coefficients fortement oscillants est étudié dans un régime de forte convection i.e., dans un régime de grand nombre de Péclet. La présence de forte convection dans le modèle microscopique se traduit par l'apparition d'une large dérive dans les profils de concentrations. On considère à la fois l'isotherme linéaire et l'isotherme non linéaire et les résultats ainsi obtenus sont comparés. Dans la deuxième partie, on généralise nos résultats concernant le transport réactif d'un seul soluté à ceux de plusieurs solutés dans un cadre linéaire. Dans ce cas, les paramètres effectifs sont obtenus en utilisant le principe de Factorisation et la convergence à deux échelles avec dérive. On étudie numériquement le comportement des paramètres effectifs par rapport au nombre de Péclet et au nombre de Damköhler. On utilise Freefem++ pour effectuer des tests numériques en dimension deux.

Mots clefs: Homogénéisation, Milieux poreux, Structures périodiques, Convergence à deux échelles, Tenseur de dispersion, Écoulements réactifs, Isothermes d'adsorption.