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Corrector Homogenization Estimates for PDE Systems with Coupled Fluxes posed in Media with Periodic Microstructures

PHD CANDIDATE

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This thesis is dedicated to the memory of my father, **Vo Hoang Oanh**, to my beloved mother, **Duong Thi Thu**, and to my younger brother, **Vo Anh Khoi**.

Declaration

This thesis is the result of my own work and includes nothing which is the outcome of work done in collaboration, except where specifically indicated in the text. I hereby declare that except where specific reference is made to the work of others, the contents of this thesis are original and have not been submitted in whole or in part for consideration for any other degree or qualification in any other University/Institute. Finally, this thesis contains fewer than 100,000 words in length, exclusive of appendices, bibliography, footnotes, tables and equations and has less than 15 figures.

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Abstract

The purpose of this thesis is the derivation of corrector estimates justifying the upscaling of systems of partial differential equations (PDEs) with coupled fluxes posed in media with microstructures (like porous media). Such models play an important role in the understanding of, for example, drug-delivery mechanisms, where the involved chemical species diffusing inside the domain are assumed to obey perhaps other transport mechanisms and certain non-dissipative nonlinear processes within the pore space and at the boundaries of the perforated media (e.g. interaction, chemical reaction, aggregation, deposition). In this thesis, our corrector estimates provide a quantitative analysis in terms of convergence rates in suitable norms, i.e. as the small homogenization parameter tends to zero, the differences between the micro- and macro-concentrations and between the corresponding micro- and macro-concentration gradients are controlled in terms of the small parameter. As preparation, we are first concerned with the weak solvability of the microscopic models as well as with the fundamental asymptotic homogenization procedures that are behind the derivation of the corresponding upscaled models. We report results on three connected mathematical problems:

1. *Asymptotic analysis of microscopic semi-linear elliptic equations/systems.* We explore the asymptotic analysis of a prototype model including the interplay between stationary diffusion and both surface and volume chemical reactions in porous media. Our interest lies in deriving homogenization limits (upscaling) for alike systems, and particularly, in justifying rigorously the obtained averaged descriptions. We prove the well-posedness of the microscopic problem ensuring also the positivity and boundedness of the involved concentrations. Then we use the structure of the two-scale expansions to derive corrector estimates delimitating quantitatively the convergence rate of the asymptotic approximates to the macroscopic limit concentrations and their gradients. High-order corrector estimates are also obtained. The semi-linear auxiliary problems are tackled by a fixed-point homogenization argument. Our techniques include also Moser-like iteration techniques, a variational formulation, two-scale asymptotic expansions as well as suitable energy estimates.

2. *Corrector estimates for a Smoluchowski-Soret-Dufour model*. We consider a thermo-diffusion system, which is a coupled system of PDEs and ODEs that account for the heat-driven diffusion dynamics of hot colloids in periodic heterogeneous media. This model describes the joint evolution of temperature and colloidal concentrations in a saturated porous tissue where the Smoluchowski interactions for aggregation process and a linear deposition process take place. By a fixed-point argument, we prove the local existence and uniqueness results for the upscaled system. To obtain the corrector estimates, we exploit the concept of macroscopic reconstructions as well as suitable integral estimates to control boundary interactions.

3. *Corrector estimates for a non-stationary Stokes-Nernst-Planck-Poisson system*. We investigate a non-stationary Stokes-Nernst-Planck-Poisson system posed in a perforated domain as originally proposed by Knabner and his co-authors (see e.g. [98] and [99]). Starting off with the setting from [99], we complete the results by proving corrector estimates for the homogenization procedure. Main difficulties are connected to the choice of boundary conditions for the Poisson part of the system as well as with the scaling of the Stokes part of the system.

Key words: Corrector estimates, PDEs with coupled fluxes, Thermo-diffusion system, Drift-diffusion-reaction system, Weak solvability, Homogenization
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Contents

CHAPTER 1

Introduction

Before delving into the main content of this thesis, we start off with a short description of what we mean by a medium with microstructures and present a couple of historical remarks on homogenization. We also get across the central points that brought us to this thesis. In particular, we begin with the idea of periodic homogenization in Section 1.1 and give a classical example in Section 1.2. In Section 1.3, we take a glimpse on existing homogenization methods. The role of Section 1.4 is to give a brief review on the chosen mathematical models as well as on the used methodologies, drawing also the main goals of this work. The outline of the thesis is presented in Section 1.5.

1.1 Background

Inhomogeneous media (media with microstructures) are omnipresent. The ubiquity of such media is apparent in both natural and engineering problems such as carbon-fibre composites in material sciences, multi-strand ropes in structural mechanics and multi-functional cellular solids in scaffolds for cell growth. This type of materials is subjected to loads or/and forcing that vary on a length scale. Often, the experimental understanding refers to a governing scale that is massively bigger than the characteristic length scales of the microstructure. The situation is even more complex since besides many length scales, many time scales are also involved.

Taking into account only length scales at a "frozen" time scale, we consider physical processes that have two separated continuous length scales: the *macroscale* and the *microscale*. The macroscale describes physical phenomena without the aid of magnifying devices, while the microscale is essentially linked to the geometrically smaller observations of the objects as viewed through e.g. a microscope. A typical example of microscale/microstructures is the output of scanning electron microscope (SEM) of a fabricated microframe in interference lithography; see Figure 1.1, e.g.

The microscale is usually characterized by some recurring shape properties where the frequency of recurrence is much smaller than the size defining the macroscale. Mathematically, this fundamental parameter is referred to as $0 < \varepsilon \ll 1$. The models posed at the microscale are called in this context the *microscopic system*. Passing to the limit $\varepsilon \to 0$ in the microscopic system is referred to as *homogenization* process and is a form of upscaling/averaging. This terminology is self-explaining, i.e. the corresponding limit model usually no longer possesses information about microstructures since the size of the recurrence is eliminated. It

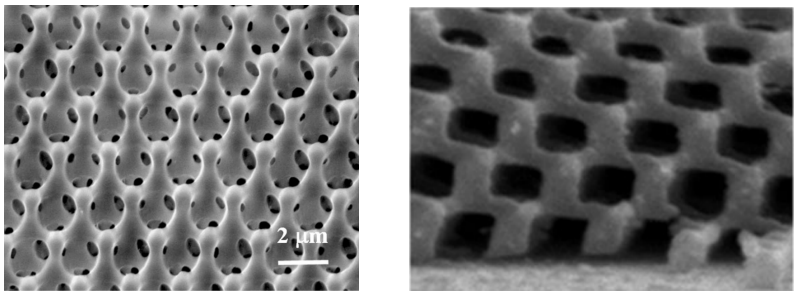

Figure 1.1: SEM image of a microframe (left) and its cross-section (right). The figures are taken from [79].

consequently reduces to a physical system posed in *homogeneous media* (an equivalent fictitious domain). This is an example of multiscale modeling. It is worth mentioning that in engineering problems, a microscopic view is helpful in accounting for many physical processes taking place deep inside the domain. On top of that, the mathematical models that resolve small length scales are unfortunately complicated and often impossible to solve fast and efficiently. The number of mesh nodes is, in fact, at least of the order of ε^{-d} (d is the spatial dimension), which is inversely proportional to the number of periodicity cells in the body. Ultimately, the complexity as well as elapsed time for computations increase dramatically as $\varepsilon \to 0$. Meanwhile, there is no difficulty in solving numerically nonlinear coupled evolution systems posed in homogeneous media.

The mathematical literature reports on two kinds of homogenization corresponding to two practical choices of microstructures: *deterministic homogenization* and *stochastic homogenization*. This thesis focuses on aspects of deterministic homogenization. For similar concepts concerning stochastic homogenization, we refer the reader for instance to [16] and [15, 14].

What concerns the deterministic framework, there is a huge mathematical literature on the periodic homogenization (here, materials are assumed to have a periodic microstructure). The homogenization process aims at replacing the initial partial differential equation with rapidly oscillating coefficients describing the composite material by the one with the corresponding effective/homogenized coefficients. Interestingly, these effective coefficients can usually be found by solving a non-oscillating partial differential equation, often of a simple nature. It is worth noting that the *perforated domain* indicates in this thesis a material with holes (empty inclusions), or equivalently solid inclusions (grains) suspended rigidly (and periodically) in air. For examples of non-periodic homogenization scenarios, see for instance, [86] and [108]. This thesis deals only with periodic scenarios.

1.2 A classical example

To illustrate the homogenization idea, we turn our attention to a one-dimensional elliptic system with an oscillating coefficient, viz.

$$\begin{cases} \dfrac{d}{dx}\left(-a^{\varepsilon}\dfrac{du^{\varepsilon}}{dx}\right) = f \quad \text{in } \Omega = (0,1)\,, \\ u^{\varepsilon}(0) = u^{\varepsilon}(1) = 0, \\ f \in L^2(\Omega)\,. \end{cases} \tag{1.2.1}$$

The oscillating coefficient a^ε is supposed to be periodic with a given period Θ and is generated by means of a bounded positive function $a \in L^\infty(\Omega)$ satisfying

$$0 < \alpha \leq a(x) \leq \beta < \infty \text{ for a.e. } x \in \Omega.$$

The coefficient is thus assigned by

$$a^\varepsilon(x) = a\left(\frac{x}{\varepsilon}\right) \text{ for } x \in \Omega.$$

Observe that the problem admits a unique solution for each fixed ε by the use of the Lax-Milgram lemma. Moreover, by the Poincaré's inequality we obtain a uniform *a priori* estimate of $\|u^\varepsilon\|_{H_0^1(\Omega)}$. In addition, if we denote the flux of u^ε by

$$\xi^\varepsilon := -a^\varepsilon \frac{du^\varepsilon}{dx},$$

then the we see that $\|\xi^\varepsilon\|_{L^2(\Omega)}$ is uniformly controlled as well.
Accordingly, we are led to the fact that there exists a subsequences, such that

$$\begin{aligned} u^\varepsilon &\rightharpoonup u^0 \text{ weakly in } H^1(\Omega), \\ \xi^\varepsilon &\rightharpoonup \xi^0 \text{ weakly in } L^2(\Omega), \\ a^\varepsilon &\rightharpoonup a^0 \text{ weakly-* in } L^\infty(\Omega). \end{aligned}$$

We denote by a^0 the mean value of a, i.e.

$$a^0 \equiv \mathscr{M}(a) = \frac{1}{|\Theta|}\int_0^\Theta a(x)\,dx.$$

We obtain $\xi_x^0 = f$ in Ω, and based on the Rellich-Kondrachov Theorem, the convergence $\xi^\varepsilon \to \xi^0$ is actually strong in $L^2(\Omega)$.
Notice that ξ^ε is the product of two weakly converging quantities. In general, this does not imply that the limit ξ^0 coincides with the product of the limit functions a^0 and u_x^0. Namely, $\xi^0 \equiv -a^0 u_x^0$ does generally not hold. In fact, we show that

$$\frac{du^0}{dx} = \mathscr{M}\left(a^{-1}\right)\xi^0,$$

which leads to the homogenized (upscaled, averaged,...) equation

$$-\frac{1}{\mathscr{M}(a^{-1})}\frac{d^2u^0}{dx^2} = f.$$

In conclusion, we have considered the periodic case with a^ε being a bounded sequence (not necessarily periodic) satisfying

$$\frac{1}{a^\varepsilon} \rightharpoonup A \text{ weakly-* in } L^\infty(\Omega), \text{ where } A^{-1} := \frac{1}{\mathscr{M}(a^{-1})}.$$

The solution u^ε is shown to converge weakly to u^0 in $H_0^1(\Omega)$, while u^0 is the unique solution of the problem:

$$\begin{cases} -A^{-1}\dfrac{d^2u^0}{dx^2} = f & \text{in } \Omega, \\ u^0(0) = u^0(1) = 0. \end{cases}$$

Let us now look at the problem (1.2.1) from a slightly different perspective, i.e. a stationary heat conduction problem in a composite material formed by a matrix and embedded fibers. Consequently, in this case the conductivity is given by

$$a^{\varepsilon}(x) = \begin{cases} a_f, & \text{if } x \in \text{fiber}, \\ a_m, & \text{if } x \in \text{matrix}. \end{cases}$$

(1.2.1) includes the continuity of both the temperature u^{ε} and of heat flux ξ^{ε} at the interface fiber/matrix. Moreover, the rapid oscillation of our conductivity herein is from its changes by the absolute value $\left|a_f - a_m\right|$ when there is a change from the point x by a value of order ε.
In any multiscale numerical scheme, the mesh-grid Δx must satisfy at least the constraint $\Delta x \ll \varepsilon$. Otherwise, the microstructure information cannot be captured. Assume that our underlying two-dimensional material has his matrix at a $\mathcal{O}(1)$ scale. Then, with the choice $\varepsilon = 10^{-5}$ (inspired from the smallest diameter of a fiber in the superconducting multifilamentary composite) and $\Delta x = 10^{-1}\varepsilon$, the order of degrees of freedom is around $\left(10 \times 10^5\right)^2 = 10^{12}$, yielding a greatly high cost of computations. We also emphasize that this is in practice even more expensive and composites are often heterogeneous on several scales, which makes naive numerical methods useless. Detailed multiscale numerical results are reported e.g. in the works by [21, 20].
Denote by ℓ and L, respectively, the characteristic lengths of the micro-cell and the macro-body. We have that $\ell \ll L$. From engineering perspectives (e.g. [13] and [12]), ℓ is a given physical parameter and cannot be changed, whilst L can somehow undertake the smallness of the scaling factor ε. Indeed, the parameter ε can be computed as the ratio of the microscale to the macroscale by $\varepsilon = \ell/L$. This means that one can choose a suitably large L to get a small enough ε. This is the reason why the homogenization procedure is often referred to as *upscaling*.

1.3 Justifying asymptotics via corrector estimates

The multiscale asymptotic expansion is an important tool in explaining multiscale problems (see, e.g. the monographs [102, 19] and [16, 27]). The basic notion of this approach consists in seeking an asymptotic expansion of the form

$$u^{\varepsilon}(x) = u_0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(x, \frac{x}{\varepsilon}\right) + \ldots \text{ for } x \in \Omega, \tag{1.3.1}$$

where u_m are Y-periodic in the second variable with Y being a unit cell, e.g.
This *ansatz* indicates that u^{ε} shall be close to some macroscopic part u_0 for a sufficiently small ε, provided that $u^{\varepsilon} \to u_0$ in some adequate topology as $\varepsilon \to 0$. Here, the function u_0 is performed as a suitable limit of u^{ε} and thus is expected to be the solution of the limit or homogenized model. The *effective coefficients* corresponding to the rapidly oscillatory ones are determined by solving the so-called *cell problems*, see Chapter 2 and Chapter 3 for more details. However, let us remark that using the aforementioned expansion for linear elliptic problems (like (1.2.1)), one can prove

$$u_0\left(x, \frac{x}{\varepsilon}\right) = \tilde{u}_0(x),$$

and $\tilde{u}_0$ is an excellent candidate as solution of a homogenized problem in which the effective conductivity does not depend on the position $x \in \Omega$, making the fictitious material homogeneous. When ε is small enough, $\tilde{u}_0$ becomes a good approximation of u^ε. Accordingly, we have replaced the composite material by a homogeneous one where their global behaviors are nearly the same. On the other hand, the *cell functions* u_m are solutions to cell problems, possessing the $\tilde{u}_0$-based structures.
Here, it is also possible to give the expected structure of the corrector estimate when using the asymptotic expansion (1.3.1). The corrector estimate is in general of the form

$$\left\| u^\varepsilon - \sum_{m=0}^{M} \varepsilon^m u_m \right\|_{H^1(\Omega^\varepsilon)} \leq C\varepsilon^{M-1},$$

where $C > 0$ is a generic constant independent of ε and $M \geq 2$ is a chosen order of the asymptotic expansion.

This type of corrector estimate is useful for multiscale finite element methods, e.g. the relation between the corrector homogenization estimate and the error estimate in conventional finite element methods is proved in [66]. In fact, the key estimate one normally wants to prove in this direction quantifies the difference between the exact solution and the so-called interpolant of the homogenized solution using the multiscale base functions. To do that, it further requires basic *a priori* error estimates of the approximation method whose proofs are based on the structure of corrector estimates (see [66] in Section 5).

1.4 Pore-scale models. Main goals

Modern approaches to modeling focus on multiple scales. Given a multiscale physical problem, one of the leading questions is to derive upscaled model equations and the corresponding structure of effective model coefficients (e.g. [37, 107]). We start off from microscopic PDE models describing the motion of populations of colloidal particles in soils and porous tissues with direct applications to drug-delivery design and control of the spread of radioactive pollutants. In particular, our background systems are mathematical models for hot-driven colloidal concentrations–the Smoluchowski-Soret-Dufour model, and for charged colloidal particles–the Stokes-Nernst-Planck-Poisson model.
A quick overview of these physical systems can be made, as follows:

- The Smoluchowski-Soret-Dufour system (SSD) (see e.g. [49] and [1] concerning the Smoluchowski interaction aiming at capturing the Alzheimer disease) models natural changes of the temperature due to a joint with the evolution of colloidal concentrations within the framework of a coupled thermo-diffusion-reaction process accounting for adsorption and desorption processes on the micro-surfaces.

- The Stokes-Nernst-Planck-Poisson (SNPP) system is well-developed to describe the dynamics of dilute electrolytes and dissolved charged particles in porous media; see e.g. [72] and [50] for detailed phenomenological descriptions. It also provides insight into the evolution of charged chemical species within a Newtonian liquid at low Reynolds

numbers. Concurrent with the Stokes equation, the charged species satisfy the Nernst-Planck-Poisson equations.

As analytically investigated in [97, 75, 99], these systems are mathematically well-posed and have been upscaled rigorously. Nevertheless, the question regarding the corrector estimates that deliminate the error made when homogenizing (averaging, upscaling, coarse graining...) these microscopic systems has not yet been studied. Thereby, the main purpose of this thesis is to estimate the speed of convergence as $\varepsilon \to 0$ of suitable norms of specific differences in micro-macro concentrations, velocities, charges, etc. and their micro-macro gradients.
As indicated in Section 1.3, the corrector estimates obtained in this framework can be further used to design convergent multiscale finite element methods (MsFEM) for the studied PDE systems (see e.g. [66] for the basic idea of the MsFEM approach). Having available corrector estimates, on the other side, allows in principle the construction of convergence proofs of multiscale numerical methods by deriving *a priori* error estimate for MsFEM applied to problems in perforated media like in [24], for instance. It is worth mentioning at this point that the existing literature on corrector estimates justifying the homogenization asymptotics is huge. One of the best studied problems is the derivation of plate theories from bulk elastic bodies with various types of perforations; see for instance the reference monographs [77, 90], but also the more recent concrete applications to transport and (static and dynamic) mechanics of membranes as indicated in [10, 11], e.g.
To obtain the corrector estimates in our framework, our strategy is to use an energy-like method and suitable macroscopic reconstructions (cf. e.g. [40] and [41]). This technique basically relies on the choice of test functions that captures in suitable norms the difference between the micro-and macro-fields and their transport fluxes. As readily expected, careful attention needs to be payed to the regularity of the limit solutions as well as of the cell functions involved in the asymptotic procedure; see e.g. [46]. Using more regularity, high-order corrector estimates can be obtained for semi-linear elliptic systems accounting for the stationary diffusion of the populations of colloidal particles. This can be done via an iteration method that uses explicitly the expected structure of the two-scale asymptotic expansion.
Note also from [31], guessing the structure of the corrector merely requires a deep understanding of cell functions up to the first order, i.e. the quantity u_1. Therefore, the corrector forms with the aid of macroscopic reconstructions: compare [39, 40] concerning the upscaling of a phase field model posed in high contrast regimes. Besides handling new nonlinear terms, a novel aspect in our context is the handling of the errors produced in the upscaling due to micro-surfaces and the presence of coupled fluxes. A similar analysis can be carried over the settings in [9, 99, 107, 45], e.g.
Besides the energy-like approach used here for a periodic homogenization case, significant contributions can be obtained using variants of the bulk and boundary unfolding operators: see, for instance, [60, 91, 46, 85, 81, 100]. Settings involving locally-periodic microstructures (correctors by special test functions adapted to the local periodicity) can be treated as in [86], e.g., while the random case is in most of the cases out of reach; see [73, 95, 119] for some details in this direction.

1.5 Outline of the thesis

This thesis is structured as follows:

We begin with the study of a stationary diffusion problem in Chapter 2 and Chapter 3, from which the nonlinear structure of the system is significantly correlated with the SSD and SNPP models. In the first part of Chapter 2, we mainly discuss the existence of a non-negative weak solution for this elliptic microscopic system by the minimization approach stated in Theorem 2.3.6. Moreover, uniqueness as well as boundedness results are shown. In the second part of this chapter, we apply the high-order asymptotic expansion to derive the structure of the limit system. Besides the use of this expansion, a general corrector estimate for homogenization limit is presented in Theorem 2.5.1, whose proof relies on energy-like estimates. These results are supplemented by extensions to the semilinear case of the auxiliary problems and to a general high-order corrector estimate postulated, respectively, in Section 3.2 and Section 3.3 of Chapter 3.

To tackle the Smoluchowski-Soret-Dufour model in Chapter 4, we introduce its mathematical description in the first part of the chapter. Here we can find also the technical assumptions as well as a mathematical interpretation of the chosen perforated domain. In addition, this part also contains the mathematical analysis of the microscopic system and corresponding upscaled systems. The corrector estimates are stated in Theorem 4.3.1.

The corrector justification for the Stokes-Nernst-Planck-Poisson model is investigated in Chapter 5. When doing so, we recall the existence of a unique weak solution of the microscopic system and the expected structure of the limit (upscaled) systems according to several scaling choices and boundary conditions. The main results are specified in Theorem 5.4.2 and Theorem 5.4.3. Besides macroscopic reconstructions and energy-like estimates, we further employ boundary layer estimates to treat the corrector structure for the Stokes equation.

Closing remarks and a list of open issues for forthcoming considerations are added in Chapter 6.

Guideline for the reader. The chapters can be read independently from each other. Whenever relevant, we state the geometrical settings of physical domains as well as the physical meaning of all quantities and balance laws behind each model. Due to the differently considered systems, the associated function spaces are defined in every chapter, albeit it perhaps do over again. Except those notations, we write $C_{\#}^{\infty}(Y)$ for the space of functions in $C^{\infty}\left(\mathbb{R}^d\right)$ that are Y-periodic. Given a Sobolev space $H\left(\mathbb{R}^d\right)$, we denote by $H_{\#}(Y)$ the space of functions in $H_{loc}\left(\mathbb{R}^d\right)$ (if it exists) that are Y-periodic, and by $H_{\#}(Y)/\mathbb{R}$ the space of those functions whose average over Y vanishes, i.e.

$$\int_Y u(y)\,dy = 0 \quad \text{for } u \in H_{\#}(Y).$$

Proofs of theorems, lemmas or propositions are either closed with the symbol $\square$, or fully presented in a concrete subsection. The concepts of two-scale convergence and related compactness results are provided in Appendix A to avoid unnecessary repetition (see, in particular, Definition A.0.1-Definition A.0.3 and Theorem A.0.2-Theorem A.0.4). Additionally, detailed statements concerning universal inequalities can be found therein.

CHAPTER 2

Asymptotic analysis of a semi-linear elliptic system in perforated domains

2.1 Introduction

We study the semi-linear elliptic boundary-value problem of the form

$$(P^\varepsilon): \begin{cases} \mathscr{A}^\varepsilon u_i^\varepsilon \equiv \nabla \cdot \left(-d_i^\varepsilon \nabla u_i^\varepsilon\right) = R_i\left(u^\varepsilon\right), & \text{in } \Omega^\varepsilon \subset \mathbb{R}^d, \\ d_i^\varepsilon \nabla u_i^\varepsilon \cdot \mathrm{n} = \varepsilon\left(a_i^\varepsilon u_i^\varepsilon - b_i^\varepsilon F_i\left(u_i^\varepsilon\right)\right), & \text{across } \Gamma^\varepsilon, \\ u_i^\varepsilon = 0, & \text{across } \Gamma^{ext}, \end{cases} \tag{2.1.1}$$

for $i = \{1, ..., N\}$ $(N \geq 2, d \in \{2, 3\})$. Following [75], this system models the diffusion in a porous medium as well as the aggregation, dissociation and surface deposition of N interacting populations of colloidal particles indexed by u_i^ε. As short-hand notation, $u^\varepsilon := \left(u_1^\varepsilon, ..., u_N^\varepsilon\right)$ points out the vector of these concentrations. Such scenarios arise in drug-delivery mechanisms in human bodies and often include cross- and thermo-diffusion which are triggers of our motivation (compare [34] for the Sorret and Dufour effects and [52, 116] for related cross-diffusion and chemotaxis-like systems).

The model (2.1.1) involves a number of parameters: d_i^ε represents molecular diffusion coefficients, R_i represents the volume reaction rate, $a_i^\varepsilon, b_i^\varepsilon$ are the so-called deposition coefficients, while F_i indicates a surface chemical reaction for the immobile species. We refer to (2.1.1) as problem (P^ε).

This chapter is organized as follows: In Section 2.2 we start off with a set of technical preliminaries focusing especially on the working assumptions on the data and the description of the microstructure of the porous medium. The weak solvability of the microscopic model is established in Section 2.3. The homogenization method is applied in Section 2.4 to the problem (P^ε). This is the place where we derive the corrector estimates and establish herewith the convergence rate of the homogenization process. A brief discussion in Section 2.5 and some concluding remarks in Section 2.6 close the chapter.

2.2 Preliminaries

2.2.1 Description of the geometry

The geometry of our porous medium is sketched in Figure 2.1 (left), together with the choice of perforation (referred here to also as "microstructure") cf. Figure 2.1 (right). We refer the reader to [65] for a concise mathematical representation of the perforated geometry. In the

same spirit, take Ω be a bounded open domain in $\mathbb{R}^d$ with a piecewise smooth boundary $\Gamma = \partial\Omega$. Let Y be the unit representative cell, i.e.

$$Y := \left\{ \sum_{i=1}^{d} \lambda_i \vec{e}_i : 0 < \lambda_i < 1 \right\},$$

where we denote by $\vec{e}_i$ by ith unit vector in $\mathbb{R}^d$.
Take Y_0 the open subset of Y with a piecewise smooth boundary ∂Y_0 in such a way that $\overline{Y_0} \subset \overline{Y}$. In the porous media terminology, Y is the unit cell made of two parts: the gas phase (pore space) $Y \backslash \overline{Y_0}$ and the solid phase Y_0.
Let $Z \subset \mathbb{R}^d$ be a hypercube. Then for $X \subset Z$ we denote by X^k the shifted subset

$$X^k := X + \sum_{i=1}^{d} k_i \vec{e}_i,$$

where $k = (k_1, ..., k_d) \in \mathbb{Z}^d$ is a vector of indices.
Setting $Y_1 = Y \backslash \overline{Y_0}$, we now define the pore skeleton by

$$\Omega_0^\varepsilon := \bigcup_{k \in \mathbb{Z}^d} \left\{ \varepsilon Y_0^k : Y_0^k \subset \Omega \right\},$$

where ε is observed as a given scale factor or homogenization parameter.
It thus comes out that the total pore space is

$$\Omega^\varepsilon := \Omega \backslash \overline{\Omega_0^\varepsilon},$$

for εY_0^k the ε-homotetic set of Y_0^k, while the total pore surface of the skeleton is denoted by

$$\Gamma^\varepsilon := \partial\Omega_0^\varepsilon = \bigcup_{k \in \mathbb{Z}^d} \left\{ \varepsilon \Gamma^k : \Gamma^k \subset \Omega \right\}.$$

The exterior boundary of Ω^ε is certainly a hypersurface in $\mathbb{R}^d$, denoted by $\Gamma^{ext} = \partial\Omega^\varepsilon \backslash \Gamma^\varepsilon$, where it has a nonzero $(d-1)$-dimensional measure, satisfies $\Gamma^{ext} \cap \Gamma^\varepsilon = \emptyset$ and coincides with Γ. Moreover, n denotes the unit normal vector to Γ^ε.
Finally, our perforated domain Ω^ε is assumed to be connected through the gas phase. Notice here that Γ^{ext} is smooth.
N.B. This chapter aims at understanding the problem in two or three space dimensions. However, all our results hold also for $d \geq 3$. Throughout this chapter, C denotes a generic constant which can change from line to line. If not otherwise stated, the constant C is independent of the choice of ε.

2.2.2 Notation. Assumptions on the data

We denote by $x \in \Omega^\varepsilon$ the macroscopic variable and by $y = x/\varepsilon$ the microscopic variable representing fast variations at the microscopic geometry. With this convention in view, we write

$$d_i^\varepsilon(x) = d_i\left(\frac{x}{\varepsilon}\right) = d_i(y).$$

A similar meaning is given to all involved "oscillating" data, e.g. to $a_i^\varepsilon(x)$, $b_i^\varepsilon(x)$.

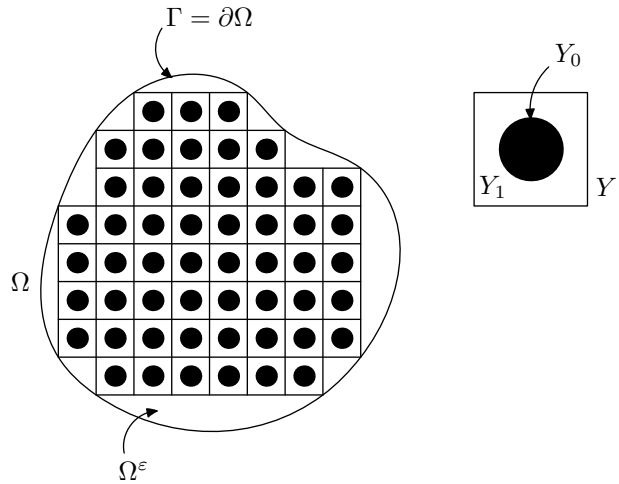

Figure 2.1: Admissible two-dimensional perforated domain (left) and basic geometry of the microstructure (right).

We now make the following set of assumptions:
(A_1) The diffusion coefficient $d_i^\varepsilon \in L^\infty\left(\mathbb{R}^d\right)$ is Y-periodic, and there exists a positive constant α_i such that

$$d_i(y)\,\xi_i\xi_j \geq \alpha_i\,|\xi|^2 \quad \text{for any } \xi \in \mathbb{R}^d.$$

(A_2) The deposition coefficients $a_i^\varepsilon, b_i^\varepsilon \in L^\infty(\Gamma^\varepsilon)$ are positive and Y-periodic.
(A_3) The reaction rates $R_i : \Omega^\varepsilon \times [0,\infty)^N \to \mathbb{R}$ and $F_i : \Gamma^\varepsilon \times [0,\infty) \to \mathbb{R}$ are Carathéodory functions, i.e. they are, respectively, continuous in $[0,\infty)^N$ and $[0,\infty)$ with respect to x variable (in the "almost all" sense), and measurable in Ω^ε and Γ^ε with essential boundedness with respect to concentrations $u_i^\varepsilon \geq 0$.
(A_4) The chemical rates R_i and F_i are sublinear in the sense that for any $p = (p_1, ..., p_N)$

$$R_i(p) \leq C\left(1 + \sum_{j=1, j\neq i}^{N} p_i p_j\right) \quad \text{for } p \geq 0,$$

$$F_i(p_i) \leq C(1 + p_i) \quad \text{for } p_i \geq 0.$$

Furthermore, assume that $R_i(p)/p_i$ is decreasing and $F_i(p_i)/p_i$ is increasing in p_i for any $p > 0$.
(A_5) For every $\varepsilon > 0$, there exist vectors (x-dependent) $r_0^\varepsilon, r_\infty^\varepsilon, f_0^\varepsilon, f_\infty^\varepsilon$ whose elements are

$$r_{0,i}^\varepsilon = \lim_{u_i^\varepsilon \to 0^+} \frac{R_i(u^\varepsilon)}{u_i^\varepsilon}, \quad r_{\infty,i}^\varepsilon = \lim_{u_i^\varepsilon \to \infty} \frac{R_i(u^\varepsilon)}{u_i^\varepsilon},$$

$$f_{0,i}^\varepsilon = \lim_{u_i^\varepsilon \to 0^+} \varepsilon\left(a_i^\varepsilon - b_i^\varepsilon \frac{F_i\left(u_i^\varepsilon\right)}{u_i^\varepsilon}\right), \quad f_{\infty,i}^\varepsilon = \lim_{u_i^\varepsilon \to \infty} \varepsilon\left(a_i^\varepsilon - b_i^\varepsilon \frac{F_i\left(u_i^\varepsilon\right)}{u_i^\varepsilon}\right).$$

(A_6) R_i and F_i satisfy the growth conditions:

$$|R_i(x,p)| \leq C\sum_{i=1}^{N}(1 + p_i) \quad \text{for } p \geq 0, \tag{2.2.1}$$

$$\left|a_i^\varepsilon p_i - b_i^\varepsilon F_i(p_i)\right| \leq C(1 + p_i) \quad \text{for } p_i \geq 0. \tag{2.2.2}$$

Let us define the function space

$$V^{\varepsilon} := \left\{ v \in H^1(\Omega^{\varepsilon}) \,|\, v = 0 \text{ on } \Gamma^{ext} \right\},$$

which is a closed subspace of the Hilbert space $H^1(\Omega^{\varepsilon})$, and thus endowed with the semi-norm

$$\|v\|_{V^{\varepsilon}} = \left(\sum_{i=1}^{d} \int_{\Omega^{\varepsilon}} \left| \frac{\partial v}{\partial x_i} \right|^2 dx \right)^{1/2} \quad \text{for all } v \in V^{\varepsilon}.$$

Obviously, this norm is equivalent to the usual H^1-norm by the Poincaré inequality. Moreover, this equivalence is uniform in ε (cf. [31, Lemma 2.1]).
We introduce the Hilbert spaces

$$\mathscr{H}(\Omega^{\varepsilon}) = L^2(\Omega^{\varepsilon}) \times \ldots \times L^2(\Omega^{\varepsilon}), \quad \mathscr{V}^{\varepsilon} = V^{\varepsilon} \times \ldots \times V^{\varepsilon},$$

with the inner products defined respectively by

$$\langle u, v \rangle_{\mathscr{H}(\Omega^{\varepsilon})} := \sum_{i=1}^{N} \int_{\Omega^{\varepsilon}} u_i v_i dx, \quad u = (u_1, \ldots, u_N), v = (v_1, \ldots, v_N) \in \mathscr{H}(\Omega^{\varepsilon}),$$

$$\langle u, v \rangle_{\mathscr{V}^{\varepsilon}} := \sum_{i=1}^{N} \sum_{j=1}^{d} \int_{\Omega^{\varepsilon}} \frac{\partial u_i}{\partial x_j} \frac{\partial v_i}{\partial x_j} dx, \quad u = (u_1, \ldots, u_N), v = (v_1, \ldots, v_N) \in \mathscr{V}^{\varepsilon}.$$

Furthermore, the notation $\mathscr{H}(\Gamma^{\varepsilon})$ indicates the corresponding product of $L^2(\Gamma^{\varepsilon})$ spaces. For $q \in (2, \infty]$, the following spaces are also used

$$\mathscr{W}^q(\Omega^{\varepsilon}) = L^q(\Omega^{\varepsilon}) \times \ldots \times L^q(\Omega^{\varepsilon}),$$
$$\mathscr{W}^q(\Gamma^{\varepsilon}) = L^q(\Gamma^{\varepsilon}) \times \ldots \times L^q(\Gamma^{\varepsilon}).$$

2.3 Well-posedness of the microscopic model

Before studying the asymptotics behaviour as $\varepsilon \to 0$ (the homogenization limit), we must ensure the well-posedness of the microstructure model. In this section we focus only on the weak solvability of the problem, the stability with respect to the initial data and all parameter being straightforward to prove. We remark at this stage that the structure of the model equation has attracted much attention. For example, Amann used in [8] the method of sub- and super- solutions to prove the existence of positive solutions when a Robin boundary condition is considered. Brezis and Oswald introduced in [22] an energy minimization approach to guarantee the existence, uniqueness and positivity results for the semi-linear elliptic problem with zero Dirichlet boundary conditions. Very recently, the authors in [55] extended the result in [22] (and also of other previous works including [25, 32]) to problems involving nonlinear boundary conditions of mixed type. For what we are concerned here, we will use Moser-like iterations technique (see the original works in [83, 84]) to prove L^{∞}-bounds for all concentrations and then follow the strategy provided in [22] to study the well-posedness of (P^{ε}).

Definition 2.3.1. A function $u^\varepsilon \in \mathscr{V}^\varepsilon$ is a weak solution to (P^ε) provided that

$$\sum_{i=1}^{N}\int_{\Omega^\varepsilon}\left(d_i^\varepsilon \nabla u_i^\varepsilon \nabla \varphi_i - R_i\left(u^\varepsilon\right)\varphi_i\right)dx - \sum_{i=1}^{N}\varepsilon\int_{\Gamma^\varepsilon}\left(a_i^\varepsilon u_i^\varepsilon - b_i^\varepsilon F_i\left(u_i^\varepsilon\right)\right)\varphi_i dS_\varepsilon = 0 \quad \text{for all } \varphi \in \mathscr{V}^\varepsilon. \tag{2.3.1}$$

Definition 2.3.2. By means of the usual variational characterization, the principal eigenvalue of (P^ε) is defined by

$$\lambda_1\left(p^\varepsilon, q^\varepsilon\right) := \inf_{u^\varepsilon \in \mathscr{V}^\varepsilon, \sum_{i=1}^{N}\left|u_i^\varepsilon\right|^2 \neq 0} \frac{\sum_{i=1}^{N}\left(\alpha\int_{\Omega^\varepsilon}\left|\nabla u_i^\varepsilon\right|^2 dx - N\int_{\Omega^\varepsilon} p_i^\varepsilon\left|u_i^\varepsilon\right|^2 dx - N\int_{\Gamma^\varepsilon} q_i^\varepsilon\left|u_i^\varepsilon\right|^2 dS_\varepsilon\right)}{\sum_{i=1}^{N}\int_{\Omega^\varepsilon}\left|u_i^\varepsilon\right|^2 dx}, \tag{2.3.2}$$

where p_i^ε and q_i^ε are measurable such that either they are simultaneously bounded from above or from below (this leads to $\lambda_1 \in (-\infty, \infty]$ or $\lambda_1 \in [-\infty, \infty)$, correspondingly). Here, we denote $\alpha := \min\{\alpha_1, ..., \alpha_N\}$.

Lemma 2.3.3. *Assume (A_1)-(A_5) and replace $\left(A_4\right)$ by (A_6). Let $u^\varepsilon \in \mathscr{V}^\varepsilon \cap \mathscr{H}\left(\Gamma^\varepsilon\right)$ be a weak solution to (P^ε), then $u^\varepsilon \in \mathscr{W}^\infty\left(\Omega^\varepsilon\right)$ and there exists an ε-independent constant $C > 0$ such that*

$$\|u^\varepsilon\|_{\mathscr{W}^\infty(\Omega^\varepsilon)} \leq C\left(1 + \|u^\varepsilon\|_{\mathscr{H}(\Omega^\varepsilon)} + \|u^\varepsilon\|_{\mathscr{H}(\Gamma^\varepsilon)}\right).$$

Proof. Let $\beta \geq 1$ and $k_i > 1$ for all $i = \overline{1,N}$. We begin by introducing a vector φ^ε of test functions $\varphi_i^\varepsilon = \min\left\{v_i^{\beta+\frac{1}{2}}, k_i^{\beta+\frac{1}{2}}\right\} - 1$ where $v_i = u_i^\varepsilon + 1$ with u_i^ε as in (2.3.1). Thus, it is straightforward to show that $\varphi^\varepsilon \in \mathscr{V}^\varepsilon \cap \mathscr{H}\left(\Gamma^\varepsilon\right)$. We have

$$\begin{aligned}
\alpha\left(\beta + \frac{1}{2}\right)\sum_{i=1}^{N}\int_{\{v_i<k_i\}} v_i^{\beta-\frac{1}{2}}\left|\nabla v_i\right|^2 &\leq \sum_{i=1}^{N}\left(\int_{\Omega^\varepsilon} R_i\left(x, u^\varepsilon\right)\varphi_i^\varepsilon dx + \int_{\Gamma^\varepsilon} F_i\left(x, u_i^\varepsilon\right)\varphi_i^\varepsilon dS_\varepsilon\right) \\
&\leq C\sum_{i=1}^{N}\int_{\Omega^\varepsilon}\left|1 + u_i^\varepsilon\right|^2 v_i^{\beta+\frac{1}{2}} dx \\
&\quad + C\sum_{i=1}^{N}\int_{\Gamma^\varepsilon}\left|1 + u_i^\varepsilon\right|^2 v_i^{\beta+\frac{1}{2}} dS_\varepsilon \\
&\leq C\sum_{i=1}^{N}\left(\int_{\Omega^\varepsilon} v_i^{\beta+\frac{3}{2}} dx + \int_{\Gamma^\varepsilon} v_i^{\beta+\frac{3}{2}} dS_\varepsilon\right),
\end{aligned} \tag{2.3.3}$$

where we have used (2.2.1) and (2.2.2).

Now, for every $i \in \{1, ..., N\}$, if we assign $\psi_i = \min\left\{v_i^{\frac{\beta+\frac{3}{2}}{2}}, k_i^{\frac{\beta+\frac{3}{2}}{2}}\right\}$, then one has

$$\left(\beta + \frac{1}{2}\right) v_i^{\beta-\frac{1}{2}}\left|\nabla v_i\right|^2 \chi_{\{v_i<k_i\}} = \frac{4\left(\beta + \frac{1}{2}\right)}{\left(\beta + \frac{3}{2}\right)^2}\left|\nabla \psi_i\right|^2. \tag{2.3.4}$$

Since Ω^ε is a Lipschitz domain, then the trace embedding $H^1\left(\Omega^\varepsilon\right) \subset L^q\left(\partial\Omega^\varepsilon\right)$ holds for $1 \leq q \leq 2^*_{\partial\Omega^\varepsilon}$, where $2^*_{\partial\Omega^\varepsilon} = 2(d-1)/(d-2)$ if $d \geq 3$, and $2^*_{\partial\Omega^\varepsilon} = \infty$ if $d = 2$ (cf. [44]). Therefore, given $q \in (2, 2^*]$ we apply this embedding to (2.3.3) with the aid of (2.3.4) and

then obtain

$$\frac{4\alpha\left(\beta+\frac{1}{2}\right)}{\left(\beta+\frac{3}{2}\right)^2}\sum_{i=1}^{N}\left[\left(\int_{\Gamma^\varepsilon}|\psi_i|^q\,dS_\varepsilon\right)^{\frac{2}{q}}-\int_{\Omega^\varepsilon}|\psi_i|^2\,dx\right]\leq C\sum_{i=1}^{N}\left(\int_{\Omega^\varepsilon}v_i^{\beta+\frac{3}{2}}dx+\int_{\Gamma^\varepsilon}v_i^{\beta+\frac{3}{2}}dS_\varepsilon\right). \tag{2.3.5}$$

We see that $\psi_i^2\leq v^{\beta+\frac{3}{2}}$ and also

$$\frac{1}{\beta+\frac{3}{2}}\leq\frac{4\left(\beta+\frac{1}{2}\right)}{\left(\beta+\frac{3}{2}\right)^2}\leq 4$$

holds for all $\beta\geq 1$. As a result, (2.3.5) yields

$$\sum_{i=1}^{N}\left(\int_{\Gamma^\varepsilon}|\psi_i|^q\,dS_\varepsilon\right)^{\frac{2}{q}}\leq C\alpha^{-1}\left(\beta+\frac{3}{2}\right)\sum_{i=1}^{N}\left(\int_{\Omega^\varepsilon}v_i^{\beta+\frac{3}{2}}dx+\int_{\Gamma^\varepsilon}v_i^{\beta+\frac{3}{2}}dS_\varepsilon\right). \tag{2.3.6}$$

Our next aim is to show that if for some $s\geq 2$ we have $u^\varepsilon\in\mathscr{W}^s(\Omega^\varepsilon)\cap\mathscr{W}^s(\Gamma^\varepsilon)$, then $u^\varepsilon\in\mathscr{W}^{ks}(\Omega^\varepsilon)\cap\mathscr{W}^{ks}(\Gamma^\varepsilon)$ for $k>1$ arbitrary at each ε-level. In fact, assume that $u^\varepsilon\in\mathscr{W}^{\beta+\frac{3}{2}}(\Omega^\varepsilon)\cap\mathscr{W}^{\beta+\frac{3}{2}}(\Gamma^\varepsilon)$ then letting $k\to\infty$ in (2.3.6) gives

$$\sum_{i=1}^{N}\left(\int_{\Gamma^\varepsilon}|v_i|^{\frac{q}{2}\left(\beta+\frac{3}{2}\right)}dS_\varepsilon\right)^{\frac{2}{q}}\leq C\left(\beta+\frac{3}{2}\right)\sum_{i=1}^{N}\left(\int_{\Omega^\varepsilon}v_i^{\beta+\frac{3}{2}}dx+\int_{\Gamma^\varepsilon}v_i^{\beta+\frac{3}{2}}dS_\varepsilon\right). \tag{2.3.7}$$

One obtains in the same manner that by the embedding $H^1(\Omega^\varepsilon)\subset L^q(\Omega^\varepsilon)$ (this is valid for $1\leq q\leq 2^*_{\Omega^\varepsilon}$ where $2^*_{\Omega^\varepsilon}=2d/(d-2)$ if $d\geq 3$, and $2^*_{\Omega^\varepsilon}=\infty$ if $d=2$; thus q given before is definitely valid), we are led to the following estimate

$$\sum_{i=1}^{N}\left(\int_{\Omega^\varepsilon}|v_i|^{\frac{q}{2}\left(\beta+\frac{3}{2}\right)}dx\right)^{\frac{2}{q}}\leq C\left(\beta+\frac{3}{2}\right)\sum_{i=1}^{N}\left(\int_{\Omega^\varepsilon}v_i^{\beta+\frac{3}{2}}dx+\int_{\Gamma^\varepsilon}v_i^{\beta+\frac{3}{2}}dS_\varepsilon\right). \tag{2.3.8}$$

Combining (2.3.7), (2.3.8) and the Minkowski inequality (see Lemma A.0.11) enables us to get

$$\left(\int_{\Omega^\varepsilon}|v_i|^{\frac{q}{2}\left(\beta+\frac{3}{2}\right)}dx+\int_{\Gamma^\varepsilon}|v_i|^{\frac{q}{2}\left(\beta+\frac{3}{2}\right)}dS_\varepsilon\right)^{\frac{2}{q}}\leq C\left(\beta+\frac{3}{2}\right)\sum_{i=1}^{N}\left(\int_{\Omega^\varepsilon}v_i^{\beta+\frac{3}{2}}dx+\int_{\Gamma^\varepsilon}v_i^{\beta+\frac{3}{2}}dS_\varepsilon\right),$$

for all $i\in\{1,\ldots,N\}$, which easily leads to, by raising to the power $1/\left(\beta+\frac{3}{2}\right)$, the fact that $u_i^\varepsilon\in L^{\frac{q}{2}\left(\beta+\frac{3}{2}\right)}(\Omega^\varepsilon)\cap L^{\frac{q}{2}\left(\beta+\frac{3}{2}\right)}(\Gamma^\varepsilon)$ for all $i\in\{1,\ldots,N\}$; and hence $u^\varepsilon\in\mathscr{W}^{\frac{q}{2}\left(\beta+\frac{3}{2}\right)}(\Omega^\varepsilon)\cap\mathscr{W}^{\frac{q}{2}\left(\beta+\frac{3}{2}\right)}(\Gamma^\varepsilon)$. The constant k is indicated by $q/2>1$. Thus, if we choose q and β such that

$$\beta+\frac{3}{2}=2\left(\frac{q}{2}\right)^n\quad\text{for } n=0,1,2,\ldots,$$

and iterating the above estimate, we obtain, by induction, that

$$\|v\|_{2\left(\frac{q}{2}\right)^n}\leq\prod_{j=0}^{n}\left(2\left(\frac{q}{2}\right)^j C\right)^{\frac{1}{2}\left(\frac{2}{q}\right)^j}\|v\|_2, \tag{2.3.9}$$

where we have denoted

$$\|v\|_r:=\sum_{i=1}^{N}\left(\int_{\Omega^\varepsilon}|v_i|^r\,dx+\int_{\Gamma^\varepsilon}|v_i|^r\,dS_\varepsilon\right)^{\frac{1}{r}}.$$

It is interesting to point out that since the series $\sum_{n=0}^{\infty}\left(\frac{2}{q}\right)^n$ and $\sum_{n=0}^{\infty} n\left(\frac{2}{q}\right)^n$ are convergent for $q>2$, we have

$$\prod_{j=0}^{n}\left(2\left(\frac{q}{2}\right)^j C\right)^{\frac{1}{2}\left(\frac{2}{q}\right)^j} < \sqrt{(2C)^{\sum_{n=0}^{\infty}\left(\frac{2}{q}\right)^n} q^{\sum_{n=0}^{\infty} n\left(\frac{2}{q}\right)^n}} = C.$$

Therefore, the constant on the right-hand side of (2.3.9) is indeed independent of n, and by passing $n\to\infty$ in (2.3.9), i.e. in the inequality,

$$\|v\|_{\mathscr{W}^{2\left(\frac{q}{2}\right)^n}(\Omega^\varepsilon)} \le C\left(\|v\|_{\mathscr{H}(\Omega^\varepsilon)} + \|v\|_{\mathscr{H}(\Gamma^\varepsilon)}\right),$$

we finally obtain

$$\|v\|_{\mathscr{W}^\infty(\Omega^\varepsilon)} \le C\left(\|v\|_{\mathscr{H}(\Omega^\varepsilon)} + \|v\|_{\mathscr{H}(\Gamma^\varepsilon)}\right).$$

Consequently, recalling $v_i = u_i^\varepsilon + 1$, we have:

$$\|u^\varepsilon\|_{\mathscr{W}^\infty(\Omega^\varepsilon)} \le C\left(1 + \|u^\varepsilon\|_{\mathscr{H}(\Omega^\varepsilon)} + \|u^\varepsilon\|_{\mathscr{H}(\Gamma^\varepsilon)}\right).$$

This step completes the proof of the lemma. □

Remark 2.3.4. *Using the trace inequality (see Lemma A.0.8) and the norm equivalence between V^ε and $H^1(\Omega^\varepsilon)$, if $u^\varepsilon \in \mathscr{V}^\varepsilon$ then the result in Lemma* 2.3.3 *reads*

$$\begin{aligned}\|u^\varepsilon\|_{\mathscr{W}^\infty(\Omega^\varepsilon)} &\le C\left(1 + \varepsilon^{-1/2}\|u^\varepsilon\|_{\mathscr{H}(\Omega^\varepsilon)} + \|u^\varepsilon\|_{\mathscr{V}^\varepsilon}\right)\\ &\le C\left(1 + \varepsilon^{-1/2}\|u^\varepsilon\|_{\mathscr{V}^\varepsilon}\right).\end{aligned}$$

Lemma 2.3.5. *Assume (A_1)-(A_5) and that $\lambda_1\left(r_\infty^\varepsilon, f_\infty^\varepsilon\right) > 0$ and $\lambda_1\left(r_0^\varepsilon, f_0^\varepsilon\right) < 0$ hold. We define the following functional*

$$J[u^\varepsilon] := \frac{1}{2}\sum_{i=1}^{N}\int_{\Omega^\varepsilon} d_i^\varepsilon \left|\nabla u_i^\varepsilon\right|^2 dx - \sum_{i=1}^{N}\int_{\Omega^\varepsilon}\mathscr{R}_i(x,u^\varepsilon)\,dx - \sum_{i=1}^{N}\int_{\Gamma^\varepsilon}\mathscr{F}_i\left(x,u_i^\varepsilon\right)dS_\varepsilon,$$

where

$$\mathscr{R}_i(x,u^\varepsilon) := \int_0^{u_i^\varepsilon} R_i\left(x,u_1^\varepsilon,\ldots s_i,\ldots,u_N^\varepsilon\right)ds_i,$$

$$\mathscr{F}_i\left(x,u_i^\varepsilon\right) := \int_0^{u_i^\varepsilon}\left(a_i^\varepsilon s - b_i^\varepsilon F_i(s)\right)ds,$$

and the nonlinear terms are extended to be $R_i(x,0)$ and $F_i(x,0)$ for $u_i^\varepsilon \le 0$. Then J is coercive on $\mathscr{V}^\varepsilon$ and lower semi-continuous for $\mathscr{V}^\varepsilon$. Moreover, there exists $\phi \in \mathscr{V}^\varepsilon$ such that $J[\phi] < 0$.

Proof. **Step 1:** (Coerciveness)
Suppose, by contradiction, that there exists a sequence $\{u^{\varepsilon,m}\} \subset \mathscr{V}^\varepsilon$ such that $\|u^{\varepsilon,m}\|_{\mathscr{V}^\varepsilon} \to \infty$ while $J[u^{\varepsilon,m}] \le C$. Setting

$$s_{i,m} = \left(\int_{\Gamma^\varepsilon}\left|u_i^{\varepsilon,m}\right|^2 dS_\varepsilon\right)^{1/2}, \quad t_{i,m} = \left(\int_{\Omega^\varepsilon}\left|u_i^{\varepsilon,m}\right|^2 dx\right)^{1/2}, \tag{2.3.10}$$

we say that $\sum_{i=1}^{N} t_{i,m}^2 \to \infty$ up to a subsequence as $m \to \infty$. Indeed, the assumption $J[u^{\varepsilon,m}] \leq C$ yields that

$$\frac{1}{2}\sum_{i=1}^{N}\int_{\Omega^\varepsilon} d_i^\varepsilon \left|\nabla u_i^{\varepsilon,m}\right|^2 dx \leq \sum_{i=1}^{N}\int_{\Omega^\varepsilon} \mathscr{R}_i\left(x, u^{\varepsilon,m}\right) dx + \sum_{i=1}^{N}\int_{\Gamma^\varepsilon} \mathscr{F}_i\left(x, u_i^{\varepsilon,m}\right) dS_\varepsilon + C, \quad (2.3.11)$$

which, in combination with (2.3.10) and $\left(\mathrm{A}_4\right)$, leads to

$$\frac{1}{2}\sum_{i=1}^{N}\int_{\Omega^\varepsilon} d_i^\varepsilon \left|\nabla u_i^{\varepsilon,m}\right|^2 dx \leq C(N)\left(1 + \sum_{i=1}^{N} t_{i,m}^2 + \sum_{i=1}^{N} s_{i,m}^2\right). \quad (2.3.12)$$

Here, if $\sum_{i=1}^{N} t_{i,m}^2$ is convergent, then $\sum_{i=1}^{N} s_{i,m}^2$ cannot be bounded. While putting

$$v_{i,m} = u_i^{\varepsilon,m} / \sum_{i=1}^{N} s_{i,m},$$

it enables us to derive that

$$\sum_{i=1}^{N}\int_{\Omega^\varepsilon} \left|\nabla v_{i,m}\right|^2 dx = \frac{\sum_{i=1}^{N}\int_{\Omega^\varepsilon} \left|\nabla u_i^{\varepsilon,m}\right|^2 dx}{\left(\sum_{i=1}^{N} s_{i,m}\right)^2} \leq \frac{\sum_{i=1}^{N}\int_{\Omega^\varepsilon} \left|\nabla u_i^{\varepsilon,m}\right|^2 dx}{\sum_{i=1}^{N} s_{i,m}^2}. \quad (2.3.13)$$

If we assign $\alpha := \min\{\alpha_1, ..., \alpha_N\} > 0$, then it follows from (4.3.15) and (2.3.13) that

$$\begin{aligned} \frac{\alpha}{2}\sum_{i=1}^{N}\int_{\Omega^\varepsilon} \left|\nabla v_{i,m}\right|^2 dx &\leq \frac{\sum_{i=1}^{N}\int_{\Omega^\varepsilon} d_i^\varepsilon \left|\nabla u_i^{\varepsilon,m}\right|^2 dx}{2\sum_{i=1}^{N} s_{i,m}^2} \\ &\leq C(N)\left(1 + \frac{\sum_{i=1}^{N} t_{i,m}^2}{\sum_{i=1}^{N} s_{i,m}^2} + \frac{1}{\sum_{i=1}^{N} s_{i,m}^2}\right) \leq C(N). \end{aligned}$$

Now, we claim that there exists $v_i \in V^\varepsilon$ such that $v_{i,m} \rightharpoonup v_i$ weakly in V^ε, and then strongly in $L^2(\Omega^\varepsilon)$ and in $L^2(\Gamma^\varepsilon)$. However, it implies here a contradiction. It is because we have $v_i \equiv 0$ in Ω^ε for all $i = \overline{1,N}$ while

$$\sum_{i=1}^{N}\int_{\Gamma^\varepsilon} |v_i|^2 dS_\varepsilon = \left(\sum_{i=1}^{N} s_i\right)^{-2} \sum_{i=1}^{N}\int_{\Gamma^\varepsilon} \left|u_i^\varepsilon\right|^2 dS_\varepsilon \geq N^{-1} > 0.$$

Let us now assume that $\sum_{i=1}^{N} t_{i,m}^2$ is divergent. By putting

$$w_{i,m} = u_i^{\varepsilon,m} / \sum_{i=1}^{N} t_{i,m},$$

we have, in the same manner, that

$$\frac{\alpha}{2}\sum_{i=1}^{N}\int_{\Omega^\varepsilon}\left|\nabla w_{i,m}\right|^2 dx \le C(N)\left(1+\frac{1}{\sum_{i=1}^{N} t_{i,m}^2}+\frac{\sum_{i=1}^{N} s_{i,m}^2}{\sum_{i=1}^{N} t_{i,m}^2}\right).$$

From (2.3.10), we know that

$$\sum_{i=1}^{N}\int_{\Omega^\varepsilon}\left|w_{i,m}\right|^2 dx = \left(\sum_{i=1}^{N} t_{i,m}\right)^{-2}\sum_{i=1}^{N}\int_{\Omega^\varepsilon}\left|u_i^{\varepsilon,m}\right|^2 dx \le 1, \tag{2.3.14}$$

and

$$\sum_{i=1}^{N}\int_{\Gamma^\varepsilon}\left|w_{i,m}\right|^2 dS_\varepsilon \ge N^{-1}\left(\sum_{i=1}^{N} t_{i,m}^2\right)^{-1}\sum_{i=1}^{N}\int_{\Gamma^\varepsilon}\left|u_i^{\varepsilon,m}\right|^2 dS_\varepsilon \ge \frac{\sum_{i=1}^{N} s_{i,m}^2}{N\sum_{i=1}^{N} t_{i,m}^2}. \tag{2.3.15}$$

Combining the trace inequality (cf. Lemma A.0.8) with (2.3.14) and (2.3.15), we obtain

$$\begin{aligned}
\frac{\sum_{i=1}^{N} s_{i,m}^2}{\sum_{i=1}^{N} t_{i,m}^2} &\le N\sum_{i=1}^{N}\int_{\Gamma^\varepsilon}\left|w_{i,m}\right|^2 dS_\varepsilon \\
&\le CN\left(2\sum_{i=1}^{N}\left(\int_{\Omega^\varepsilon}\left|w_{i,m}\right|^2 dx\right)^{1/2}\left(\int_{\Omega^\varepsilon}\left|\nabla w_{i,m}\right|^2 dx\right)^{1/2}+\varepsilon^{-1}\sum_{i=1}^{N}\int_{\Omega^\varepsilon}\left|w_{i,m}\right|^2 dx\right) \\
&\le CN\left(2\sum_{i=1}^{N}\left(\int_{\Omega^\varepsilon}\left|\nabla w_{i,m}\right|^2 dx\right)^{1/2}+\varepsilon^{-1}\right).
\end{aligned}$$

It yields that

$$\sum_{i=1}^{N}\int_{\Omega^\varepsilon}\left|\nabla w_{i,m}\right|^2 dx \le \frac{2C(N)}{\alpha}\left[\sum_{i=1}^{N}\left(\int_{\Omega^\varepsilon}\left|\nabla w_{i,m}\right|^2 dx\right)^{1/2}+C(\varepsilon)+\left(\sum_{i=1}^{N} t_{i,m}^2\right)^{-1}\right],$$

which finally leads to

$$\left|\left(\int_{\Omega^\varepsilon}\left|\nabla w_{i,m}\right|^2 dx\right)^{1/2}-\frac{C(N)}{\alpha}\right| \le C(N,\varepsilon)\left(1+\left(\sum_{i=1}^{N} t_{i,m}^2\right)^{-1}\right)^{1/2}, \tag{2.3.16}$$

for all $i=\overline{1,N}$.

Therefore, $\int_{\Omega^\varepsilon}\left|\nabla w_{i,m}\right|^2 dx$ is bounded by the inequality (2.3.16). So, up to a subsequence, $w_{i,m} \rightharpoonup w_i$ weakly in V^ε, and then strongly in $L^2(\Omega^\varepsilon)$ and $L^2(\Gamma^\varepsilon)$. In addition, it can be proved that $\sum_{i=1}^{N}\int_{\Omega^\varepsilon}|w_i|^2 dx \ge N^{-1} > 0$, and from (2.3.11), it gives us that

$$\frac{\alpha}{2}\sum_{i=1}^{N}\int_{\Omega^\varepsilon}\left|\nabla w_{i,m}\right|^2 dx \le \frac{C}{\sum_{i=1}^{N} t_{i,m}^2}+\sum_{i=1}^{N}\int_{\Omega^\varepsilon}\frac{\mathscr{R}_i(x,u^{\varepsilon,m})}{\sum_{i=1}^{N} t_{i,m}^2}dx+\sum_{i=1}^{N}\int_{\Gamma^\varepsilon}\frac{\mathscr{F}_i\left(x,u_i^{\varepsilon,m}\right)}{\sum_{i=1}^{N} t_{i,m}^2}dS_\varepsilon. \tag{2.3.17}$$

We now consider the second integral on the right-hand side of the above inequality, then the third one is totally similar. Using the fact that $w_{i,m} \to w_i$ strongly in $L^2(\Omega^\varepsilon)$ and the assumptions (A_4)-(A_5) in combination with the Fatou lemma, we get

$$\limsup_{m\to\infty} \sum_{i=1}^{N} \int_{\Omega^\varepsilon} \frac{\mathscr{R}_i(x, u^{\varepsilon,m})}{\sum_{i=1}^{N} t_{i,m}^2} dx \le \frac{N}{2} \sum_{i=1}^{N} \int_{\Omega^\varepsilon \cap \{w>0\}} r_{\infty,i}^\varepsilon \left|w_{i,m}\right|^2 dx,$$

where we have also applied the following inequalities

$$N^{-1}\left(\sum_{i=1}^{N} t_{i,m}^2\right)^{-1} \le \left(\sum_{i=1}^{N} t_{i,m}\right)^{-2} \le \left|w_{i,m}\right|^2 \left|u_i^{\varepsilon,m}\right|^{-2},$$

$$\limsup_{u_i^\varepsilon \to \infty} \frac{\mathscr{R}_i(x, u^\varepsilon)}{\left|u_i^\varepsilon\right|^2} \le \frac{1}{2} r_{\infty,i}^\varepsilon(x) \quad \text{for a.e. } x \in \Omega^\varepsilon.$$

Thus, passing to the limit in (2.3.17) we are led to

$$\frac{\alpha}{2} \sum_{i=1}^{N} \int_{\Omega^\varepsilon} |\nabla w_i|^2 dx \le \frac{N}{2} \left(\sum_{i=1}^{N} \int_{\Omega^\varepsilon \cap \{w>0\}} r_{\infty,i}^\varepsilon |w_i|^2 dx + \sum_{i=1}^{N} \int_{\Gamma^\varepsilon \cap \{w>0\}} f_{\infty,i}^\varepsilon |w_i|^2 dS_\varepsilon \right).$$

Recall that $\lambda_1\left(r_\infty^\varepsilon, f_\infty^\varepsilon\right) > 0$, it then gives us that $w_i^+ \equiv 0$ for all $i = \overline{1,N}$. As a consequence, $w_i \equiv 0$ while it contradicts the above result $\sum_{i=1}^{N} \int_{\Omega^\varepsilon} |w_i|^2 dx \ge N^{-1}$.

Hence, J is coercive.

Step 2: (Lower semi-continuity)

It can be proved as in [22, 55] that: if $u^{\varepsilon,m} \rightharpoonup u^\varepsilon$ in $\mathscr{V}^\varepsilon$, then we obtain

$$\limsup_{m\to\infty} \int_{\Omega^\varepsilon} \mathscr{R}_i(x, u^{\varepsilon,m}) dx \le \int_{\Omega^\varepsilon} \mathscr{R}_i(x, u^\varepsilon) dx,$$

$$\limsup_{m\to\infty} \int_{\Gamma^\varepsilon} \mathscr{F}_i\left(x, u_i^{\varepsilon,m}\right) dS_\varepsilon \le \int_{\Gamma^\varepsilon} \mathscr{F}_i\left(x, u_i^\varepsilon\right) dS_\varepsilon,$$

by using the growth assumptions (A_4) in combination with the Fatou lemma. Thus, J is lower semi-continuous.

This result tells us that J achieves the global minimum at a function $u^\varepsilon \in \mathscr{V}^\varepsilon$. If we replace u^ε by $(u^\varepsilon)^+$, u^ε can be supposed to be non-negative. Moreover, the last step shows that u^ε is non-trivial.

Step 3: (Non-triviality of the minimisers)

What we need to prove now is that there exists $\phi \in \mathscr{V}^\varepsilon$ such that $J[\phi] < 0$. In fact, given $\psi \in \mathscr{V}^\varepsilon \cap \mathscr{W}^\varepsilon$ satisfying $\|\psi\|_{\mathscr{W}^\varepsilon} = 1$ and

$$\alpha \sum_{i=1}^{N} \int_{\Omega^\varepsilon} |\nabla \psi_i|^2 dx < N \sum_{i=1}^{N} \left(\int_{\Omega^\varepsilon} r_{0,i}^\varepsilon |\psi_i|^2 dx + \int_{\Gamma^\varepsilon} f_{0,i}^\varepsilon |\psi_i|^2 dS_\varepsilon \right).$$

In fact, here we assume that ψ is non-negative. By the assumptions (A_4)-(A_5), we have

$$\liminf_{\delta\to 0^+} \frac{\mathscr{R}_i(x, \delta\psi)}{\delta^2} \ge \frac{1}{2} r_{0,i}^\varepsilon(x) |\psi|^2 \ge \frac{1}{2} r_{0,i}^\varepsilon(x) |\psi_i|^2 \quad \text{for a.e. } x \in \Omega^\varepsilon,$$

and

$$\liminf_{\delta\to 0^+}\frac{\mathscr{F}_i(x,\delta\psi_i)}{\delta^2}\geq\frac{1}{2}f_{0,i}^{\varepsilon}(x)\left|\psi_i\right|^2\quad\text{for a.e. } x\in\Gamma^{\varepsilon}.$$

This coupling with the Fatou lemma enable us to obtain the following

$$\begin{aligned}\sum_{i=1}^{N}\liminf_{\delta\to 0^+}\int_{\Omega^{\varepsilon}}\frac{\mathscr{R}_i(x,\delta\psi)}{\delta^2}dx+\sum_{i=1}^{N}\liminf_{\delta\to 0^+}\frac{\mathscr{F}_i(x,\delta\psi_i)}{\delta^2}\\ \geq\frac{1}{2}\sum_{i=1}^{N}\left(\int_{\Omega^{\varepsilon}}r_{0,i}^{\varepsilon}\left|\psi_i\right|^2dx+\int_{\Gamma^{\varepsilon}}f_{0,i}^{\varepsilon}\left|\psi_i\right|^2dS_{\varepsilon}\right),\end{aligned}$$

which leads to

$$\limsup_{\delta\to 0^+}\frac{J[\delta\psi]}{\delta^2}<0.$$

Hence, to complete the proof, we need to choose $\phi=\delta\psi$. □

Theorem 2.3.6. *Assume* (A_1)-(A_5) *and* $\lambda_1\left(r_{\infty}^{\varepsilon},f_{\infty}^{\varepsilon}\right)>0$, $\lambda_1\left(r_0^{\varepsilon},f_0^{\varepsilon}\right)<0$ *hold. Then* (P^{ε}) *admits at least a non-negative weak solution* $u^{\varepsilon}\in\mathscr{V}^{\varepsilon}\cap\mathscr{W}^{\infty}(\Omega^{\varepsilon})$.

Proof. We begin the proof by introducing the approximate system

$$\left(P^{k,\varepsilon}\right):\begin{cases}\nabla\cdot\left(-d_i^{\varepsilon}\nabla u_i^{\varepsilon}\right)=R_i^k(u^{\varepsilon}), & \text{in } \Omega^{\varepsilon}\subset\mathbb{R}^d,\\ d_i^{\varepsilon}\nabla u_i^{\varepsilon}\cdot\mathrm{n}=G_i^k\left(u_i^{\varepsilon}\right), & \text{on } \Gamma^{\varepsilon},\\ u_i^{\varepsilon}=0, & \text{on } \Gamma^{ext},\end{cases}$$

in which we have defined that for each integer $k>0$ the truncated reaction rates

$$R_i^k(u^{\varepsilon}):=\begin{cases}\max\left\{-ku_i^{\varepsilon},R_i(u^{\varepsilon})\right\}, & \text{if } u_i^{\varepsilon}\geq 0,\\ R_i(0), & \text{if } u_i^{\varepsilon}<0,\end{cases}$$

and

$$G_i^k\left(u_i^{\varepsilon}\right):=\begin{cases}\varepsilon\max\left\{-ku_i^{\varepsilon},a_i^{\varepsilon}u_i^{\varepsilon}-b_i^{\varepsilon}F_i\left(u_i^{\varepsilon}\right)\right\}, & \text{if } u_i^{\varepsilon}\geq 0,\\ -\varepsilon b_i^{\varepsilon}F_i(0), & \text{if } u_i^{\varepsilon}<0.\end{cases}$$

It is easy to check that our truncated functions R_i^k and G_i^k fulfill both $\left(\mathrm{A}_4\right)$ and (A_6). In addition, if we set elements $R_{0,i}^k,R_{\infty,i}^k,G_{0,i}^k,G_{\infty,i}^k$ as functions in (A_5) by R_i^k and G_i^k, one may prove that

$$r_{0,i}^{\varepsilon}\leq R_{0,i}^k,\ r_{\infty,i}^{\varepsilon}\leq R_{\infty,i}^k,\ f_{0,i}^{\varepsilon}\leq G_{0,i}^k,\ f_{\infty,i}^{\varepsilon}\leq G_{\infty,i}^k\quad\text{for all } i\in\{1,\ldots,N\},$$

and $\lambda_1\left(R_0^k,G_0^k\right)<0$ and $\lambda_1\left(R_{\infty}^k,G_{\infty}^k\right)>0$ for k large (see, e.g. [55]).
Thanks to Lemma 2.3.5, the problem $\left(P^{k,\varepsilon}\right)$ admits a global non-trivial and non-negative minimizer, denoted by $u^{k,\varepsilon}$, which belongs to $\mathscr{V}^{\varepsilon}$ and it is associated with the following functional

$$J^k[u^{\varepsilon}]:=\frac{1}{2}\sum_{i=1}^{N}\int_{\Omega^{\varepsilon}}d_i^{\varepsilon}\left|\nabla u_i^{\varepsilon}\right|dx-\sum_{i=1}^{N}\int_{\Omega^{\varepsilon}}\mathscr{R}_i^k(x,u^{\varepsilon})dx-\sum_{i=1}^{N}\int_{\Gamma^{\varepsilon}}\mathscr{F}_i^k\left(x,u_i^{\varepsilon}\right)dS_{\varepsilon}.$$

Furthermore, $u^{k,\varepsilon}$ defines a weak solution to the problem $\left(P^{k,\varepsilon}\right)$ for every k and thus, $u^{k,\varepsilon}\in\mathscr{W}^{\infty}(\Omega^{\varepsilon})$ by Lemma 2.3.3.
Now, we assign a vector v^{ε} whose elements are defined by $v_i^{\varepsilon}:=\min\left\{u_i^{\varepsilon},u_i^{k,\varepsilon}\right\}$ where $u\in\mathscr{V}^{\varepsilon}$ is the global minimizer constructed from the functional J. We shall prove that $J[v^{\varepsilon}]\leq J[u^{\varepsilon}]$.

Note that when doing so, $v^\varepsilon \in \mathscr{W}^\infty(\Omega^\varepsilon)$ and then define a weak solution $u \in \mathscr{V}^\varepsilon \cap \mathscr{W}^\infty(\Omega^\varepsilon)$ to (P^ε).
In fact, one has

$$J^k\left[u^{k,\varepsilon}\right] \le J[\phi] \quad \text{for all } \phi \in \mathscr{V}^\varepsilon.$$

Then by choosing ϕ such that $\phi_i := \max\left\{u_i^\varepsilon, u_i^{k,\varepsilon}\right\}$ we have

$$\begin{aligned}
&\sum_{i=1}^N \int_{\left\{u_i^{k,\varepsilon} < u_i^\varepsilon\right\} \cap \Omega^\varepsilon} \left(\frac{1}{2} d_i^\varepsilon \left|\nabla u_i^{k,\varepsilon}\right|^2 - \mathscr{R}_i^k\left(x, u^{k,\varepsilon}\right)\right) dx - \sum_{i=1}^N \int_{\left\{u_i^{k,\varepsilon} < u_i^\varepsilon\right\} \cap \Gamma^\varepsilon} \mathscr{F}_i^k\left(x, u_i^{k,\varepsilon}\right) dS_\varepsilon \\
&\le \sum_{i=1}^N \int_{\left\{u_i^{k,\varepsilon} < u_i^\varepsilon\right\} \cap \Omega^\varepsilon} \left(\frac{1}{2} d_i^\varepsilon \left|\nabla u_i^\varepsilon\right|^2 - \mathscr{R}_i^k\left(x, u^\varepsilon\right)\right) dx - \sum_{i=1}^N \int_{\left\{u_i^{k,\varepsilon} < u_i^\varepsilon\right\} \cap \Gamma^\varepsilon} \mathscr{F}_i^k\left(x, u_i^\varepsilon\right) dS_\varepsilon. \quad (2.3.18)
\end{aligned}$$

In addition, by the choice of J (see in Lemma 2.3.5) we deduce that

$$\begin{aligned}
J[v^\varepsilon] - J[u^\varepsilon] = &\sum_{i=1}^N \int_{\left\{u_i^{k,\varepsilon} < u_i^\varepsilon\right\} \cap \Omega^\varepsilon} \frac{1}{2} d_i^\varepsilon \left(\left|\nabla u_i^{k,\varepsilon}\right|^2 - \left|\nabla u_i^\varepsilon\right|\right) dx \\
&- \sum_{i=1}^N \int_{\left\{u_i^{k,\varepsilon} < u_i^\varepsilon\right\} \cap \Omega^\varepsilon} \left(\mathscr{R}_i\left(x, u^{k,\varepsilon}\right) - \mathscr{R}_i\left(x, u^\varepsilon\right)\right) dx \\
&- \sum_{i=1}^N \int_{\left\{u_i^{k,\varepsilon} < u_i^\varepsilon\right\} \cap \Gamma^\varepsilon} \left(\mathscr{F}_i\left(x, u_i^{k,\varepsilon}\right) - \mathscr{F}_i\left(x, u_i^\varepsilon\right)\right) dS_\varepsilon. \quad (2.3.19)
\end{aligned}$$

On the other hand, (2.3.18) yields

$$\sum_{i=1}^N \int_{\left\{u_i^{k,\varepsilon} < u_i^\varepsilon\right\} \cap \Omega^\varepsilon} \left[\mathscr{R}_i^k\left(x, u^{k,\varepsilon}\right) - \mathscr{R}_i^k\left(x, u^\varepsilon\right) - \left(\mathscr{R}_i\left(x, u^{k,\varepsilon}\right) - \mathscr{R}_i\left(x, u^\varepsilon\right)\right)\right] \le 0, \quad (2.3.20)$$

and

$$\sum_{i=1}^N \int_{\left\{u_i^{k,\varepsilon} < u_i^\varepsilon\right\} \cap \Gamma^\varepsilon} \left[\mathscr{F}_i^k\left(x, u^{k,\varepsilon}\right) - \mathscr{F}_i^k\left(x, u^\varepsilon\right) - \left(\mathscr{F}_i\left(x, u^{k,\varepsilon}\right) - \mathscr{F}_i\left(x, u^\varepsilon\right)\right)\right] \le 0. \quad (2.3.21)$$

Hence, combining (2.3.18)-(2.3.21) we complete the proof of the lemma. This tells us that under assumptions (A_1)-(A_5) the problem (P^ε) admits a non-negative, non-trivial and bounded weak vector of solutions u^ε at each ε-level. □

Remark 2.3.7. *If $R_i(u^\varepsilon) \ge -Mu_i^\varepsilon$ in Ω^ε (or for each subdomain of Ω^ε if rigorously stated) for some ε-dependent constant $M > 0$ and all $i \in \{1, ..., N\}$, then (P^ε) has at least a positive, non-trivial and bounded weak solution u^ε by the Hopf strong maximum principle. Furthermore, one may prove in the same vein in [55, Lemma 13] that the solution is unique by using vectors of test functions $\varphi_\delta^\varepsilon$ and ψ_δ^ε whose elements are given by*

$$\varphi_{\delta,i}^\varepsilon = \frac{\left(u_i^\varepsilon + \delta\right)^2 - \left(v_i^\varepsilon + \delta\right)^2}{u_i^\varepsilon + \delta}, \ \psi_{\delta,i}^\varepsilon = \frac{\left(u_i^\varepsilon + \delta\right)^2 - \left(v_i^\varepsilon + \delta\right)^2}{v_i^\varepsilon + \delta},$$

where u_i^ε and v_i^ε are two solutions of (P^ε) at each layer $i \in \{1, ..., N\}$, which are expected to equal to each other.

Remark 2.3.8. *In the case of zero Neumann boundary condition on Γ^ε, if the nonlinearity R_i is globally Lipschitz with the Lipschitz constant, denoted by L_i, independent of the scale ε for any $i \in \{1, ..., N\}$, then we may use an iterative scheme to deal with the existence and uniqueness of solutions to our problem. In fact, for $n \in \mathbb{N}$ such an iterative scheme is given by*

$$\left(P_n^\varepsilon\right): \begin{cases} \nabla \cdot \left(-d_i^\varepsilon \nabla u_i^{\varepsilon,n+1}\right) = R_i\left(u^{\varepsilon,n}\right), & \text{in } \Omega^\varepsilon, \\ d_i^\varepsilon \nabla u_i^{\varepsilon,n+1} \cdot n = 0, & \text{on } \Gamma^\varepsilon, \\ u_i^{\varepsilon,n+1} = 0, & \text{on } \Gamma^{ext}, \end{cases} \tag{2.3.22}$$

where the starting point is $u^{\varepsilon,0} = 0$.
This global Lipschitz assumption is an alternative to $\left(A_4\right)$ for R_i and it is termed as $\left(A_4'\right)$.

Theorem 2.3.9. *Assume (A_1) and (A_3) hold (without F_i) and suppose that the nonlinearity R_i satisfy $\left(A_4'\right)$ replaced by $\left(A_4\right)$. Then, the problem (P^ε) with zero Neumann boundary condition on Γ^ε has a unique solution in $\mathscr{V}^\varepsilon$ if the constant $\alpha^{-1} \max_{1 \le i \le N} \{L_i\} N$ is small enough.*

Proof. It is worth noting that the problem (2.3.22) admits a unique solution in $\mathscr{V}^\varepsilon$ for any n. Then, the functional $w_i^{\varepsilon,n} = u_i^{\varepsilon,n+1} - u_i^{\varepsilon,n} \in V^\varepsilon$ satisfies the following problem:

$$\begin{cases} \nabla \cdot \left(-d_i^\varepsilon \nabla w_i^{\varepsilon,n}\right) = R_i\left(u^{\varepsilon,n}\right) - R_i\left(u^{\varepsilon,n-1}\right), & \text{in } \Omega^\varepsilon, \\ d_i^\varepsilon \nabla w_i^{\varepsilon,n} \cdot \mathrm{n} = 0, & \text{on } \Gamma^\varepsilon, \\ w_i^{\varepsilon,n} = 0. & \text{on } \Gamma^{ext}. \end{cases}$$

Using the test function $\psi_i \in V^\varepsilon$ we arrive at

$$\left\langle d_i^\varepsilon w_i^{\varepsilon,n}, \psi_i \right\rangle_{V^\varepsilon} = \left\langle R_i\left(u^{\varepsilon,n}\right) - R_i\left(u^{\varepsilon,n-1}\right), \psi_i \right\rangle_{L^2(\Omega^\varepsilon)}.$$

We may consider an estimate for the above expression:

$$\alpha \sum_{i=1}^N \left|\left\langle w_i^{\varepsilon,n}, \psi_i \right\rangle_{V^\varepsilon}\right| \le \sum_{i=1}^N L_i N \left|\left\langle w_i^{\varepsilon,n-1}, \psi_i \right\rangle_{L^2(\Omega^\varepsilon)}\right|. \tag{2.3.23}$$

Thanks to Hölder's and Poincaré inequalities (cf. Lemma A.0.10 and Lemma A.0.9), we have

$$\sum_{i=1}^N \left|\left\langle w_i^{\varepsilon,n}, \psi_i \right\rangle_{V^\varepsilon}\right| \le C_p \alpha^{-1} \max_{1 \le i \le N} \{L_i\} N \left\|w^{\varepsilon,n-1}\right\|_{\mathscr{V}^\varepsilon} \|\psi\|_{\mathscr{V}^\varepsilon},$$

where $C_p > 0$ is the Poincaré constant independent of the choice of ε, but the dimension d of the media (see, e.g. [31, Lemma 2.1] and [33]).
If the constant $\alpha^{-1} \max_{1 \le i \le N} \{L_i\} N$ is small enough such that $\kappa_p := C_p \alpha^{-1} \max_{1 \le i \le N} \{L_i\} N < 1$, then choosing $\psi_i = w_i^{\varepsilon,n}$ for $i \in \{1, ..., N\}$ we obtain that

$$\|w^{\varepsilon,n}\|_{\mathscr{V}^\varepsilon} \le \kappa_p \left\|w^{\varepsilon,n-1}\right\|_{\mathscr{V}^\varepsilon}.$$

Consequently, for some $k \in \mathbb{N}$ we get

$$\begin{aligned} \left\|u^{\varepsilon,n+k} - u^{\varepsilon,n}\right\|_{\mathscr{V}^\varepsilon} &\le \left\|u^{\varepsilon,n+k} - u^{\varepsilon,n+k-1}\right\|_{\mathscr{V}^\varepsilon} + ... + \left\|u^{\varepsilon,n+1} - u^{\varepsilon,n}\right\|_{\mathscr{V}^\varepsilon} \\ &\le \kappa_p^{n+k-1} \left\|u^{\varepsilon,1} - u^{\varepsilon,0}\right\|_{\mathscr{V}^\varepsilon} + ... + \kappa_p^n \left\|u^{\varepsilon,1} - u^{\varepsilon,0}\right\|_{\mathscr{V}^\varepsilon} \\ &\le \kappa_p^n \left(\kappa_p^{k-1} + \kappa_p^{k-2} + ... + 1\right) \left\|u^{\varepsilon,1}\right\|_{\mathscr{V}^\varepsilon} \\ &\le \frac{\kappa_p^n \left(1 - \kappa_p^k\right)}{1 - \kappa_p} \left\|u^{\varepsilon,1}\right\|_{\mathscr{V}^\varepsilon}. \end{aligned} \tag{2.3.24}$$

Therefore, $\{u^{\varepsilon,n}\}$ is a Cauchy sequence in $\mathscr{V}^\varepsilon$, and then there exists uniquely $u^\varepsilon \in \mathscr{V}^\varepsilon$ such that $u^{\varepsilon,n} \to u^\varepsilon$ strongly in $\mathscr{V}^\varepsilon$ as $n \to \infty$. Remarkably, this convergence combining with the Lipschitz property of R_i leads to the fact that $R_i(u^{\varepsilon,n}) \to R_i(u^\varepsilon)$ strongly in $\mathscr{V}^\varepsilon$ as $n \to \infty$. As a result, the function u^ε is the solution of the problem (P^ε) when passing to the limit in n.
In addition, when $k \to \infty$, it follows from (2.3.24) that

$$\|u^{\varepsilon,n} - u^\varepsilon\|_{\mathscr{V}^\varepsilon} \leq \frac{\kappa_p^n}{1-\kappa_p} \left\|u^{\varepsilon,1}\right\|_{\mathscr{V}^\varepsilon},$$

which implies the convergence rate of the linearization and guarantees the stability of the problem (P^ε). □

2.4 Homogenization asymptotics. Corrector estimates

2.4.1 Two-scale asymptotic expansions

For every $i \in \{1, ..., N\}$, we introduce the following Mth-order expansion ($M \geq 2$):

$$u_i^\varepsilon(x) = \sum_{m=0}^{M} \varepsilon^m u_{i,m}(x,y) + \mathscr{O}\left(\varepsilon^{M+1}\right), \quad x \in \Omega^\varepsilon, \tag{2.4.1}$$

where $u_{i,m}(x,\cdot)$ is Y-periodic for $0 \leq m \leq M$.
It follows from (3.2.3) that

$$\begin{aligned}\nabla u_i^\varepsilon &= \left(\nabla_x + \varepsilon^{-1}\nabla_y\right)\left(\sum_{m=0}^{M} \varepsilon^m u_{i,m} + \mathscr{O}\left(\varepsilon^{M+1}\right)\right)\\ &= \varepsilon^{-1}\nabla_y u_{i,0} + \sum_{m=0}^{M-1} \varepsilon^m \left(\nabla_x u_{i,m} + \nabla_y u_{i,m+1}\right) + \mathscr{O}\left(\varepsilon^M\right).\end{aligned} \tag{2.4.2}$$

Using the relation of the operator $\mathscr{A}^\varepsilon$ and (3.2.5), we compute that

$$\mathscr{A}^\varepsilon u_i^\varepsilon = \left(\nabla_x + \varepsilon^{-1}\nabla_y\right)\cdot\left(-d_i(y)\left[\varepsilon^{-1}\nabla_y u_{i,0} + \sum_{m=0}^{M-1}\varepsilon^m\left(\nabla_x u_{i,m} + \nabla_y u_{i,m+1}\right)\right]\right) + \mathscr{O}\left(\varepsilon^{M-1}\right),$$

then after collecting those having the same powers of ε, we obtain

$$\begin{aligned}\mathscr{A}^\varepsilon u_i^\varepsilon &= \varepsilon^{-2}\nabla_y\cdot\left(-d_i(y)\nabla_y u_{i,0}\right)\\ &\quad + \varepsilon^{-1}\left[\nabla_x\cdot\left(-d_i(y)\nabla_y u_{i,0}\right) + \nabla_y\cdot\left(-d_i(y)\left(\nabla_x u_{i,0} + \nabla_y u_{i,1}\right)\right)\right]\\ &\quad + \sum_{m=0}^{M-2}\varepsilon^m\left[\nabla_x\cdot\left(-d_i(y)\left(\nabla_x u_{i,m} + \nabla_y u_{i,m+1}\right)\right)\right.\\ &\quad \left. + \nabla_y\cdot\left(-d_i(y)\left(\nabla_x u_{i,m+1} + \nabla_y u_{i,m+2}\right)\right)\right] + \mathscr{O}\left(\varepsilon^{M-1}\right).\end{aligned} \tag{2.4.3}$$

In the same vein, we take into consideration the boundary condition at Γ^ε as follows:

$$\begin{aligned}-d_i^\varepsilon \nabla u_i^\varepsilon\cdot \mathrm{n} &:= -d_i(y)\left(\varepsilon^{-1}\nabla_y u_{i,0} + \sum_{m=0}^{M-1}\varepsilon^m\left(\nabla_x u_{i,m} + \nabla_y u_{i,m+1}\right)\right)\cdot \mathrm{n}\\ &= \varepsilon b_i(y) F_i\left(\sum_{m=0}^{M-1}\varepsilon^m u_{i,m}\right) - a_i(y)\sum_{m=0}^{M-1}\varepsilon^{m+1}u_{i,m} + \mathscr{O}\left(\varepsilon^M\right).\end{aligned} \tag{2.4.4}$$

It is worth noting that in order to investigate the convergence analysis, we give assumptions that allow to pull the ε-dependent quantities out of the nonlinearities R_i and F_i:

$$R_i\left(\sum_{m=0}^{M}\varepsilon^m u_{1,m},\ldots,\sum_{m=0}^{M}\varepsilon^m u_{N,m}\right)=\sum_{m=0}^{M}\varepsilon^m\bar{R}_i\left(u_{1,m},\ldots,u_{N,m}\right)+\mathscr{O}\left(\varepsilon^{M+1}\right), \tag{2.4.5}$$

$$F_i\left(\sum_{m=0}^{M}\varepsilon^m u_{i,m}\right)=\sum_{m=0}^{M}\varepsilon^m\bar{F}_i\left(u_{i,m}\right)+\mathscr{O}\left(\varepsilon^{M+1}\right), \tag{2.4.6}$$

in which $\bar{R}_i$ and $\bar{F}_i$ are global Lipschitz functions corresponding to the Lipschitz constant L_i and K_i, respectively, for $i\in\{1,\ldots,N\}$.
From now on, collecting the coefficients of the same powers of ε in (3.2.6) and (3.2.7) in combination with using (3.2.8) and (2.4.6), we are led to the following systems of elliptic problems, which we refer to the auxiliary problems:

$$\begin{cases}\mathscr{A}_0 u_{i,0}=0, & \text{in } Y_1,\\ -d_i(y)\nabla_y u_{i,0}\cdot \mathrm{n}=0, & \text{on } \partial Y_0,\\ u_{i,0} \text{ is } Y-\text{periodic in } y,\end{cases} \tag{2.4.7}$$

$$\begin{cases}\mathscr{A}_0 u_{i,1}=-\mathscr{A}_1 u_{i,0}, & \text{in } Y_1,\\ -d_i(y)\left(\nabla_x u_{i,0}+\nabla_y u_{i,1}\right)\cdot \mathrm{n}=0, & \text{on } \partial Y_0,\\ u_{i,1} \text{ is } Y-\text{periodic in } y,\end{cases} \tag{2.4.8}$$

$$\begin{cases}\mathscr{A}_0 u_{i,m+2}=\bar{R}_i(u_m)-\mathscr{A}_1 u_{i,m+1}-\mathscr{A}_2 u_{i,m}, & \text{in } Y_1,\\ -d_i(y)\left(\nabla_x u_{i,m+1}+\nabla_y u_{i,m+2}\right)\cdot \mathrm{n}=b_i(y)\bar{F}_i\left(u_{i,m}\right)-a_i(y)u_{i,m}, & \text{on } \partial Y_0,\\ u_{i,m+2} \text{ is } Y-\text{periodic in } y,\end{cases} \tag{2.4.9}$$

for $0\le m\le M-2$.
Here, the notation u_m is ascribed to the vector containing elements $u_{i,m}$ for all $i\in\{1,\ldots,N\}$, and we have denoted by

$$\begin{aligned}\mathscr{A}_0&:=\nabla_y\cdot\left(-d_i(y)\nabla_y\right),\\ \mathscr{A}_1&:=\nabla_x\cdot\left(-d_i(y)\nabla_y\right)+\nabla_y\cdot\left(-d_i(y)\nabla_x\right),\\ \mathscr{A}_2&:=\nabla_x\cdot\left(-d_i(y)\nabla_x\right).\end{aligned}$$

For the first auxiliary problem (3.2.9), it is trivial to prove that the solution to (3.2.9) is independent of y, and hence we obtain

$$u_{i,0}(x,y)=\tilde{u}_{i,0}(x). \tag{2.4.10}$$

For the second auxiliary problem (3.2.10), we recall the result in [93, Lemma 2.1] to ensure the existence and uniqueness of periodic solutions to the elliptic problem, which is called the solvability condition. In this case, this condition satisfies itself because we easily get from the PDE in (3.2.10) that

$$-\int_{\partial Y_1} d_i(y)\nabla_y u_{i,1}\cdot \mathrm{n}dS_y=\int_{\partial Y_0} d_i(y)\nabla_x\tilde{u}_{i,0}\cdot \mathrm{n}dS_y,$$

by Gauß's theorem. Thus, it claims the existence of a unique weak solution to (3.2.10).

Moreover, this solution is sought by using separation of variables:

$$u_{i,1}(x,y) = -\chi_i(y)\cdot\nabla_x\tilde{u}_{i,0}(x) + \mathscr{C}_i(x). \tag{2.4.11}$$

Substituting (2.4.11) into (3.2.10), we obtain the ith cell problem:

$$\begin{cases} \mathscr{A}_0\chi_i = \nabla_y d_i(y), & \text{in } Y_1, \\ -d_i(y)\nabla_y\chi_i\cdot \mathrm{n} = d_i(y)\cdot \mathrm{n}, & \text{on } \partial Y_0, \\ \chi_i \text{ is } Y-\text{periodic in } y, \end{cases} \tag{2.4.12}$$

in which the field $\chi_i(y)$ is called cell function. Additionally, by the definition of the mean value, we have

$$\mathscr{M}_Y(\chi_i) := \frac{1}{|Y|}\int_{Y_1}\chi_i dy = 0. \tag{2.4.13}$$

As a consequence, it can be proved that χ_i belongs to the space $H^1_\#(Y_1)/\mathbb{R}$ and satisfies (2.4.13).

Now, it only remains to consider the third auxiliary problem (3.2.11). Assume that we have in mind the functions u_m and u_{m+1}, then to find u_{m+2} let us remark that the right-hand side of the PDE in (3.2.11) can be rewritten as

$$\begin{aligned} \bar{R}_i(u_m) - \mathscr{A}_1 u_{i,m+1} - \mathscr{A}_2 u_{i,m} = \bar{R}_i(u_m) &+ \nabla_y\cdot\big(d_i(y)\nabla_x u_{i,m+1}\big) \\ &+ \nabla_x\cdot\big(d_i(y)\big(\nabla_x u_{i,m} + \nabla_y u_{i,m+1}\big)\big). \end{aligned} \tag{2.4.14}$$

We define the operator $\mathscr{L}_i(\psi)$ for $i\in\{1,...,N\}$ by multiplying (2.4.14) by a test function $\psi\in C^\infty_\#(Y_1)$, as follows:

$$\begin{aligned} \mathscr{L}_i(\psi) := &\int_{Y_1}\bar{R}_i(u_m)\psi dy + \int_{Y_1}\nabla_y\cdot\big(d_i(y)\nabla_x u_{i,m+1}\big)\psi dy \\ &+ \int_{Y_1}\nabla_x\cdot\big(d_i(y)\big(\nabla_x u_{i,m} + \nabla_y u_{i,m+1}\big)\big)\psi dy \\ &= \int_{Y_1}\bar{R}_i(u_m)\psi dy - \int_{Y_1} d_i(y)\nabla_x u_{i,m+1}\cdot\nabla_y\psi dy \\ &+ \int_{Y_1}\nabla_x\cdot\big(d_i(y)\big(\nabla_x u_{i,m} + \nabla_y u_{i,m+1}\big)\big)\psi dy. \end{aligned}$$

To apply the Lax-Milgram type lemma provided by [31, Lemma 2.2], we need $\mathscr{L}_i(\psi_1) = \mathscr{L}_i(\psi_2)$ for $\psi_1,\psi_2\in H^1_\#(Y_1)/\mathbb{R}$ with $\psi_1\simeq\psi_2$, or it is equivalent to

$$\int_{Y_1}\bar{R}_i(u_m)(\psi_1-\psi_2)dy + \int_{Y_1}\nabla_x\cdot\big(d_i(y)\big(\nabla_x u_{i,m} + \nabla_y u_{i,m+1}\big)\big)(\psi_1-\psi_2)dy = 0. \tag{2.4.15}$$

Note that $\psi_1-\psi_2$ is independent of y. Hence, (2.4.15) becomes

$$\int_{Y_1}\nabla_x\cdot\big(-d_i(y)\big(\nabla_x u_{i,m} + \nabla_y u_{i,m+1}\big)\big)dy = \int_{Y_1}\bar{R}_i(u_m)dy. \tag{2.4.16}$$

For simplicity, we first take $m=0$. Remind from (2.4.10) and (2.4.11) that $u_{i,0}$ and $u_{i,1}$ are known, while the term $R_i(u_0)$ depends on x only, then one has

$$\int_{Y_1}\nabla_x\cdot\big(-d_i(y)\big(-\nabla_y\chi_i\nabla_x\tilde{u}_{i,0} + \nabla_x\tilde{u}_{i,0}\big)\big)dy = |Y_1|\bar{R}_i(u_0),$$

or equivalently,

$$\int_{Y_1} \nabla_x \cdot \left(-d_i(y)\left(-\nabla_y \chi_i + \mathbb{I}\right)\nabla_x \tilde{u}_{i,0}\right) dy = |Y_1| \bar{R}_i(u_0).$$

Thus, if we set the homogenized (or effective) coefficient

$$q_i = \frac{1}{|Y|}\int_{Y_1} d_i(y)\left(-\nabla_y \chi_i + \mathbb{I}\right) dy,$$

the $\tilde{u}_{i,0}$ must satisfy (in the "almost all" sense)

$$-\nabla_x \cdot \left(q_i \nabla_x \tilde{u}_{i,0}\right) = |Y|^{-1}|Y_1|\bar{R}_i(u_0), \quad \text{in } \Omega. \tag{2.4.17}$$

On the other hand, it is associated with $\tilde{u}_{i,0} = 0$ at Γ^{ext} and still satisfies the ellipticity condition.
Let us now determine $u_{i,2}$. At first, the PDE in (3.2.11) (for $m = 0$) is given by

$$\mathscr{A}_0 u_{i,2} = \bar{R}_i(u_0) - d_i(y)\nabla_y \chi_i \nabla_x^2 \tilde{u}_{i,0} - \nabla_y\left(d_i(y)\chi_i\right)\nabla_x^2 \tilde{u}_{i,0} + d_i(y)\nabla_x^2 \tilde{u}_{i,0}, \quad \text{in } Y_1. \tag{2.4.18}$$

Next, the boundary condition reads

$$-d_i(y)\nabla_y u_{i,2} \cdot \mathrm{n} = b_i(y)\bar{F}_i\left(u_{i,0}\right) - a_i(y)u_{i,0} - d_i(y)\chi_i \nabla_x^2 \tilde{u}_{i,0} \cdot \mathrm{n}, \quad \text{on } \partial Y_0.$$

Note that (2.4.18) can be rewritten as

$$\mathscr{A}_0 u_{i,2} - \nabla_y \cdot \left(d_i(y)\chi_i \nabla_x^2 \tilde{u}_{i,0}\right) = \bar{R}_i(u_0) - d_i(y)\left(\nabla_y \chi_i - \mathbb{I}\right)\nabla_x^2 \tilde{u}_{i,0}.$$

Using the relation (2.4.17), we have

$$\mathscr{A}_0 u_{i,2} + \mathscr{A}_0\left(\chi_i \nabla_x^2 \tilde{u}_{i,0}\right) = -|Y_1|^{-1}|Y|\nabla_x \cdot \left(q_i \nabla_x \tilde{u}_{i,0}\right) - d_i(y)\left(\nabla_y \chi_i - \mathbb{I}\right)\nabla_x^2 \tilde{u}_{i,0}. \tag{2.4.19}$$

Therefore, (2.4.19) allows us to look for $u_{i,2}$ of the form

$$u_{i,2}(x,y) = \theta_i(y)\nabla_x^2 \tilde{u}_{i,0}, \tag{2.4.20}$$

in which such a function θ_i is the solution of the following problem

$$\begin{cases} \mathscr{A}_0\left(\nabla_y \theta_i - \chi_i\right) = -|Y_1|^{-1}|Y| q_i - d_i(y)\left(\nabla_y \chi_i - \mathbb{I}\right), & \text{in } Y_1, \\ -d_i(y)\left(\nabla_y \theta_i - \chi_i\right) \cdot \mathrm{n} = b_i(y)\bar{F}_i\left(u_{i,0}\right) - a_i(y)u_{i,0}, & \text{on } \partial Y_0, \\ \theta_i \text{ is } Y-\text{periodic in } y. \end{cases} \tag{2.4.21}$$

In conclusion, we have derived an expansion of $u_i^\varepsilon(x)$ up to the second-order corrector. In particular, we deduced that

$$u_i^\varepsilon(x) = \tilde{u}_{i,0}(x) - \varepsilon \chi_i\left(\frac{x}{\varepsilon}\right) \cdot \nabla_x \tilde{u}_{i,0}(x) + \varepsilon^2 \theta_i\left(\frac{x}{\varepsilon}\right)\nabla_x^2 \tilde{u}_{i,0}(x) + \mathscr{O}\left(\varepsilon^3\right), \quad x \in \Omega^\varepsilon, \tag{2.4.22}$$

where $\tilde{u}_{i,0}$ can be solved by the microscopic problem (3.2.9), χ_i satisfies the cell problem (2.4.12), and θ_i satisfies the cell problem (2.4.21). Moreover, the homogenized equation is defined in (2.4.17).

For the time being, it remains to derive the macroscopic equation from the PDE for $u_{i,2}$ in (3.2.11) for $m=0$. When doing so, the following solvability condition has to be fulfilled:

$$\int_{Y_1}\left(\bar{R}_i\left(u_0\right)-\mathscr{A}_1 u_{i,1}-\mathscr{A}_2\tilde{u}_{i,0}\right)dy=\int_{\partial Y_0}\left(b_i\left(y\right)\bar{F}_i\left(\tilde{u}_{i,0}\right)-a_i\left(y\right)\tilde{u}_{i,0}+d_i\left(y\right)\nabla_x u_{i,1}\cdot \mathrm{n}\right)dS_y. \tag{2.4.23}$$

The left-hand side of (2.4.23) can be rewritten as

$$\int_{Y_1}\bar{R}_i\left(u_0\right)dy+\int_{Y_1}\nabla_y\cdot\left(d_i\left(y\right)\nabla_x u_{i,1}\right)dy+\int_{Y_1}\nabla_x\cdot\left(d_i\left(y\right)\left(\nabla_x\tilde{u}_{i,0}+\nabla_y u_{i,1}\right)\right)dy. \tag{2.4.24}$$

Let us consider the last two integrals in (2.4.24). In fact, we have

$$\begin{aligned}\int_{Y_1}\nabla_x\left(d_i\left(y\right)\nabla_x\tilde{u}_{i,0}\right)dy&=\nabla_x\cdot\left[\left(\int_{Y_1}d_i\left(y\right)dy\right)\nabla_x\tilde{u}_{i,0}\right]\\&=\left(\int_{Y_1}d_i\left(y\right)dy\right):\nabla_x\nabla_x\tilde{u}_{i,0},\end{aligned} \tag{2.4.25}$$

where we have used the inner product (or exactly, double dot product) between two matrices

$$A:B:=\mathrm{tr}\left(A^TB\right)=\sum_{ij}a_{ij}b_{ij}.$$

In addition, by periodicity and Gauß's theorem we obtain

$$\int_{Y_1}\nabla_y\cdot\left(d_i\left(y\right)\nabla_x u_{i,1}\right)dy=\int_{\partial Y_0}d_i\left(y\right)\nabla_x u_{i,1}\cdot \mathrm{n}dS_y. \tag{2.4.26}$$

Next, employing the double dot product again, we get

$$\int_{Y_1}\nabla_x\cdot\left(d_i\left(y\right)\nabla_y u_{i,1}\right)dy=-\int_{Y_1}\left(d_i\left(y\right)\nabla_y\chi_i\right)dy:\nabla_x\nabla_x\tilde{u}_{i,0}. \tag{2.4.27}$$

Combining (2.4.23), (2.4.25)-(2.4.27) yields the macroscopic equation:

$$\left(\int_{Y_1}\left(d_i\left(y\right)-d_i\left(y\right)\nabla_y\chi_i\right)dy\right):\nabla_x\nabla_x\tilde{u}_{i,0}=\left\langle b_i\right\rangle\bar{F}_i\left(\tilde{u}_{i,0}\right)-\left\langle a_i\right\rangle\tilde{u}_{i,0}-|Y_1|\bar{R}_i\left(u_0\right),$$

where we have denoted by

$$\left\langle a_i\right\rangle:=\int_{\partial Y_0}a_i\left(y\right)dy \text{ and } \left\langle b_i\right\rangle:=\int_{\partial Y_0}b_i\left(y\right)dy.$$

Furthermore, this equation is associated with the boundary condition $\tilde{u}_{i,0}=0$ at Γ^{ext}.

2.4.2 Corrector estimates. Justification of the asymptotics

From the point of view of applications, upper bound estimates on convergence rates over the space $\mathscr{V}^\varepsilon$ in terms of quantitative analysis tell how fast one can approximate both u^ε, the solution of systems (P^ε), and ∇u^ε by the asymptotic expansion (2.4.22). On the other hand,

it also gives rise to the question that: how much information on data will we need via such averaging techniques?
We introduce the well-known cut-off function $m^\varepsilon \in C_c^\infty(\Omega)$ such that $\varepsilon |\nabla m^\varepsilon| \le C$ and

$$m^\varepsilon(x) := \begin{cases} 0, & \text{if } \operatorname{dist}(x,\Gamma) \le \varepsilon, \\ 1, & \text{if } \operatorname{dist}(x,\Gamma) \ge 2\varepsilon. \end{cases}$$

For $i \in \{1,...,N\}$, we define the function Ψ_i^ε by

$$\Psi_i^\varepsilon := \varphi_i^\varepsilon + (1-m^\varepsilon)\left(\varepsilon u_{i,1} + \varepsilon^2 u_{i,2}\right),$$

where we have denoted by

$$\varphi_i^\varepsilon := u_i^\varepsilon - \left(u_{i,0} + \varepsilon u_{i,1} + \varepsilon^2 u_{i,2}\right).$$

Due to the auxiliary problems (3.2.9)-(3.2.11), we have

$$\mathscr{A}^\varepsilon \varphi_i^\varepsilon = R_i(u^\varepsilon) - \bar{R}_i(u_0) - \varepsilon\left(\mathscr{A}_2 u_{i,1} + \mathscr{A}_1 u_{i,2}\right) - \varepsilon^2 \mathscr{A}_2 u_{i,2}, \quad x \in \Omega^\varepsilon, \tag{2.4.28}$$

while on the boundary Γ^ε, the function φ_i^ε satisfies

$$-d_i^\varepsilon \nabla_x \varphi_i^\varepsilon \cdot \mathrm{n} = \varepsilon^2 d_i^\varepsilon \nabla_x u_{i,2} \cdot \mathrm{n} + \varepsilon\left[a_i^\varepsilon\left(u_{i,0} - u_i^\varepsilon\right) + b_i^\varepsilon\left(F_i\left(u_i^\varepsilon\right) - \bar{F}_i\left(u_{i,0}\right)\right)\right]. \tag{2.4.29}$$

Rewriting the above information, the function φ_i^ε satisfies the following system:

$$\begin{cases} \mathscr{A}^\varepsilon \varphi_i^\varepsilon = R_i(u^\varepsilon) - \bar{R}_i(u_0) + \varepsilon g_i^\varepsilon, & \text{in } \Omega^\varepsilon, \\ -d_i^\varepsilon \nabla_x \varphi_i^\varepsilon \cdot \mathrm{n} = \varepsilon^2 h_i^\varepsilon \cdot \mathrm{n} + \varepsilon l_i^\varepsilon, & \text{on } \Gamma^\varepsilon, \end{cases} \tag{2.4.30}$$

where we have denoted by

$$\begin{aligned} g_i^\varepsilon :=& -d_i\left(\frac{x}{\varepsilon}\right)\chi_i\left(\frac{x}{\varepsilon}\right)\nabla_x^3 \tilde{u}_{i,0} + d_i\left(\frac{x}{\varepsilon}\right)\theta_i\left(\frac{x}{\varepsilon}\right)\nabla_x^3 \tilde{u}_{i,0} \\ &+ \nabla_y\left(d_i\left(\frac{x}{\varepsilon}\right)\theta_i\left(\frac{x}{\varepsilon}\right)\right)\nabla_x^3 \tilde{u}_{i,0} + \varepsilon d_i\left(\frac{x}{\varepsilon}\right)\theta_i\left(\frac{x}{\varepsilon}\right)\nabla_x^4 \tilde{u}_{i,0}, \\ h_i^\varepsilon :=& d_i\left(\frac{x}{\varepsilon}\right)\theta_i\left(\frac{x}{\varepsilon}\right)\nabla_x^3 \tilde{u}_{i,0}, \\ l_i^\varepsilon :=& a_i\left(\frac{x}{\varepsilon}\right)\left(\tilde{u}_{i,0} - u_i^\varepsilon\right) + b_i\left(\frac{x}{\varepsilon}\right)\left(F_i\left(u_i^\varepsilon\right) - \bar{F}_i\left(\tilde{u}_{i,0}\right)\right). \end{aligned}$$

Now, multiplying the PDE in (3.2.16) by $\varphi_i \in V_\varepsilon$ for $i \in \{1,...,N\}$ and integrating by parts, we get that

$$\begin{aligned} \left\langle d_i^\varepsilon \varphi_i^\varepsilon, \varphi_i \right\rangle_{V^\varepsilon} =& \left\langle R_i(u^\varepsilon) - \bar{R}_i(u_0), \varphi_i \right\rangle_{L^2(\Omega^\varepsilon)} + \varepsilon \left\langle g_i^\varepsilon, \varphi_i \right\rangle_{L^2(\Omega^\varepsilon)} \\ &- \varepsilon \left\langle l_i^\varepsilon, \varphi_i \right\rangle_{L^2(\Gamma^\varepsilon)} - \varepsilon^2 \int_{\Gamma^\varepsilon} h_i^\varepsilon \cdot \mathrm{n} \varphi_i dS_\varepsilon. \end{aligned} \tag{2.4.31}$$

To guarantee all the derivatives appearing in g_i^ε (up to higher order correctors), $\tilde{u}_{i,0}$, which is the solution to (2.4.17), needs to be smooth enough, says $L^\infty(\Omega)$ (cf. [3]), and the cell functions χ_i and θ_i to (2.4.12) and (2.4.21), respectively, belong at least to $H_\#^1(Y_1)$ as derived above. Consequently, it allows us to estimate g_i^ε by an ε-independent constant, i.e.

$$\left\| g_i^\varepsilon \right\|_{L^2(\Omega^\varepsilon)} \le C \quad \text{for all } i \in \{1,...,N\}. \tag{2.4.32}$$

Furthermore, it is easy to estimate the integral including h_i^ε in (3.2.17) by the following (see, e.g. [31]):

$$\int_{\Gamma^\varepsilon} h_i^\varepsilon \cdot \mathrm{n} dS_\varepsilon \approx C\varepsilon^{-1},$$

which leads to

$$\left\| h_i^\varepsilon \cdot \mathrm{n} \right\|_{L^2(\Gamma^\varepsilon)} \leq C\varepsilon^{-1/2}. \tag{2.4.33}$$

Now, it remains to estimate the third integral in (3.2.17). Thanks to (A_2) and (2.4.6), we may have

$$\left| \left\langle l_i^\varepsilon, \varphi_i \right\rangle_{L^2(\Gamma^\varepsilon)} \right| \leq C\left(1+\bar{K}_i\right) \left\| u_i^\varepsilon - \tilde{u}_{i,0} \right\|_{L^2(\Gamma^\varepsilon)} \|\varphi_i\|_{L^2(\Gamma^\varepsilon)}. \tag{2.4.34}$$

In the same vein, we get

$$\left| \left\langle R_i(u^\varepsilon) - \bar{R}_i(u_0), \varphi_i \right\rangle_{L^2(\Omega^\varepsilon)} \right| \leq C\bar{L}_i \|u^\varepsilon - \tilde{u}_0\|_{\mathscr{V}^\varepsilon} \|\varphi_i\|_{L^2(\Omega^\varepsilon)}. \tag{2.4.35}$$

Combining (3.2.17)-(2.4.35) with (A_1) and putting $\bar{L} := \max\left\{\bar{L}_1, ..., \bar{L}_N\right\}$ and $\bar{K} := 1 + \max\left\{\bar{K}_1, ..., \bar{K}_N\right\}$, we are led to the estimate:

$$\begin{aligned} \alpha \sum_{i=1}^N \left| \left\langle \varphi_i^\varepsilon, \varphi_i \right\rangle_{V^\varepsilon} \right| &\leq C\left(\bar{L}\|u^\varepsilon - \tilde{u}_0\|_{\mathscr{V}^\varepsilon} + \varepsilon\right) \|\varphi\|_{\mathscr{V}^\varepsilon} \\ &\quad + C\left(\bar{K}\varepsilon \|u^\varepsilon - \tilde{u}_0\|_{\mathscr{H}(\Gamma^\varepsilon)} + \varepsilon^{3/2}\right) \|\varphi\|_{\mathscr{H}(\Gamma^\varepsilon)} \\ &\leq C\left(\varepsilon + \varepsilon^{1/2}\right) \|\varphi\|_{\mathscr{V}^\varepsilon} \leq C\varepsilon^{1/2} \|\varphi\|_{\mathscr{V}^\varepsilon}, \end{aligned} \tag{2.4.36}$$

where we have made use of the trace inequality $\|\varphi\|_{\mathscr{H}(\Gamma^\varepsilon)} \leq C\varepsilon^{-1/2} \|\varphi\|_{\mathscr{V}^\varepsilon}$ (cf. Lemma A.0.8) and the Poincaré inequality $\|\varphi\|_{\mathscr{H}(\Omega^\varepsilon)} \leq C \|\varphi\|_{\mathscr{V}^\varepsilon}$.
Recall that our aim is to estimate $\|\Psi^\varepsilon\|_{\mathscr{V}^\varepsilon}$, it remains to control the following term:

$$\left\langle (1-m^\varepsilon)\left(\varepsilon u_{i,1} + \varepsilon^2 u_{i,2}\right), \varphi_i \right\rangle_{V^\varepsilon} \text{ for } \varphi_i \in V^\varepsilon.$$

In fact, one easily has that

$$\begin{aligned} \sum_{i=1}^N \left| \left\langle (1-m^\varepsilon)\left(\varepsilon u_{i,1} + \varepsilon^2 u_{i,2}\right), \varphi_i \right\rangle_{V^\varepsilon} \right| &\leq C\varepsilon \|\nabla(1-m^\varepsilon)\|_{\mathscr{H}(\Omega^\varepsilon)} \|\varphi\|_{\mathscr{V}^\varepsilon} \\ &\quad + C\left\| (1-m^\varepsilon)\nabla\left(\varepsilon u_1 + \varepsilon^2 u_2\right) \right\|_{\mathscr{H}(\Omega^\varepsilon)} \|\varphi\|_{\mathscr{V}^\varepsilon} \\ &\leq C\left(\varepsilon^{1/2} + \varepsilon^{3/2}\right) \|\varphi\|_{\mathscr{V}^\varepsilon} \leq C\varepsilon^{1/2} \|\varphi\|_{\mathscr{V}^\varepsilon}, \end{aligned} \tag{2.4.37}$$

where we have used

$$\|\nabla(1-m^\varepsilon)\|^2_{\mathscr{H}(\Omega^\varepsilon)} \leq N\left(\int_{\Omega^\varepsilon \cap \{x | \mathrm{dist}(x,\Gamma) \leq 2\varepsilon\}} |\nabla m^\varepsilon|^2 dx\right) \leq C\varepsilon^{-1},$$

$$\left\| (1-m^\varepsilon)\nabla\left(\varepsilon u_1 + \varepsilon^2 u_2\right) \right\|^2_{\mathscr{H}(\Omega^\varepsilon)} \leq N\varepsilon^2 |\Omega^\varepsilon| \int_{\Omega^\varepsilon \cap \{x | \mathrm{dist}(x,\Gamma) \leq 2\varepsilon\}} |\nabla m^\varepsilon|^2 dx \leq C\varepsilon^3.$$

Hence, by using the triangle inequality in (2.4.36) and (2.4.37) it yields that

$$\sum_{i=1}^N \left| \left\langle \Psi_i^\varepsilon, \varphi_i \right\rangle_{V^\varepsilon} \right| \leq C\varepsilon^{1/2} \|\varphi\|_{\mathscr{V}^\varepsilon},$$

which finally leads to

$$\|\Psi^\varepsilon\|_{\mathscr{V}^\varepsilon} \leq C\varepsilon^{1/2},$$

by choosing $\varphi = \Psi^\varepsilon$.
All in all, we can now state of the following theorem.

Theorem 2.4.1. *Let u^ε be the solution of the elliptic system (P^ε) with assumptions (A_1)-(A_3) and* (3.2.8)-(2.4.6) *up to $M = 2$. Suppose the unique pair $(u_0, u_m) \in \mathscr{W}^\infty(\Omega) \times \mathscr{W}^\infty\left(\Omega; H^1_\#(Y_1)/\mathbb{R}\right)$ for $m \in \{1,2\}$. The following corrector with second order for the homogenization limit holds:*

$$\left\|u^\varepsilon - u_0 - m^\varepsilon\left(\varepsilon u_1 + \varepsilon^2 u_2\right)\right\|_{\mathscr{V}^\varepsilon} \leq C\varepsilon^{1/2},$$

where u_0, u_1 and u_2 are vectors whose elements are defined by (2.4.10), (2.4.11) *and* (2.4.20), *respectively.*

2.5 Discussion

In real-world applications, the nonlinear reaction term R_i is often locally Lipschitz. However, relying on Lemma 2.3.3 the L^∞-type estimate of the positive solution makes the nonlinearity globally Lipschitz. The telling example can be seen through the mass action kinetic deterministic model of the simplest autocatalytic reaction $X_1 + X_2 \rightleftharpoons 2X_1$, which implies $N = 2$ species with the rates $R_1(u_1, u_2) = u_1u_2 - u_1^2 = -R_2(u_1, u_2)$. Considering the first rate R_1 for simplicity, we have

$$|R_1(u_1,u_2) - R_1(v_1,v_2)| \leq \max\left\{\|u_2\|_{L^\infty}, \|u_1\|_{L^\infty} + \|v_1\|_{L^\infty}\right\}(|u_1 - v_1| + |u_2 - v_2|).$$

In addition, for $M = 1$ we compute that

$$R_1\left(u_{1,0} + \varepsilon u_{1,1}, u_{2,0} + \varepsilon u_{2,1}\right) = u_{1,0}u_{2,0} + \varepsilon\left(u_{1,1}u_{2,0} + u_{1,0}u_{2,1} - 2u_{1,0}u_{1,1}\right) + \mathscr{O}\left(\varepsilon^2\right). \quad (2.5.1)$$

Consequently, it follows from (2.5.1) that

$$R_1\left(\sum_{m\in\{0,1\}} \varepsilon^m u_{1,m}, \sum_{m\in\{0,1\}} \varepsilon^m u_{2,m}\right) = \sum_{m\in\{0,1\}} \varepsilon^m\left[(1-m)u_{1,0}u_{2,0} + m\left(u_{1,1}u_{2,0} + u_{1,0}u_{2,1} - 2u_{1,0}u_{1,1}\right)\right] + \mathscr{O}\left(\varepsilon^2\right).$$

which implies $\bar{R}_1 := (1-m)u_{1,0}u_{2,0} + m\left(u_{1,1}u_{2,0} + u_{1,0}u_{2,1} - 2u_{1,0}u_{1,1}\right)$.
If $u_{i,m}, v_{i,m} \in L^\infty(\Omega)$ for all i, m, we thus arrive at

$$\left|\bar{R}_1\left(u_{1,0}, u_{1,1}, u_{2,0}, u_{2,1}\right) - \bar{R}_1\left(v_{1,0}, v_{1,1}, v_{2,0}, v_{2,1}\right)\right| \leq L_1 \sum_{m\in\{0,1\}, i\in\{1,2\}} \left|u_{i,m} - v_{i,m}\right|,$$

where we compute that

$$L_1 = 4\max\left\{\left\|u_{2,0}\right\|_{L^\infty(\Omega)}, \left\|v_{1,0}\right\|_{L^\infty(\Omega)}, \left\|v_{1,1}\right\|_{L^\infty(\Omega)}, \left\|v_{2,1}\right\|_{L^\infty(\Omega)}, \left\|u_{1,0}\right\|_{L(\Omega^\varepsilon)}, 1\right\}.$$

A similar discussion for the nonlinear surface rates F_i. In particular, note that that if L^∞ bounds are available (up to the boundary) then also the exponential function $F(u) = e^u$ can be treated conveniently.

We may repeat the homogenization procedure by the auxiliary problems (3.2.9)-(3.2.11) to obtain not only the general expansion of the concentrations and corresponding problems, but also the higher order of corrector estimate due to the $\tilde{u}_0$-based construction of u_m. Taking the M-level expansion (3.2.3) into consideration, the general corrector can be found easily. Indeed, by induction we have from (2.4.28) that for $x \in \Omega^\varepsilon$

$$\begin{aligned}
\mathscr{A}^\varepsilon \varphi_i^\varepsilon &= \mathscr{A}^\varepsilon u_i^\varepsilon - \varepsilon^{-2}\mathscr{A}_0 u_{i,0} - \varepsilon^{-1}\left(\mathscr{A}_0 u_{i,1} + \mathscr{A}_1 u_{i,0}\right) \\
&- \sum_{m=0}^{M-2} \varepsilon^m \left(\mathscr{A}_0 u_{i,m+2} + \mathscr{A}_1 u_{i,m+1} + \mathscr{A}_2 u_{i,m}\right) \\
&- \varepsilon^{M-1}\left(\mathscr{A}_1 u_{i,M} + \mathscr{A}_2 u_{i,M-1}\right) - \varepsilon^M \mathscr{A}_2 u_{i,M} \\
&= R_i\left(u^\varepsilon\right) - \sum_{m=0}^{M-2} \varepsilon^m \bar{R}_i\left(u_m\right) - \varepsilon^{M-1}\left(\mathscr{A}_1 u_{i,M} + \mathscr{A}_2 u_{i,M-1}\right) - \varepsilon^M \mathscr{A}_2 u_{i,M},
\end{aligned}$$

while (2.4.29) becomes

$$-d_i^\varepsilon \nabla_x \varphi_i^\varepsilon \cdot \mathrm{n} = \varepsilon^M d_i^\varepsilon \nabla_x u_{i,M} + \varepsilon\left[a_i^\varepsilon\left(\sum_{m=0}^{M-2}\varepsilon^m u_{i,m} - u_i^\varepsilon\right) + b_i^\varepsilon\left(F\left(u_i^\varepsilon\right) - \sum_{m=0}^{M-2}\varepsilon^m \bar{F}\left(u_{i,m}\right)\right)\right].$$

Thanks to the assumptions (3.2.8) and (2.4.6), we are totally in a position to prove the generalization of Theorem 2.4.1. Since we just need to follow the above procedure, we shall give the following theorem while skipping the proof.

Theorem 2.5.1. *Let u^ε be the solution of the elliptic system (P^ε) with assumptions (A_1)-(A_3) and (3.2.8)-(2.4.6) up to M-level of expansion. Suppose that the unique pair $(u_0, u_m) \in \mathscr{W}^\infty(\Omega^\varepsilon) \times \mathscr{W}^\infty\left(\Omega^\varepsilon; H^1_\#(Y_1)/\mathbb{R}\right)$ for all $0 \le m \le M$. The following correctors for the homogenization limit hold:*

$$\left\| u^\varepsilon - \sum_{m=0}^{M} \varepsilon^m u_m \right\|_{\mathscr{V}^\varepsilon} \le C\varepsilon^{M-1},$$

$$\left\| u^\varepsilon - u_0 - m^\varepsilon \sum_{m=1}^{M} \varepsilon^m u_m \right\|_{\mathscr{V}^\varepsilon} \le C \sum_{m=1}^{M} \varepsilon^{m-1/2}.$$

2.6 Concluding remarks

In this chapter, we have proved results on the weak solvability and homogenization of a microscopic semi-linear elliptic system posed in perforated media. The model presented in this chapter explores the interplay between stationary diffusion and both surface and volume chemical reactions in porous media. More precisely, we have derived homogenization limits (upscaling) for alike systems and particularly justified rigorously the obtained averaged descriptions. Based on Moser-like iteration techniques with the minimization approach, we have proved the well-posedness of the microscopic problem ensuring also the positivity and boundedness of the involved concentrations. Then, we have used the structure of the formal two-scale expansions and followed energy-like estimates to derive corrector estimates delimitating this way the convergence rate of the asymptotic approximates to the macroscopic limit concentrations.

Let us mention that by the same approach, we can also derive general high-order corrector estimates. We observe, on the other side, that the linearity of the auxiliary problems typically relies on the structure of the reaction term. These results shall be given in Chapter 3 as an extension of this chapter.

It is worth noting that the correctors estimates stated in Theorem 2.4.1 and Theorem 2.5.1 can be improved if one handles the eventual boundary layers occurring due to the presence of the Dirichlet condition $u_i^\varepsilon = 0$ holding across Γ^{ext}. A major gain would be to be able to account for the effect of the presence of the corners on the convergence speed of the homogenization limit. We expect that the working techniques used in [17] are applicable also in our setting; compare to [117] for additional related references on boundary layers correctors, and plan to approach this matter in a forthcoming work.

CHAPTER 3

Notes on semi-linear auxiliary problems and a high-order corrector estimate

3.1 Introduction

This chapter has a two-fold target:

1. to elucidate the cases where auxiliary problems are semi-linear;
2. to derive additional high-order corrector estimates.

Henceforward, this chapter is structured as follows. In Section 3.2, we show that the structure of the volume reaction rate may lead to the semi-linear auxiliary problems. We then present a simple and efficient monotone iterations, based on [92, 71], to derive also the structure of high-order correctors for the homogenization limit. On the other hand, Section 3.3 is devoted to generalizing all aforementioned corrector estimates by the same arguments and techniques. It is worth noting that the domain $\Omega^\varepsilon \subset \mathbb{R}^d$ considered here approximates a porous medium. The precise description of Ω^ε is already showed in [65] and further in Chapter 2. In Figure 2.1 (left), we sketch an admissible geometry of our medium, pointing out the sample micro-structure in Figure 2.1 (right). We also follow the notation from the previous chapter. Finally, we end up with this chapter by Section 3.4 in which some open problems are discussed and provided.

3.2 Derivation of semi-linear auxiliary problems

3.2.1 Problem setting

We are concerned with the study of the semi-linear elliptic boundary-value problem of the form

$$\begin{cases} \mathscr{A}^\varepsilon u^\varepsilon = R(u^\varepsilon), & \text{in } \Omega^\varepsilon, \\ u^\varepsilon = 0, & \text{across } \Gamma^{ext}, \\ \nabla u^\varepsilon \cdot \mathrm{n} = 0, & \text{across } \Gamma^\varepsilon, \end{cases} \tag{3.2.1}$$

where the operator $\mathscr{A}^\varepsilon u^\varepsilon := \nabla\cdot(-d^\varepsilon \nabla u^\varepsilon)$ involves d^ε termed as the molecular diffusion while R represents the volume reaction rate. We take into account the following assumptions:
(A_1) the diffusion coefficient $d^\varepsilon \in L^\infty\left(\mathbb{R}^d\right)$ for $d \in \mathbb{N}$ is Y-periodic and symmetric, and it guarantees the ellipticity of $\mathscr{A}^\varepsilon$ as follows:

$$d^\varepsilon \xi_i \xi_j \geq \alpha |\xi|^2 \quad \text{for any } \xi \in \mathbb{R}^d;$$

(A_2) the reaction coefficient $R \in L^\infty(\Omega^\varepsilon \times \mathbb{R})$ is globally L-Lipschitzian, i.e. there exists $L > 0$ independent of ε such that

$$|R(u) - R(v)| \leq L\,|u - v| \quad \text{for } u, v \in \mathbb{R}.$$

Remark 3.2.1. *Recall that we denote the space V^ε by*

$$V^\varepsilon := \left\{ v \in H^1(\Omega^\varepsilon) | v = 0 \text{ on } \Gamma^{ext} \right\} \tag{3.2.2}$$

endowed with the norm

$$\|v\|_{V^\varepsilon} = \left(\int_{\Omega^\varepsilon} |\nabla v|^2 \, dx \right)^{1/2}.$$

This norm is equivalent (uniformly in the homogenization parameter ε) to the usual H^1 norm by the Poincaré inequality.

3.2.2 Main results

We begin with the Mth-order expansion ($M \geq 2$) which reads

$$u^\varepsilon(x) = \sum_{m=0}^{M} \varepsilon^m u_m(x, y) + \mathscr{O}\left(\varepsilon^{M+1}\right), \quad x \in \Omega^\varepsilon, \tag{3.2.3}$$

where $u_m(x, \cdot)$ is Y-periodic for $0 \leq m \leq M$.
Following standard homogenization procedures, we deduce the so-called auxiliary problems (see e.g. [16]). To do so, we consider the functional $\Phi(x, y)$ depending on two variables: the macroscopic x and $y = x/\varepsilon$ the microscopic presentation, and denote $\Phi^\varepsilon(x) = \Phi(x, y)$. The simple chain rule allows us to derive the fact that

$$\nabla \Phi^\varepsilon(x) = \nabla_x \Phi\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^{-1} \nabla_y \Phi\left(x, \frac{x}{\varepsilon}\right). \tag{3.2.4}$$

The quantities ∇u^ε and $\mathscr{A}^\varepsilon u^\varepsilon$ must be expanded correspondingly. In fact, it follows from (3.2.4) and (3.3.1) that

$$\begin{aligned} \nabla u^\varepsilon &= \left(\nabla_x + \varepsilon^{-1} \nabla_y\right) \left(\sum_{m=0}^{M} \varepsilon^m u_m + \mathscr{O}\left(\varepsilon^{M+1}\right) \right) \\ &= \varepsilon^{-1} \nabla_y u_0 + \sum_{m=0}^{M-1} \varepsilon^m \left(\nabla_x u_m + \nabla_y u_{m+1}\right) + \mathscr{O}\left(\varepsilon^M\right). \end{aligned} \tag{3.2.5}$$

Using the structure of the operator $\mathscr{A}^\varepsilon$, we obtain the following:

$$\begin{aligned} \mathscr{A}^\varepsilon u^\varepsilon = {} & \varepsilon^{-2} \nabla_y \cdot \left(-d(y) \nabla_y u_0\right) \\ & + \varepsilon^{-1} \left[\nabla_x \cdot \left(-d(y) \nabla_y u_0\right) + \nabla_y \cdot \left(-d(y) \left(\nabla_x u_0 + \nabla_y u_1\right)\right) \right] \\ & + \sum_{m=0}^{M-2} \varepsilon^m \left[\nabla_x \cdot \left(-d(y) \left(\nabla_x u_m + \nabla_y u_{m+1}\right)\right) \right. \\ & \left. + \nabla_y \cdot \left(-d(y) \left(\nabla_x u_{m+1} + \nabla_y u_{m+2}\right)\right) \right] + \mathscr{O}\left(\varepsilon^{M-1}\right). \end{aligned} \tag{3.2.6}$$

Concerning the boundary condition at Γ^ε, we note:

$$d^\varepsilon \nabla u^\varepsilon \cdot \mathrm{n} = d_i(y)\left(\varepsilon^{-1}\nabla_y u_0 + \sum_{m=0}^{M-1}\varepsilon^m\left(\nabla_x u_m + \nabla_y u_{m+1}\right)\right)\cdot \mathrm{n}. \tag{3.2.7}$$

From here on, we introduce the following key structure of the reaction term:

$$R\left(\sum_{m=0}^{M}\varepsilon^m u_m\right) = \sum_{m=0}^{M}\varepsilon^{m-r}R(u_m) + \mathscr{O}\left(\varepsilon^{M-r+1}\right) \quad \text{for } r\in\mathbb{Z}, r\le 2. \tag{3.2.8}$$

At this point we see, if $r\in\{1,2\}$ solving nonlinear auxiliary problems is then needed. To see the impediment, let us focus on $r=2$. By collecting the coefficients of the same powers of ε in (3.2.6) and (3.2.7), we are led to the following systems, which we refer to the auxiliary problems:

$$\begin{cases} \mathscr{A}_0 u_0 = R(u_0), & \text{in } Y_1,\\ -d(y)\nabla_y u_0\cdot \mathrm{n} = 0, & \text{on } \partial Y_0,\\ u_0 \text{ is } Y-\text{periodic in } y, \end{cases} \tag{3.2.9}$$

$$\begin{cases} \mathscr{A}_0 u_1 = R(u_1) - \mathscr{A}_1 u_0, & \text{in } Y_1,\\ -d(y)\left(\nabla_x u_0 + \nabla_y u_1\right)\cdot \mathrm{n} = 0, & \text{on } \partial Y_0,\\ u_1 \text{ is } Y-\text{periodic in } y, \end{cases} \tag{3.2.10}$$

$$\begin{cases} \mathscr{A}_0 u_{m+2} = R(u_{m+2}) - \mathscr{A}_1 u_{m+1} - \mathscr{A}_2 u_m, & \text{in } Y_1,\\ -d(y)\left(\nabla_x u_{m+1} + \nabla_y u_{m+2}\right)\cdot \mathrm{n} = 0, & \text{on } \partial Y_0,\\ u_{m+2} \text{ is } Y-\text{periodic in } y, \end{cases} \tag{3.2.11}$$

for $0\le m\le M-2$.
Here, we have denoted

$$\begin{aligned} \mathscr{A}_0 &:= \nabla_y\cdot\left(-d(y)\nabla_y\right),\\ \mathscr{A}_1 &:= \nabla_x\cdot\left(-d(y)\nabla_y\right) + \nabla_y\cdot\left(-d(y)\nabla_x\right),\\ \mathscr{A}_2 &:= \nabla_x\cdot\left(-d(y)\nabla_x\right). \end{aligned} \tag{3.2.12}$$

Remark 3.2.2. *In the case $r\le 0$, it is trivial to not only prove the well-posedness of these auxiliary problems* (3.3.8)-(3.3.10)*, but also to compute the solutions by many approaches due to its linearity. For details, the reader is referred here to [31].*

The idea is now to linearize the auxiliary problems. Inspired by the fact that a fixed-point homogenization argument seems to be applicable in this framework, and also by the way *a priori* error estimates are proven for difference schemes, we suggest an iteration technique to "linearize" the involved PDE systems. We start the procedure by choosing the initial point $u_m^{(0)} = 0$ for $m\in\{0,\dots,M\}$. As next step, we consider the following systems corresponding to the nonlinear auxiliary problems:

$$\begin{cases} \mathscr{A}_0 u_0^{(n_0)} = R\left(u_0^{(n_0-1)}\right), & \text{in } Y_1,\\ -d(y)\nabla_y u_0^{(n_0)}\cdot \mathrm{n} = 0, & \text{on } \partial Y_0,\\ u_0^{(n_0)} \text{ is } Y-\text{periodic in } y, \end{cases} \tag{3.2.13}$$

$$\begin{cases} \mathscr{A}_0 u_1^{(n_1)} = R\left(u_1^{(n_1-1)}\right) - \mathscr{A}_1 u_0^{(n_0)}, & \text{in } Y_1, \\ -d(y)\left(\nabla_x u_0^{(n_0)} + \nabla_y u_1^{(n_1)}\right)\cdot \mathrm{n} = 0, & \text{on } \partial Y_0, \\ u_1^{(n_1)} \text{ is } Y-\text{periodic in } y, \end{cases} \tag{3.2.14}$$

$$\begin{cases} \mathscr{A}_0 u_{m+2}^{(n_{m+2})} = R\left(u_{m+2}^{(n_{m+2}-1)}\right) - \mathscr{A}_1 u_{m+1}^{(n_{m+1})} - \mathscr{A}_2 u_m^{(n_m)}, & \text{in } Y_1, \\ -d(y)\left(\nabla_x u_{m+1}^{(n_{m+1})} + \nabla_y u_{m+2}^{(n_{m+2})}\right)\cdot \mathrm{n} = 0, & \text{on } \partial Y_0, \\ u_{m+2}^{(n_{m+2})} \text{ is } Y-\text{periodic in } y, \end{cases} \tag{3.2.15}$$

for $0 \le m \le M-2$. Note that the quantity n_m is independent of ε.
Since the approximate auxiliary problems became linear, standard procedures are able to find the solutions $u_m^{(n_m)}$ for $0 \le m \le M$. Note that these problems admit a unique solution (see, e.g. [31, Lemma 2.2]) on V, i.e. the quotient space of V_{Y_1} defined by

$$V_{Y_1} := \left\{\varphi | \varphi \in H^1(Y_1), \varphi \text{ is } Y-\text{periodic}\right\}.$$

If $\kappa_p := C_p L \alpha^{-1} < 1$ holds (here C_p is the Poincaré constant depending only on the dimension of Y_1), then we easily obtain that for every m, $\left\{u_m^{(n_m)}\right\}$ is a Cauchy sequence in $H^1(Y_1)$. Hereby, it naturally claims the existence and uniqueness of the nonlinear auxiliary problems (3.3.8)-(3.3.10). Moreover, the convergence rate of the iteration procedure is given by

$$\left\|u_m^{(n_m)} - u_m\right\|_{H^1(Y_1)} \le \frac{\kappa_p^{n_m}}{1-\kappa_p^{n_m}} \left\|u_m^{(1)}\right\|_{H^1(Y_1)}.$$

For more details in this sense, see [71, Theorem 2.2].
To prove the corrector estimate, we suppose that the solutions of the auxiliary problems (3.3.8)-(3.3.10) belong to the space $L^\infty(\Omega^\varepsilon; V)$. Let us introduce the following function:

$$\varphi^\varepsilon := u^\varepsilon - \sum_{m=0}^{M} \varepsilon^m u_m.$$

Relying on the auxiliary problems (3.3.8)-(3.3.10), note that the function φ^ε satisfies the following system:

$$\begin{cases} \mathscr{A}^\varepsilon \varphi^\varepsilon = R(u^\varepsilon) - \sum_{m=0}^{M-2} \varepsilon^{m-2} R(u_m) \\ \qquad\qquad -\varepsilon^{M-1}\left(\mathscr{A}_1 u_M + \mathscr{A}_2 u_{M-1}\right) - \varepsilon^M \mathscr{A}_2 u_M, & \text{in } \Omega^\varepsilon, \\ -d^\varepsilon \nabla_x \varphi^\varepsilon \cdot \mathrm{n} = \varepsilon^M d^\varepsilon \nabla_x u_M \cdot \mathrm{n}, & \text{on } \Gamma^\varepsilon. \end{cases} \tag{3.2.16}$$

Now, multiplying the PDE in (3.2.16) by $\varphi \in V^\varepsilon$ and integrating by parts, we arrive at

$$\begin{aligned} \langle d^\varepsilon \varphi^\varepsilon, \varphi\rangle_{V^\varepsilon} = &\left\langle R(u^\varepsilon) - \sum_{m=0}^{M-2} \varepsilon^{m-2} R(u_m), \varphi \right\rangle_{L^2(\Omega^\varepsilon)} \\ &- \varepsilon^{M-1}\left\langle \mathscr{A}_1 u_M + \mathscr{A}_2 u_{M-1} + \varepsilon \mathscr{A}_2 u_M, \varphi\right\rangle_{L^2(\Omega^\varepsilon)} \\ &- \varepsilon^M \int_{\Gamma^\varepsilon} d^\varepsilon \nabla_x u_M \cdot \mathrm{n} \varphi \, dS_\varepsilon. \end{aligned} \tag{3.2.17}$$

From here on, we estimate the integrals on the right-hand side of (3.3.13), which is a standard procedure; see [31] for similar calculations. Thus, we claim that

$$\left|\left\langle R(u^\varepsilon)-\sum_{m=0}^{M-2}\varepsilon^{m-2}R(u_m),\varphi\right\rangle_{L^2(\Omega^\varepsilon)}\right|\leq CL\left\|u^\varepsilon-\sum_{m=0}^{M}\varepsilon^m u_m+\mathscr{O}\left(\varepsilon^{M-1}\right)\right\|_{V^\varepsilon}\|\varphi\|_{L^2(\Omega^\varepsilon)}, \tag{3.2.18}$$

where we have essentially used the global Lipschitz condition on the reaction term, the assumption (3.2.8), and the Poincaré inequality (cf. Lemma **??**). Next, we get

$$\varepsilon^{M-1}\left|\langle\mathscr{A}_1u_M+\mathscr{A}_2u_{M-1}+\varepsilon\mathscr{A}_2u_M,\varphi\rangle_{L^2(\Omega^\varepsilon)}\right|\leq C\varepsilon^{M-1}\|\varphi\|_{L^2(\Omega^\varepsilon)}, \tag{3.2.19}$$

while using the trace inequality (cf. Lemma A.0.8) to deal with the the last integral, it gives

$$\varepsilon^M\left|\int_{\Gamma^\varepsilon}d^\varepsilon\nabla_x u_M\cdot\mathrm{n}\varphi dS_\varepsilon\right|\leq C\varepsilon^{M-1}\|\varphi\|_{L^2(\Omega^\varepsilon)}. \tag{3.2.20}$$

Combining (3.3.14)-(3.3.17), we provide that

$$\alpha\left|\langle\varphi^\varepsilon,\varphi\rangle_{V^\varepsilon}\right|\leq C\varepsilon^{M-1}\|\varphi\|_{L^2(\Omega^\varepsilon)},$$

which finally leads to $\|\varphi^\varepsilon\|_{V^\varepsilon}\leq C\varepsilon^{M-1}$ by choosing $\varphi=\varphi^\varepsilon$, very much in the spirit of energy estimates.
Ultimately, we state our results in the frame of the following theorems.

Theorem 3.2.3. *Suppose* (3.2.8) *holds for* $r\in\{1,2\}$ *and assume* $\kappa_p:=C_pL\alpha^{-1}<1$ *for the given Poincaré constant. Let* $\left\{u_m^{(n_m)}\right\}_{n_m\in\mathbb{N}}$ *be the schemes that approximate the nonlinear auxiliary problems* (3.2.13)-(3.2.15). *Then* (3.2.13)-(3.2.15) *admit a unique solution* u_m *for all* $m\in\{0,...,M\}$ *with the speed of convergence:*

$$\left\|u_m^{(n_m)}-u_m\right\|_{H^1(Y_1)}\leq\frac{C\kappa_p^n}{1-\kappa_p^n}\text{ for all }n_m\in\mathbb{N}\text{ and }m\in\{0,...,M\},$$

where $C>0$ *is a generic* ε*-independent constant and* $n:=\max\{n_0,...,n_M\}$.

Theorem 3.2.4. *Let* u^ε *be the solution of the elliptic system* (3.2.1) *with the assumptions* (A_1)-(A_2) *stated above and suppose that* (3.2.8) *holds for* $r\in\{1,2\}$. *For* $m\in\{0,\ldots,M\}$ *with* $M\geq 2$, *we consider* u_m *the solutions of the auxiliary problems* (3.2.13)-(3.2.15). *Then we obtain the following corrector estimate:*

$$\left\|u^\varepsilon-\sum_{m=0}^{M}\varepsilon^m u_m\right\|_{V^\varepsilon}\leq C\varepsilon^{M-1},$$

where $C>0$ *is a generic* ε*-independent constant.*

Remark 3.2.5. *If the Lipschitz constant* L *depends on the homogenization parameter* ε *for a given order of* $\mathscr{O}(\varepsilon^q)$, $q\in\mathbb{R}$, *then the same result can be obtained. In fact, such a constant only appears in* (3.3.14). *Then an increase in the order* M *of the expansion is necessary to guarantee the convergence when* q *is negative. Note that, the more the order* M *is exploited, the more complicated becomes the computation procedure. On the other hand, such* M*-dependence broadens the applicability of our approach. For instance, a simple example having an* ε*-dependent* L *and satisfying* (3.2.8) *is* $R(u)=\varepsilon^{-1}u$. *Here one has* $L=\varepsilon^{-1}$ *and* $r=1$, *and hence, with* $M\geq 3$ *the corrector estimate is of the order* $\mathscr{O}\left(\varepsilon^{M-2}\right)$.

Remark 3.2.6. *An improved version of the above iterations can be proposed by adding a stabilization term. For example, if the quantity* $L_s\left(u_0^{(n_0)}-u_0^{(n_0-1)}\right)$ *(with* L_s *being a free-to-choose positive number) is inserted into the right-hand side of the PDE of the auxiliary problem* (3.2.13)*, we are led to a new mild restriction* $(L+L_s)\,C_p/\min\{\alpha,L_s\}<1$.

Remark 3.2.7. *The structural condition* (3.2.8) *must be viewed here as a prototype. Modifying it accordingly allows the treatment of many classes of reaction rates, including those mentioned in [63, 94, 96]. Note that although in many multiscale problems the impediment* $r\in\{1,2\}$ *is not present, the high-order corrector (as well as the technicalities coming with its derivation) are still available. It is worth noting that extensions can also include Arrhenius-like laws (i.e. exponential rates of the type* $R(u)=e^{|u|}$*). The control of the oscillations can be then done in terms of the elementary inequality* $\left|e^a-e^b\right|\le\max\left\{e^a\,|a-b|\,,e^b\,|a-b|\right\}$*, for* $a,b\ge 0$*, provided* L^∞*-bounds on the solution are available.*

3.3 A high-order corrector estimate

3.3.1 Problem setting

Recalling the macroscopic elliptic system we have considered in Chapter 2, i.e.

$$\mathscr{A}^\varepsilon u_i^\varepsilon\equiv\nabla\cdot\left(-d_i^\varepsilon\nabla u_i^\varepsilon\right)=R_i\left(u_1^\varepsilon,...,u_N^\varepsilon\right)\quad\text{in }\Omega^\varepsilon,$$

associated with the boundary conditions

$$d_i^\varepsilon\nabla u_i^\varepsilon\cdot\mathrm{n}=\varepsilon\left(a_i^\varepsilon u_i^\varepsilon-b_i^\varepsilon F_i\left(u_i^\varepsilon\right)\right)\quad\text{across }\Gamma^\varepsilon,$$

$$u_i^\varepsilon=0\quad\text{across }\Gamma^{ext},$$

for $i\in\{1,...,N\}$ with $N\ge 2$ being the number of involved concentrations. For simplicity, we once again refer to this problem as (P^ε).
This problem is connected to the Smoluchowski-Soret-Dufour modeling of the evolution of temperature and colloid concentrations [34, 75]. Here, $u^\varepsilon:=\left(u_1^\varepsilon,...,u_N^\varepsilon\right)$ denotes the vector of the concentrations, d_i^ε represents the molecular diffusion with R_i being the volume reaction rate and a_i^ε, b_i^ε are deposition coefficients, whilst F_i indicates a surface chemical reaction for the immobile species. Notice that the quantity ε is called the homogenization parameter or the scale factor. Denote by $x\in\Omega^\varepsilon$ the macroscopic variable and by $y=x/\varepsilon$ the microscopic variable representing high oscillations at the microscopic geometry. Henceforward, we understand throughout this subsection the following convention:

$$d_i^\varepsilon(x)=d_i\left(\frac{x}{\varepsilon}\right)=d_i(y),\quad x\in\Omega^\varepsilon,y\in Y_1,$$

with the same meaning for all the oscillating data such as a_i^ε, b_i^ε, e.g.
Our above-mentioned corrector estimate evaluation starts from the two--scale asymptotic expansion up to Mth-level ($M\ge 2$) given by

$$u_i^\varepsilon(x)=\sum_{m=0}^{M}\varepsilon^m u_{i,m}(x,y)+\mathscr{O}\left(\varepsilon^{M+1}\right),\quad x\in\Omega^\varepsilon,\tag{3.3.1}$$

where $u_{i,m}(x,\cdot)$ is Y-periodic for $0\le m\le M$ and $i\in\{1,...,N\}$.

It is worth noting that in Chapter 2, we have analyzed the solvability of (P^ε) using the energy minimization approach and derived the upscaled equations as well as the corresponding effective coefficients. Furthermore, we showed that using the separation of variables, the functions $u_{i,m}(x,y)$ for $0 \le m \le M$ can be structured as, e.g.

$$\begin{aligned} u_{i,0}(x,y) &= \tilde{u}_{i,0}(x), \\ u_{i,1}(x,y) &= -\chi_{i,1}(y) \cdot \nabla_x \tilde{u}_{i,0}(x), \\ u_{i,2}(x,y) &= \chi_{i,2}(y) \nabla_x^2 \tilde{u}_{i,0}(x), \end{aligned}$$

with $\tilde{u}_{i,0}(x)$ being determined uniquely from the auxiliary problem and $\chi_{i,m}$ satisfy the corresponding cell problems. One can also rule out the $\tilde{u}_{i,0}$-based construction of $u_{i,m}$ that $u_{i,m}(x,y) = (-1)^m \chi_{i,m}(y) \nabla_x^m \tilde{u}_{i,0}(x)$ for $1 \le m \le M$.
In this scenario, we wish to obtain the error estimate up to a high-order expansion for the differences of concentrations and their gradients, albeit some types have been investigated so far. In particular, we prove in this part a corrector in the form of

$$u^\varepsilon - \sum_{k=0}^{K} \varepsilon^k u_k - m^\varepsilon \sum_{m=K+1}^{M} \varepsilon^m u_m, \tag{3.3.2}$$

in which we fix $K \in \mathbb{N}$ such that $0 \le K \le M-2$ and $m^\varepsilon \in C_c^\infty(\Omega)$ is a cut-off function such that $\varepsilon |\nabla m^\varepsilon| \le C$ and

$$m^\varepsilon(x) := \begin{cases} 0, & \text{if } \operatorname{dist}(x,\Gamma) \le \varepsilon, \\ 1, & \text{if } \operatorname{dist}(x,\Gamma) \ge 2\varepsilon, \end{cases}$$

(see [31] for more properties of m^ε).
With the above definition of m^ε, the second term in (3.3.2) vanishes everywhere except in a neighborhood of the boundary of Ω^ε. In other words, the appearance of m^ε provides that the speed of convergence in the interior of the material is better than the rate at the vicinity of the boundary, albeit the standard result expected that $\|u^\varepsilon - u_0\|_{H^1(\Omega^\varepsilon)} \le C\varepsilon^{1/2}$. It is then easy to see that (3.3.2) includes the cases

$$u^\varepsilon - \sum_{m=0}^{M} \varepsilon^m u_m \quad \text{and} \quad u^\varepsilon - u_0 - m^\varepsilon \sum_{m=1}^{M} \varepsilon^m u_m, \quad M \ge 2,$$

reported in Theorem 2.5.1 and further in [31].
The similarity between Theorem 3.3.1 and Theorem 2.5.1 in Chapter 2 is that under the energy-type method, we employ the cut-off function m^ε to distinguish the speeds of convergence in H^1-norm of the limit u_0 in the interior part of the perforated material and at the boundary of inclusions. The main difference consists in showing that if $K = M-2$, the corrector (3.3.5) yields the order of $\mathcal{O}(\varepsilon^{M-\frac{3}{2}})$, whilst it only gives the order $\mathcal{O}(\varepsilon^{\frac{1}{2}})$ in Theorem 2.5.1.
Further comments can be found in Remark 3.3.2 and Remark 3.3.3, discussing the *a priori* assumptions on the smoothness of the limit u_0 and on the structure of the cell problems for arbitrarily high-order correctors.
With V^ε postulated in (3.2.2), we define $\mathscr{V}^\varepsilon := V^\varepsilon \times \ldots \times V^\varepsilon$ as well as some other function spaces such as $\mathscr{W}^{p,q}(\Omega^\varepsilon) := W^{p,q}(\Omega^\varepsilon) \times \ldots \times W^{p,q}(\Omega^\varepsilon)$ the Sobolev space of functions with index of differentiability $p \in \mathbb{N}$ and integrability q and $\mathscr{W}^q(\Omega^\varepsilon) := L^q(\Omega^\varepsilon) \times \ldots \times L^q(\Omega^\varepsilon)$ for $q \in (2,\infty]$.

To handle the corrector estimates, we need the following assumptions:
(A_1) The diffusion coefficient $d_i^\varepsilon \in L^\infty\left(\mathbb{R}^d\right)$ is Lipschitz and Y-periodic, and there exists a positive constant α_i such that

$$d_i(y)\,\xi_i\xi_j \geq \alpha_i\,|\xi|^2 \quad \text{for any } \xi \in \mathbb{R}^d.$$

(A_2) The deposition coefficients $a_i^\varepsilon, b_i^\varepsilon \in L^\infty(\Gamma^\varepsilon)$ are positive and Y-periodic.
(A_3) The reaction rates $R_i : \Omega^\varepsilon \times [0,\infty)^N \to \mathbb{R}$ and $F_i : \Gamma^\varepsilon \times [0,\infty) \to \mathbb{R}$ are Carathéodory functions. Moreover, they satisfy the structural assumptions:

$$R_i\left(\sum_{m=0}^{M}\varepsilon^m u_{1,m},\ldots,\sum_{m=0}^{M}\varepsilon^m u_{N,m}\right) = \sum_{m=0}^{M}\varepsilon^m \bar{R}_i\left(u_{1,m},\ldots,u_{N,m}\right) + \mathscr{O}\left(\varepsilon^{M+1}\right), \tag{3.3.3}$$

$$F_i\left(\sum_{m=0}^{M}\varepsilon^m u_{i,m}\right) = \sum_{m=0}^{M}\varepsilon^m \bar{F}_i\left(u_{i,m}\right) + \mathscr{O}\left(\varepsilon^{M+1}\right), \tag{3.3.4}$$

where $\bar{R}_i$ and $\bar{F}_i$ are global Lipschitz functions with the Lipschitz constants L_i and K_i for $i \in \{1,\ldots,N\}$, in the sense that

$$\left|\bar{R}_i\left(u_{1,m},\ldots,u_{N,m}\right) - \bar{R}_i\left(v_{1,m},\ldots,v_{N,m}\right)\right| \leq L_i \sum_{i=1}^{N}\left|u_{i,m} - v_{i,m}\right|,$$

$$\left|\bar{F}_i\left(u_{1,m},\ldots,u_{N,m}\right) - \bar{F}_i\left(v_{1,m},\ldots,v_{N,m}\right)\right| \leq K_i \sum_{i=1}^{N}\left|u_{i,m} - v_{i,m}\right|,$$

for every $0 \leq m \leq M$.

3.3.2 Main results

Theorem 3.3.1. *Assume* (A_1)-(A_3) *hold. Let* u^ε *be the vector of solutions of the elliptic system* (P^ε). *Consider the high-order asymptotic expansion* (3.3.1) *up to* M*-level* ($M \geq 2$) *and take* $u_0 \in \mathscr{W}^{M+2,\infty}(\Omega^\varepsilon) \cap \mathscr{W}^{M+1,\infty}(\Gamma^\varepsilon)$ *and* $u_m \in \mathscr{W}^\infty\left(\Omega^\varepsilon; H^1_\#(Y_1)/\mathbb{R}\right)$ *for all* $0 \leq m \leq M$. *For a fixed* $K \in \mathbb{N}$ *such that* $0 \leq K \leq M-2$, *the following corrector estimate holds:*

$$\left\|u^\varepsilon - \sum_{k=0}^{K}\varepsilon^k u_k - m^\varepsilon \sum_{m=K+1}^{M}\varepsilon^m u_m\right\|_{\mathscr{V}^\varepsilon} \leq C\left(\varepsilon^{M-1} + \varepsilon^M + \sum_{m=K+1}^{M}\left(\varepsilon^{m-\frac{1}{2}} + \varepsilon^{m+\frac{1}{2}}\right)\right), \tag{3.3.5}$$

where $C > 0$ *is a generic* ε*-independent constant.*

Proof. Before giving the proof, let us recall the structural inequalities of the cut-off function m^ε. The following useful estimates (cf. [40]) hold true:

$$\|1 - m^\varepsilon\|_{L^2(\Omega^\varepsilon)} \leq C\varepsilon^{1/2}, \quad \varepsilon\,\|\nabla m^\varepsilon\|_{L^2(\Omega^\varepsilon)} \leq C\varepsilon^{1/2}. \tag{3.3.6}$$

To bound from above in terms of ε the quantity (3.3.2), we can reduce the discussion to the corrector at ith concentration which is defined as

$$\Psi_i^\varepsilon := u_i^\varepsilon - \sum_{k=0}^{K}\varepsilon^k u_{i,k} - m^\varepsilon \sum_{m=K+1}^{M}\varepsilon^m u_{i,m} \quad \text{for } i \in \{1,\ldots,N\}.$$

We observe that Ψ_i^ε can be decomposed further as

$$\Psi_i^\varepsilon = \underbrace{u_i^\varepsilon - \sum_{m=0}^{M} \varepsilon^m u_{i,m}}_{\varphi_i^\varepsilon} + \underbrace{(1-m^\varepsilon) \sum_{m=K+1}^{M} \varepsilon^m u_{i,m}}_{\gamma_i^\varepsilon}. \tag{3.3.7}$$

As in Chapter 3, we use the auxiliary problems

$$\begin{cases} \mathscr{A}_0 u_{i,0} = 0, & \text{in } Y_1, \\ -d_i(y) \nabla_y u_{i,0} \cdot \mathrm{n} = 0, & \text{on } \partial Y_0, \\ u_{i,0} \text{ is } Y-\text{periodic in } y, \end{cases} \tag{3.3.8}$$

$$\begin{cases} \mathscr{A}_0 u_{i,1} = -\mathscr{A}_1 u_{i,0}, & \text{in } Y_1, \\ -d_i(y) \left(\nabla_x u_{i,0} + \nabla_y u_{i,1}\right) \cdot \mathrm{n} = 0, & \text{on } \partial Y_0, \\ u_{i,1} \text{ is } Y-\text{periodic in } y, \end{cases} \tag{3.3.9}$$

$$\begin{cases} \mathscr{A}_0 u_{i,m+2} = \bar{R}_i(u_m) - \mathscr{A}_1 u_{i,m+1} - \mathscr{A}_2 u_{i,m}, & \text{in } Y_1, \\ -d_i(y) \left(\nabla_x u_{i,m+1} + \nabla_y u_{i,m+2}\right) \cdot \mathrm{n} = b_i(y) \bar{F}_i\left(u_{i,m}\right) - a_i(y) u_{i,m}, & \text{on } \partial Y_0, \\ u_{i,m+2} \text{ is } Y-\text{periodic in } y, \end{cases} \tag{3.3.10}$$

for $0 \le m \le M-2$.
In (3.3.8)-(3.3.10), the operators $\mathscr{A}_0$, $\mathscr{A}_1$ and $\mathscr{A}_2$ are defined in (3.2.12), respectively.
By induction, one can easily obtain that the first part of decomposition (3.3.7), the function φ_i^ε, satisfies the following equation:

$$\mathscr{A}^\varepsilon \varphi_i^\varepsilon = R_i(u^\varepsilon) - \sum_{m=0}^{M-2} \varepsilon^m \bar{R}_i(u_m) - \varepsilon^{M-1}\left(\mathscr{A}_1 u_{i,M} + \mathscr{A}_2 u_{i,M-1}\right) - \varepsilon^M \mathscr{A}_2 u_{i,M} \quad \text{in } \Omega^\varepsilon, \tag{3.3.11}$$

associated with the following boundary condition at Γ^ε

$$\begin{aligned} -d_i^\varepsilon \nabla_x \varphi_i^\varepsilon \cdot \mathrm{n} &= \varepsilon^M d_i^\varepsilon \nabla_x u_{i,M} \cdot \mathrm{n} \\ &\quad + \varepsilon \left[a_i^\varepsilon \left(\sum_{m=0}^{M-2} \varepsilon^m u_{i,m} - u_i^\varepsilon \right) + b_i^\varepsilon \left(F_i\left(u_i^\varepsilon\right) - \sum_{m=0}^{M-2} \varepsilon^m \bar{F}_i\left(u_{i,m}\right) \right) \right]. \end{aligned} \tag{3.3.12}$$

Multiplying (3.3.11) by $\varphi_i \in V^\varepsilon$, integrating the result by parts, and finally using (3.3.12), we arrive at

$$\begin{aligned} \int_{\Omega^\varepsilon} d_i^\varepsilon \nabla \varphi_i^\varepsilon \cdot \nabla \varphi_i dx &= \left\langle R_i(u^\varepsilon) - \sum_{m=0}^{M-2} \varepsilon^m \bar{R}_i(u_m), \varphi_i \right\rangle_{L^2(\Omega^\varepsilon)} \\ &\quad - \varepsilon^{M-1} \left\langle \mathscr{A}_1 u_{i,M} + \mathscr{A}_2 u_{i,M-1} + \varepsilon \mathscr{A}_2 u_{i,M}, \varphi_i \right\rangle_{L^2(\Omega^\varepsilon)} \\ &\quad - \varepsilon \left\langle a_i^\varepsilon \left(\sum_{m=0}^{M-2} \varepsilon^m u_{i,m} - u_i^\varepsilon \right), \varphi_i \right\rangle_{L^2(\Gamma^\varepsilon)} \\ &\quad - \varepsilon \left\langle b_i^\varepsilon \left(F_i\left(u_i^\varepsilon\right) - \sum_{m=0}^{M-2} \varepsilon^m \bar{F}_i\left(u_{i,m}\right) \right), \varphi_i \right\rangle_{L^2(\Gamma^\varepsilon)} \\ &\quad - \varepsilon^M \int_{\Gamma^\varepsilon} d_i^\varepsilon \nabla_x u_{i,M} \cdot \mathrm{n} \varphi_i dS_\varepsilon. \end{aligned} \tag{3.3.13}$$

We can now gain the first part of the corrector (3.3.5), i.e. we shall estimate each integral (having the same orders of ε) on the right-hand side of (3.3.13), which we denote by $\mathscr{I}_1$, $\mathscr{I}_2$, $\mathscr{I}_3$ and $\mathscr{I}_4$, respectively.
Let $\bar{L} := \max\left\{\bar{L}_1, ..., \bar{L}_N\right\}$. Using the structural assumption (3.3.3) in combination with the inequality $\left\|\bar{R}_i(u_m)\right\|_{L^2(\Omega^\varepsilon)} \leq \bar{L}\left\|u_m\right\|_{\mathscr{W}^2(\Omega^\varepsilon)} + \left\|\bar{R}_i(0)\right\|_{L^2(\Omega^\varepsilon)}$ for all $0 \leq m \leq M$, we see that

$$\begin{aligned}\left|\left\langle R_i(u^\varepsilon) - \sum_{m=0}^{M-2}\varepsilon^m \bar{R}_i(u_m), \varphi_i\right\rangle_{L^2(\Omega^\varepsilon)}\right| &\leq \Big[\varepsilon^{M-1}\left(\bar{L}\left\|u_{M-1}\right\|_{\mathscr{W}^2(\Omega^\varepsilon)} + \left\|\bar{R}_i(0)\right\|_{L^2(\Omega^\varepsilon)}\right)\\ &\quad + \varepsilon^M\left(\bar{L}\left\|u_M\right\|_{\mathscr{W}^2(\Omega^\varepsilon)} + \left\|\bar{R}_i(0)\right\|_{L^2(\Omega^\varepsilon)}\right)\Big]\left\|\varphi_i\right\|_{L^2(\Omega^\varepsilon)}\\ &\leq C\left(\varepsilon^{M-1} + \varepsilon^M\right)\left\|\varphi_i\right\|_{L^2(\Omega^\varepsilon)}. \end{aligned} \tag{3.3.14}$$

Direct computations give

$$\begin{aligned}\mathscr{A}_1 u_{i,M} &= (-1)^{M+1}\left[d_i\left(\frac{x}{\varepsilon}\right)\chi_{i,M}\left(\frac{x}{\varepsilon}\right) + \nabla_y\left(d_i\left(\frac{x}{\varepsilon}\right)\chi_{i,M}\left(\frac{x}{\varepsilon}\right)\right)\right]\nabla_x^{M+1}\tilde{u}_{i,0},\\ \mathscr{A}_2 u_{i,M-1} &= (-1)^M d_i\left(\frac{x}{\varepsilon}\right)\chi_{i,M-1}\left(\frac{x}{\varepsilon}\right)\nabla_x^{M+1}\tilde{u}_{i,0},\\ \mathscr{A}_2 u_{i,M} &= (-1)^{M+1} d_i\left(\frac{x}{\varepsilon}\right)\chi_{i,M}\left(\frac{x}{\varepsilon}\right)\nabla_x^{M+2}\tilde{u}_{i,0}.\end{aligned}$$

Due to $u_{i,0} \in W^{M+2,\infty}(\Omega^\varepsilon)$ and $u_{i,m} \in L^\infty\left(\Omega^\varepsilon; H^1_\#(Y_1)/\mathbb{R}\right)$ for all $0 \leq m \leq M$ in combination with (A_1), the second integral $\mathscr{I}_2$ can be bounded from above by

$$\varepsilon^{M-1}\left|\left\langle \mathscr{A}_1 u_{i,M} + \mathscr{A}_2 u_{i,M-1} + \varepsilon\mathscr{A}_2 u_{i,M}, \varphi_i\right\rangle_{L^2(\Omega^\varepsilon)}\right| \leq C\varepsilon^{M-1}\left\|\varphi_i\right\|_{L^2(\Omega^\varepsilon)}. \tag{3.3.15}$$

Let $\bar{K} := 1 + \max\left\{\bar{K}_1, ..., \bar{K}_N\right\}$. For the integral $\mathscr{I}_3$, we proceed as in the proof of (3.3.14). We thus claim that

$$\begin{aligned}\varepsilon\left|\left\langle a_i^\varepsilon\left(\sum_{m=0}^{M-2}\varepsilon^m u_{i,m} - u_i^\varepsilon\right) + b_i^\varepsilon\left(F_i\left(u_i^\varepsilon\right) - \sum_{m=0}^{M-2}\varepsilon^m \bar{F}_i\left(u_{i,m}\right)\right), \varphi_i\right\rangle_{L^2(\Gamma^\varepsilon)}\right|\\ \leq C\left(\varepsilon^{M-1} + \varepsilon^M\right)\left\|\varphi_i\right\|_{L^2(\Omega^\varepsilon)},\end{aligned} \tag{3.3.16}$$

in which we use (3.3.1) and (3.3.4) together with (A_2) and the Hölder inequality, as well as the trace inequality. On top of that, it yields for the last integral $\mathscr{I}_4$ that

$$\begin{aligned}\varepsilon^M\left|\int_{\Gamma^\varepsilon} d_i^\varepsilon \nabla_x u_{i,M}\cdot \mathrm{n}\varphi_i dS_\varepsilon\right| &\leq \varepsilon^M\left\|d_i^\varepsilon\nabla_x u_{i,M}\cdot\mathrm{n}\right\|_{L^2(\Gamma^\varepsilon)}\left\|\varphi_i\right\|_{L^2(\Gamma^\varepsilon)}\\ &\leq C\varepsilon^{M-1}\left\|\varphi_i\right\|_{L^2(\Omega^\varepsilon)},\end{aligned} \tag{3.3.17}$$

where we follow the computations that $\left\|d_i^\varepsilon\nabla_x u_{i,M}\cdot\mathrm{n}\right\|_{L^2(\Gamma^\varepsilon)} \leq C\varepsilon^{-1/2}$ and apply again the trace inequality.
Combining (3.3.13)-(3.3.17), we observe that

$$\left|\left\langle\varphi_i^\varepsilon, \varphi_i\right\rangle_{V^\varepsilon}\right| \leq C\left(\varepsilon^{M-1} + \varepsilon^M\right)\left\|\varphi_i\right\|_{L^2(\Omega^\varepsilon)} \quad \text{for } \varphi_i \in V^\varepsilon \text{ and } i \in \{1, ..., N\}, \tag{3.3.18}$$

which then leads to $\left\|\varphi_i^\varepsilon\right\|_{V^\varepsilon} \leq C\varepsilon^{M-1}$ by choosing $\varphi_i = \varphi_i^\varepsilon$ for $i \in \{1, ..., N\}$.
It remains to estimate the second part of decomposition (3.3.7). We consider the following quantity:

$$\left\langle\gamma_i^\varepsilon, \varphi_i\right\rangle_{V^\varepsilon} \quad \text{for } \varphi_i \in V^\varepsilon \text{ and } i \in \{1, ..., N\}.$$

At this stage, the following estimate is straightforward due to (3.3.6):

$$\begin{aligned}
\left|\left\langle (1-m^\varepsilon)\sum_{m=K+1}^{M}\varepsilon^m u_{i,m},\varphi_i\right\rangle_{V^\varepsilon}\right| &\le C\left\|\nabla(1-m^\varepsilon)\left(\sum_{m=K+1}^{M}\varepsilon^m u_{i,m}\right)\right\|_{L^2(\Omega^\varepsilon)}\|\varphi_i\|_{V^\varepsilon}\\
&\quad + C\left\|(1-m^\varepsilon)\nabla\left(\sum_{m=K+1}^{M}\varepsilon^m u_{i,m}\right)\right\|_{L^2(\Omega^\varepsilon)}\|\varphi_i\|_{V^\varepsilon}\\
&\le C\sum_{m=K+1}^{M}\varepsilon^m\|\nabla(1-m^\varepsilon)\|_{L^2(\Omega^\varepsilon)}\|\varphi_i\|_{V^\varepsilon}\\
&\quad + C\sum_{m=K+1}^{M}\varepsilon^m\|1-m^\varepsilon\|_{L^2(\Omega^\varepsilon)}\|\varphi_i\|_{V^\varepsilon}\\
&\le C\sum_{m=K+1}^{M}\left(\varepsilon^{m-\frac{1}{2}}+\varepsilon^{m+\frac{1}{2}}\right)\|\varphi_i\|_{V^\varepsilon}\ \text{ for all } \varphi_i\in V^\varepsilon. \quad (3.3.19)
\end{aligned}$$

Thanks to the triangle inequality, we combine (3.3.18) and (3.3.19) to get

$$\left|\left\langle \Psi_i^\varepsilon,\varphi_i\right\rangle_{V^\varepsilon}\right| \le C\left(\varepsilon^{M-1}+\varepsilon^M+\sum_{m=K+1}^{M}\left(\varepsilon^{m-\frac{1}{2}}+\varepsilon^{m+\frac{1}{2}}\right)\right)\|\varphi_i\|_{V^\varepsilon}\quad \text{for } \varphi_i\in V^\varepsilon.$$

By choosing $\varphi_i=\Psi_i^\varepsilon$ and then by simplifying both sides of the resulting estimate by $\left\|\Psi_i^\varepsilon\right\|_{V^\varepsilon}$, we obtain that

$$\left\|\Psi_i^\varepsilon\right\|_{V^\varepsilon}\le C\left(\varepsilon^{M-1}+\varepsilon^M+\sum_{m=K+1}^{M}\left(\varepsilon^{m-\frac{1}{2}}+\varepsilon^{m+\frac{1}{2}}\right)\right).$$

This completes the proof of Theorem 3.3.1. □

Remark 3.3.2. *To obtain high-order corrector estimates, the limit u_0 has to be very smooth as stated e.g. in Theorem* 3.3.1. *The reason is that at the Mth level of expansion, we need ε-independent L^∞-bounds of the terms $\nabla_x^{M+1}\tilde{u}_{i,0}$, $\nabla_x^{M+2}\tilde{u}_{i,0}$ in Ω^ε and of $\nabla_x^M\tilde{u}_{i,M}$ on Γ^ε. To support this approach, recall that u_0 is solution of a homogenized system $\nabla_x\cdot(-q_i\nabla_x u_{i,0})=\bar{R}_i(u_0), i\in\{1,...,N\}$ in which q_i are (positive constant) homogenized coefficients given by*

$$q_i=\frac{1}{|Y_1|}\int_{Y_1}d_i(y)(-\nabla_y\chi_{i,1}+\mathbb{I})dy,$$

while $\mathbb{I}$ stands for the identity matrix. This homogenized system is associated with the zero Dirichlet boundary condition at Γ^{ext} and still satisfies the ellipticity condition.
Note that if we suppose, for simplicity, that $\bar{R}_i$ is linear functions with respect to u_0, then the homogenized system becomes the nonhomogeneous elliptic equation in the vectorial form. Therefore, we can apply the classical results in [3, Theorem 12.4] to guarantee that the derivatives of u_0 up to the desired order are in $L^\infty(\Omega)$. Thus, the needed smoothness of u_0 when dealing with the high-order correctors ($M\ge 2$) is obtainable. This result can be used similarly when we consider the correctors for $u^\varepsilon-u_0$ and $u^\varepsilon-u_0-\varepsilon u_1$ derived from (3.3.2) *with $K=0$ and $K=1$, respectively.*

Remark 3.3.3. *From the high-order auxiliary problems* (3.3.8)-(3.3.10) *and the fact already stated that $u_{i,m}(x,y)=(-1)^m\chi_{i,m}(y)\nabla_x^m\tilde{u}_{i,0}(x)$ for $1\le m\le M$, one can derive the corres-*

ponding cell problems for the high-order corrector:

$$\begin{cases} \mathscr{A}_0 \chi_{i,1} = \nabla_y d_i(y), & \text{in } Y_1, \\ -d_i(y) \nabla_y \chi_{i,1} \cdot n = d_i(y) \cdot n, & \text{on } \partial Y_0, \\ \chi_{i,1} \text{ is } Y-\text{periodic in } y, \end{cases}$$

and

$$\begin{cases} \nabla_y \cdot \left(-d_i(y)\left(\nabla_y \chi_{i,m+2} - \chi_{i,m+1}\right)\right) \nabla_x^{m+2} \tilde{u}_{i,0} \\ = (-1)^m \bar{R}_i \left((-1)^m \chi_{1,m} \nabla_x^m \tilde{u}_{1,0}, \ldots, (-1)^m \chi_{N,m} \nabla_x^m \tilde{u}_{N,0}\right) \\ \qquad -(d_i(y) - \mathbb{I}) \nabla_y \chi_{i,m+1}(y) \nabla_x^{m+2} \tilde{u}_{i,0}, & \text{in } Y_1, \\ -d_i(y)\left(\nabla_y \chi_{i,m+2} - \chi_{i,m+1}\right) \nabla_x^{m+2} \tilde{u}_{i,0} \cdot n \\ = (-1)^m b_i(y) \bar{F}_i \left((-1)^m \chi_{i,m} \nabla_x^m \tilde{u}_{i,0}\right) - a_i(y) \chi_{i,m} \nabla_x^m \tilde{u}_{i,0}, & \text{on } \partial Y_0, \\ \chi_{i,m+2} \text{ is } Y-\text{periodic in } y, \end{cases}$$

where $x \in \Omega$ is viewed here as the involved parameter, while $0 \le m \le M-2$ with $i \in \{1, \ldots, N\}$. Obviously, these problems are linear and ensuring their solvability is standard.
We also remark that from elliptic regularity theory in [103, 56], since Y_1 is a non-convex polygon, the above cell system for $\chi_{i,m}$ only admits a unique solution whose regularity is $H^{1+s}(Y_1)$ for $s \in (-1/2, 1/2)$ (cf. [103]), and we cannot go further from this regularity no matter how smooth the involved terms are. In addition, the non-existence result for this type of problems can be found e.g. in [56, Theorem 14.11].

3.4 Concluding remarks

In Section 3.2, we have shown that the structure of the volume reaction rate affects the structure of the auxiliary problems. In particular, we have focused on the monotone iterations to gain also the high-order homogenization corrector. The single-species model can be adapted to handle more complex scenarios including, for instance, nonlinearities posed at the boundary of perforations. In Section 3.3, a general high-order corrector estimate has been proved in Theorem 2.5.1. In parallel with that, the corresponding cell problems for the high-order corrector are also constructed. Let us remark that the price one has to pay for getting a high-order corrector estimate is very expensive since the structure of the components in the expansion is based on the limit function $\tilde{u}_0$. More precisely, it requires $\tilde{u}_0 \in \mathscr{W}^{M+2,\infty}(\Omega^\varepsilon) \cap \mathscr{W}^{M+1,\infty}(\Gamma^\varepsilon)$ at the Mth order of expansion.
In the near future, we can study the following microscopic system:

$$\begin{cases} \mathscr{A}^\varepsilon u^\varepsilon = \varepsilon^\alpha R(u^\varepsilon) & \text{in } \Omega^\varepsilon, \\ u^\varepsilon = 0 & \text{across } \Gamma^{ext}, \\ \nabla u^\varepsilon \cdot \mathrm{n} = \varepsilon^\beta F(u^\varepsilon) & \text{across } \Gamma^\varepsilon. \end{cases} \tag{3.4.1}$$

This is a semi-linear elliptic Dirichlet-Robin problem sometimes also referred to as a semi-linear elliptic problem with Fourier boundary condition. The parameters α and β represent scaling choices potentially arising in applications with coextensive scales on both the domain and micro-surfaces. The study of (3.4.1) connects e.g. with the works done in [26, 29, 28, 99]. The main difficulty is the presence of arbitrary scaling parameters.

CHAPTER 4

Correctors justification for a Smoluchowski-Soret-Dufour system in perforated domains

4.1 Introduction

Diffusion and heat conduction, taken separately, are well understood processes at a large variety of space scales. However, as soon as diffusion interplays with the conduction of heat, it appears that the structure of the model equations is not so clear as one would expect, especially if one wants to describe settings away from the somewhat better understood thermodynamic equilibrium, where statistical mechanics is the main investigation tool.

Driven by possible applications in the context of efficient drug-delivery and in the design of intelligent packaging materials, we wish to understand mathematically the upscaling of the following basic thermo-diffusion scenario: We look at a population of colloidal particles (monomers) driven by a flux linearly combining Fick and Fourier contributions. We assume that monomers undergo a Smoluchowski-like dynamics producing populations of i-mers that finally meet and travel through a transversal porous membrane. The microscopic boundaries (i.e. those at the level of the membrane pores) are active in the sense that they host adsorption and desorption of clusters of colloidal particles.

The starting PDE model is formulated in [74] by Krehel and his co-authors. Their thermo-diffusion system is posed in a perforated medium with uniform periodicity inside the domain. As main outcome, they prove both the global weak solvability of the model as well as the periodic homogenization limit. As byproduct, they also obtain the precise structure of the effective transport parameters. Now, is the moment to: Justify the two-scale asymptotics by proving corrector/error estimates for the homogenization limit for periodic arrangements of membrane pores/microstructures.

In our context, the structure of the corrector estimate for the involved concentrations and temperature fields we wish to prove is

$$\begin{aligned}\left\|\theta^\varepsilon-\theta_0^\varepsilon\right\|^2_{L^2((0,T)\times\Omega^\varepsilon)}+\left\|u^\varepsilon-u_0^\varepsilon\right\|^2_{L^2((0,T)\times\Omega^\varepsilon)}+\left\|\nabla\left(\theta^\varepsilon-\theta_1^\varepsilon\right)\right\|^2_{L^2((0,T)\times\Omega^\varepsilon)}\\ +\left\|\nabla\left(u^\varepsilon-u_1^\varepsilon\right)\right\|^2_{L^2((0,T)\times\Omega^\varepsilon)}+\varepsilon\left\|v^\varepsilon-v_0^\varepsilon\right\|^2_{L^2((0,T)\times\Gamma^\varepsilon)}\leq C\varepsilon,\end{aligned} \tag{4.1.1}$$

where $C>0$ is a generic constant independent of the choice of the scale parameter $\varepsilon>0$.

This chapter is structured as follows: Section 4.2 is devoted to the presentation of the Smoluchowski-Soret-Dufour model and the geometry of our perforated domain. In this section, we

also list a couple of preliminary results about the weak solvability of both the microscopic and limit models (recalling from [74]). Our main result is Theorem 4.3.1, as presented in Section 4.3. We then introduce the derivation of the difference system resulting from the microscopic problem and the "macroscopically reconstructed" system. On top of that, we prepare in this part a few helpful integral estimates. The proof of Theorem 4.3.1 is provided in Subsection 4.3.3. We conclude the paper with the remarks from Section 4.4.

4.2 Setting of the problem

4.2.1 The coupled thermo-diffusion model

A geometrical interpretation of porous medium

Let Ω be a bounded open domain in $\mathbb{R}^d$ ($d \in \{2,3\}$) with $\partial\Omega \in C^{0,1}$. Without loss of generality, we reduce ourselves to consider Ω as the parallelepiped $(0,a_1) \times ... \times (0,a_d)$ with $a_i > 0, i \in \{1,...,d\}$. Let Y be the representative unit cell defined by

$$Y := \left\{ \sum_{i=1}^{d} \lambda_i \vec{e}_i : 0 < \lambda_i < 1 \right\},$$

where $\vec{e}_i$ is the ith unit vector in $\mathbb{R}^d$.
Let Y_0 be an open subset of Y with a Lipschitz boundary $\Gamma = \partial Y_0$ which is divided into two disjoint closed parts Γ_N and Γ_R with a nonzero $(d-1)$-dimensional measure, i.e. $\Gamma = \Gamma_N \cup \Gamma_R$ with $\Gamma_N \cap \Gamma_R = \emptyset$.
Let $Z \in \mathbb{R}^d$ be a hypercube. Then for $X \subset Z$ we denote by X^k the shifted subset

$$X^k := X + \sum_{i=1}^{d} k_i \vec{e}_i,$$

where $k = (k_1,...,k_d) \in \mathbb{Z}^d$ is a vector of indices.
Assume that a scale factor $\varepsilon > 0$ is given. The pore skeleton is then defined as the union of εY_0^k the ε-homothetic sets of Y_0^k, i.e.

$$\Omega_0^\varepsilon := \bigcup_{k \in \mathbb{Z}^d} \left\{ \varepsilon Y_0^k : Y_0^k \subset \Omega \right\}.$$

Thus, the total pore space we have in mind is $\Omega^\varepsilon = \Omega \backslash \Omega_0^\varepsilon$.
Set $Y_1 := Y \backslash \overline{Y_0}$. The unit cell Y is made of two parts including the gas phase Y_1 and the solid phase Y_0. We denote the total pore surface of the skeleton by $\Gamma^\varepsilon := \partial\Omega_0^\varepsilon$. The pore surface Γ^ε consists of two parts satisfying $\Gamma^\varepsilon = \Gamma_N^\varepsilon \cup \Gamma_R^\varepsilon$ where Γ_N^ε and Γ_R^ε are disjoint closed sets possessing a nonzero $(d-1)$-dimensional measure. The Neumann boundary Γ_N^ε indicates the insulation for the heat flow, whilst at Γ_R^ε we allow for a flux of mass through a Robin-type condition. The union of the cell regions εY_1^k (without the solid grains εY_0^k) represents the total available space for thermo-diffusion.
In Figure 4.1 and Figure 4.2, we show an admissible two-dimensional domain with microstructures. We let throughout the paper $\mathrm{n} := (n_1,...,n_d)$ be the unit outward normal vector on the boundary $\partial\Omega^\varepsilon$. The representation of the periodic geometries is inspired from [65, 69, 99]

and references cited therein, but other possibilities exist as well. The practical problem usually delimitates the freedom in choosing the precise structure of Y_0; see Figure 4.2 for a couple of options.

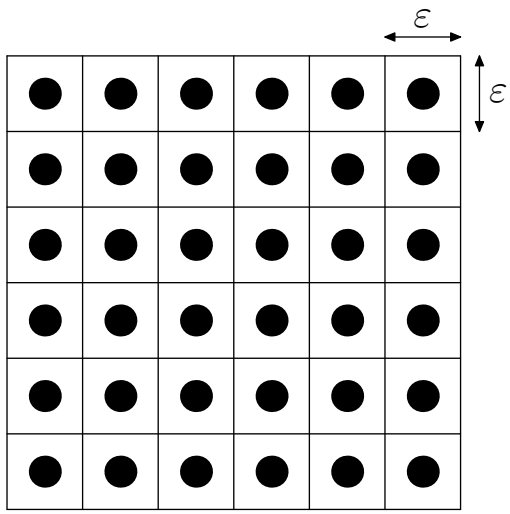

Figure 4.1: An admissible two-dimensional perforated domain.

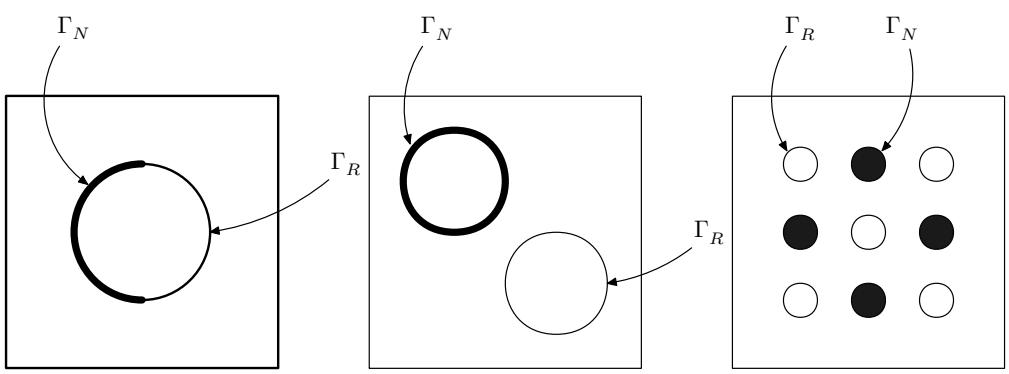

Figure 4.2: Possible choices for Y_0. The choice of (a) fits to the geometry described in Figure 4.1.

Model description

Before describing the microscopic problem (which we refer to as (P^ε)), we define some useful notation. For $\delta > 0$, let ∇^δ be the so-called mollified gradient

$$\nabla^\delta f(x) := \nabla\left[\int_{B(x,\delta)} J_\delta(x-y) f(y)\, dy\right],$$

where J_δ is a mollifier (see e.g. [43]) and $B(x,\delta)$ is the ball centered in $x \in \Omega$ with radius δ. The radius δ is assumed to be an ε-independent constant.

We denote by $x \in \Omega^\varepsilon$ the macroscopic variable and by $y = x/\varepsilon$ the microscopic variable representing fast variations at the microscopic geometry. With this convention, we write

$$\kappa^\varepsilon(x) = \kappa\left(\frac{x}{\varepsilon}\right) = \kappa(y).$$

The same convention applies to all the other oscillating coefficients involved in our problem. Let $m \geq 1$ be the number of balance equations in the system. We denote by $\mathscr{A}_{\mathbb{T}}^\varepsilon$ the second-order elliptic operator in divergence form with rapidly oscillating coefficients, i.e.

$$\mathscr{A}_{\mathbb{T}}^\varepsilon := \nabla \cdot \left(-\mathbb{T}\left(\frac{x}{\varepsilon}\right)\nabla\right) = \frac{\partial}{\partial x_i}\left[-\tau_{ij}\left(\frac{x}{\varepsilon}\right)\frac{\partial}{\partial x_j}\right], \tag{4.2.1}$$

where the Einstein summation convention is used.
Concerning the structure of $\mathscr{A}_{\mathbb{T}}^\varepsilon$, we assume that for all $y \in Y$, $\mathbb{T}(y) = \left(\tau_{ij}(y)\right) : \mathbb{R}^d \to \mathbb{R}^{d^2}$ for $1 \leq i, j \leq d$ is a second-order tensor that depends on the position vector y and satisfies an uniform (in ε) ellipticity condition. Depending on the situation, we have either $\mathbb{T}$ is the tensor κ (heat conductivity) or the tensor d_i (diffusion coefficients).
In this framework, we consider that maximum $N > 2$ colloidal species are involved in the thermo-diffusion process. We denote by $\left(\theta^\varepsilon, u_i^\varepsilon, v_i^\varepsilon\right)$ for $i \in \{1, ..., N\}$ the triplet of real-valued solutions of our thermo-diffusion model, i.e. a system of coupled ordinary differential equations with semi-linear parabolic equations for the evolution of temperature and colloid concentrations. Denote by $u^\varepsilon := \left(u_1^\varepsilon, ..., u_N^\varepsilon\right)$ the vector of all active colloidal concentrations u_i^ε. We assume that these species obey the population balance equation as postulated [109], i.e.

$$R_i(s) := \frac{1}{2}\sum_{k+j=i}\beta_{kj}s_k s_j - \sum_{j=1}^{N}\beta_{ij}s_i s_j, \quad (\text{with } R_i : \mathbb{R}^N \to \mathbb{R}, i \in \{1, ..., N\})$$

theoretically representing a quadratic-like rate of change of s_i. The presence of coagulation coefficients $\beta_{ij} > 0$ accounts for the rate aggregation and fragmentation between populations of particles of size i and j. For further modeling details, we refer the reader to [42, 57, 58] and [75], e.g.
We denote the parabolic cylinders as $Q_T^\varepsilon := (0, T) \times \Omega^\varepsilon$ and $Q_T := (0, T) \times \Omega$. Now, we detail the structure of our microscopic problem (P^ε). For $i \in \{1, ..., N\}$, we consider the following coupled thermo-diffusion system:

$$\partial_t \theta^\varepsilon + \mathscr{A}_\kappa^\varepsilon \theta^\varepsilon = \tau^\varepsilon \sum_{i=1}^{N} \nabla^\delta u_i^\varepsilon \cdot \nabla\theta^\varepsilon \quad \text{in } Q_T^\varepsilon, \tag{4.2.2}$$

$$\partial_t u_i^\varepsilon + \mathscr{A}_{d_i}^\varepsilon u_i^\varepsilon = \rho_i^\varepsilon \nabla^\delta \theta^\varepsilon \cdot \nabla u_i^\varepsilon + R_i(u^\varepsilon) \quad \text{in } Q_T^\varepsilon, \tag{4.2.3}$$

$$\partial_t v_i^\varepsilon = a_i^\varepsilon u_i^\varepsilon - b_i^\varepsilon v_i^\varepsilon \quad \text{on } (0, T) \times \Gamma^\varepsilon, \tag{4.2.4}$$

subject to the boundary conditions

$$-\kappa^\varepsilon \nabla\theta^\varepsilon \cdot \mathrm{n} = 0 \quad \text{on } (0, T) \times \Gamma_N^\varepsilon, \tag{4.2.5}$$

$$-\kappa^\varepsilon \nabla\theta^\varepsilon \cdot \mathrm{n} = \varepsilon g_0^\varepsilon \theta^\varepsilon \quad \text{on } (0, T) \times \Gamma_R^\varepsilon, \tag{4.2.6}$$

$$-\kappa^\varepsilon \nabla\theta^\varepsilon \cdot \mathrm{n} = 0 \quad \text{on } (0, T) \times \partial\Omega, \tag{4.2.7}$$

$$-d_i^\varepsilon \nabla u_i^\varepsilon \cdot \mathrm{n} = \varepsilon\left(a_i^\varepsilon u_i^\varepsilon - b_i^\varepsilon v_i^\varepsilon\right) \quad \text{on } (0, T) \times \Gamma^\varepsilon, \tag{4.2.8}$$

$$-d_i^\varepsilon \nabla u_i^\varepsilon \cdot \mathrm{n} = 0 \quad \text{on } (0, T) \times \partial\Omega, \tag{4.2.9}$$

κ^ε	heat conductivity (tensor)
τ^ε	Soret coefficient (tensor)
g_0^ε	heat absorption (scalar)
d_i^ε	diffusion coefficients (tensor)
ρ_i^ε	Dufour coefficients (tensor)
$a_i^\varepsilon, b_i^\varepsilon$	deposition rate coefficients (scalars)

Table 4.1: Physical parameters in the microscopic problem (P^ε).

and the initial data

$$\theta^\varepsilon(0,x) = \theta^{\varepsilon,0}(x) \quad \text{for } x \in \Omega^\varepsilon, \tag{4.2.10}$$

$$u_i^\varepsilon(0,x) = u_i^{\varepsilon,0}(x) \quad \text{for } x \in \Omega^\varepsilon, \tag{4.2.11}$$

$$v_i^\varepsilon(0,x) = v_i^{\varepsilon,0}(x) \quad \text{for } x \in \Gamma^\varepsilon. \tag{4.2.12}$$

Henceforward, (4.2.2)-(4.2.12) form our microscopic problem (P^ε).

Remark 4.2.1. *Our thermo-diffusion system is made of $N+1$ equations where the short-hand explanation for physical parameters in this model can be found in Table 4.1. Physically, equation* (4.2.2) *describes the changes of the temperature θ^ε in Ω^ε according to a heat conduction equation with a production term depending on $\nabla^\delta u_i^\varepsilon$, whilst the colloidal concentration u_i^ε is assumed to satisfy N reaction-diffusion like equations given by* (4.2.3) *with a chemical reaction term depending on $\nabla^\delta \theta^\varepsilon$. This type of special right-hand sides is mimicking the so-called Soret and Dufour effects. In* (4.2.8)*, v_i^ε denotes the mass of the deposited species on the boundary of the pore skeleton Γ^ε. These quantities are also supposed to satisfy the following ordinary differential equations* (4.2.4).

We make use of the following assumptions:
(A_1) The positive coefficients $\kappa^\varepsilon, \tau^\varepsilon, d_i^\varepsilon, \rho_i^\varepsilon \in [H^1(\Omega^\varepsilon)]^{d^2} \cap [L^\infty(\Omega^\varepsilon)]^{d^2}$, $g_0^\varepsilon \in L^\infty(\Gamma_R^\varepsilon)$ and $a_i^\varepsilon, b_i^\varepsilon \in L^\infty(\Gamma^\varepsilon)$ are Y-periodic. Also, there exist positive constants $\kappa_{\min}$, $\kappa_{\max}$, $\tau_{\min}$, $\tau_{\max}$, $d_{\min}$, $d_{\max}$, $\rho_{\min}$, $\rho_{\max}, a_{\min}, a_{\max}, b_{\min}, b_{\max}$ such that $\kappa_{\min} \le \kappa_{jk} \le \kappa_{\max}$, $\tau_{\min} \le \tau_{jk} \le \tau_{\max}$, $d_{\min} \le d_i^{jk} \le d_{\max}$, $\rho_{\min} \le \rho_i^{jk} \le \rho_{\max}$, $a_{\min} \le a_i^\varepsilon \le a_{\max}$, $b_{\min} \le b_i^\varepsilon \le b_{\max}$ for $i \in \{1,...,N\}$ and $j,k \in \{1,...,d\}$. Furthermore, there also exist positive constants α_i for $i \in \{0,...,N\}$ such that

$$\kappa_{jk}(y)\xi_j\xi_k \ge \alpha_0 |\xi|^2 \text{ and } d_i^{jk}(y)\xi_j\xi_k \ge \alpha_i |\xi|^2$$

for any $\xi \in \mathbb{R}^d$, $i \in \{1,...,N\}$, j and $k \in \{1,...,d\}$ to guarantee the ellipticity of the operators $\mathscr{A}_\kappa^\varepsilon$ and $\mathscr{A}_{d_i}^\varepsilon$.
The parameter δ is fixed such that $\delta \gg \varepsilon$, pointing out a length scale comparable with $\operatorname{diam}(\Omega)$ not interfering with the perforations.
(A_2) The positive initial conditions satisfy $\theta^{\varepsilon,0} \in L^\infty(\Omega^\varepsilon) \cap H^1(\Omega^\varepsilon)$, $u_i^{\varepsilon,0} \in L^\infty(\Omega^\varepsilon) \cap H^1(\Omega^\varepsilon)$, $v_i^{\varepsilon,0} \in L^\infty(\Gamma^\varepsilon)$ for $i \in \{1,...,N\}$, such that we can find $C_0 > 0$ satisfying

$$\left\|\theta^{\varepsilon,0}\right\|_{H^1(\Omega^\varepsilon)} + \sum_{i=1}^N \left(\left\|u_i^{\varepsilon,0}\right\|_{H^1(\Omega^\varepsilon)} + \left\|v_i^{\varepsilon,0}\right\|_{L^\infty(\Gamma^\varepsilon)}\right) \le C_0,$$

where C_0 is independent of the choice of ε.

Remark 4.2.2. *By the definitions of $\kappa, \tau, d_i, \rho_i$ and (A_1), there exist positive constants that bound from below and above these coefficients on Y for each choice of ε.*
The presence of $\delta > 0$ in the model equations is needed to keep (an uniform in ε) control on the terms $\nabla^\delta u_i^\varepsilon \cdot \nabla\theta^\varepsilon$ and $\nabla^\delta \theta^\varepsilon \cdot \nabla u_i^\varepsilon$. In 1D, the presence of δ is not essential since by compactness arguments it can be removed (see e.g. [62] for a compactness argument used to remove such δ arising in a similar system modeling consolidation of saturated porous media). In higher space dimensions, a complete removal of δ is not possible, see [4, Theorem 2.2].
A working example for the mollifier is given by

$$J_\delta(x) := \begin{cases} C exp\left(\dfrac{1}{|x|^2 - \delta^2}\right), & |x| < \delta, \\ 0, & |x| \geq \delta, \end{cases}$$

where the constant $C > 0$ is selected such that $\int_{\mathbb{R}^d} J_\delta(x)\,dx = 1$. Then, for $f \in L^1(\Omega^\varepsilon)$ the mollified gradient is

$$\nabla^\delta f := \nabla\left[\int_{B(x,\delta)} J_\delta(x-y)\bar{f}(y)\,dy\right],$$

with

$$\bar{f}(x) := \begin{cases} f(x), & x \in \Omega^\varepsilon, \\ 0, & x \in \mathbb{R}^d \backslash \Omega^\varepsilon. \end{cases}$$

We remark that the function $\bar{f}$ is well-defined in $L^1(B(x,\delta))$ for $x \in \Omega^\varepsilon$ since the intersection $\Omega^\varepsilon \cap B(x,\delta)$ is Lebesgue measurable. According to [43], there holds $\nabla^\delta f \in C^\infty(\Omega^\varepsilon)$ and there exists $C_\delta > 0$ such that for all $f \in L^2(\Omega^\varepsilon)$, the following inequality holds

$$\left\|\nabla^\delta f\right\|_{L^\infty(\Omega)} \leq C_\delta \|f\|_{L^2(\Omega^\varepsilon)}.$$

In this scenario, one can choose $\delta > 2\varepsilon diam(Y)$.

Unless otherwise specified, all the constants C are independent of the homogenization parameter ε, but the precise values may differ from line to line or even within a single chain of estimates. Throughout this paper, we use the superscript ε to emphasize the dependence on the heterogeneity of the material characterized by the homogenization parameter ε. In the sequel, we use dS_ε where S_ε can be viewed as a common notation for a boundary of any surface. Moreover, the notation $|\cdot|$ for a domain indicates in this work the volume of that domain.

4.2.2 Preliminary results

In this subsection, we present the fact already known concerning the weak solvability and periodic homogenization of (P^ε). It is important to note that, for our choice of Y_0, the interior extension from $H^1(\Omega^\varepsilon)$ into $H^1(\Omega)$ exists with extension constants independent of ε (see [65, Lemma 5] and [31, Theorem 2.10]).

Definition 4.2.3. The weak formulation of (P^ε)
For $i \in \{1, ..., N\}$, the triplet $\left(\theta^\varepsilon, u_i^\varepsilon, v_i^\varepsilon\right)$ satisfying

$$\theta^\varepsilon, u_i^\varepsilon \in H^1\left(0,T;L^2(\Omega^\varepsilon)\right) \cap L^\infty\left(0,T;H^1(\Omega^\varepsilon)\right) \cap L^\infty((0,T)\times\Omega^\varepsilon),$$

$$v_i^\varepsilon \in H^1\left(0,T;L^2\left(\Gamma^\varepsilon\right)\right)\cap L^\infty\left((0,T)\times\Gamma^\varepsilon\right).$$

is a weak solution to (P^ε) provided that

$$\begin{cases} \displaystyle\int_{\Omega^\varepsilon}\partial_t\theta^\varepsilon\varphi dx+\int_{\Omega^\varepsilon}\kappa^\varepsilon\nabla\theta^\varepsilon\cdot\nabla\varphi dx+\varepsilon\int_{\Gamma_R^\varepsilon}g_0\theta^\varepsilon\varphi dS_\varepsilon=\int_{\Omega^\varepsilon}\tau^\varepsilon\sum_{i=1}^N\nabla^\delta u_i^\varepsilon\cdot\nabla\theta^\varepsilon\varphi dx, \\ \displaystyle\int_{\Omega^\varepsilon}\partial_t u_i^\varepsilon\phi_i dx+\int_{\Omega^\varepsilon}d_i^\varepsilon\nabla u_i^\varepsilon\cdot\nabla\phi_i dx+\varepsilon\int_{\Gamma^\varepsilon}\left(a_i^\varepsilon u_i^\varepsilon-b_i^\varepsilon v_i^\varepsilon\right)\phi_i dS_\varepsilon \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\displaystyle=\int_{\Omega^\varepsilon}R_i\left(u^\varepsilon\right)\phi_i dx+\int_{\Omega^\varepsilon}\rho_i^\varepsilon\nabla^\delta\theta^\varepsilon\cdot\nabla u_i^\varepsilon\phi_i dx, \\ \displaystyle\varepsilon\int_{\Gamma^\varepsilon}\partial_t v_i^\varepsilon\psi_i dS_\varepsilon=\varepsilon\int_{\Gamma^\varepsilon}\left(a_i^\varepsilon u_i^\varepsilon-b_i^\varepsilon v_i^\varepsilon\right)\psi_i dS_\varepsilon, \end{cases} \tag{4.2.13}$$

for all $(\varphi,\phi_i,\psi_i)\in H^1(\Omega^\varepsilon)\times H^1(\Omega^\varepsilon)\times L^2(\Gamma^\varepsilon)$.

Theorem 4.2.4. Well-posedness and Positivity of solution
Assume (A_1)-(A_2) *and* $i\in\{1,...,N\}$. *The microscopic problem* (P^ε) *admits a unique solution* $\left(\theta^\varepsilon,u_i^\varepsilon,v_i^\varepsilon\right)$ *in the sense of Definition 5.3.1, belonging to*

$$K(T,M):=\left\{z\in L^2((0,T)\times\Omega^\varepsilon):|z|\le M \text{ a.e. in } (0,T)\times\Omega^\varepsilon\right\}$$

for some $M>0$. *Additionally,*

$$\theta^\varepsilon,u_i^\varepsilon\in H^1\left(0,T;L^2\left(\Omega^\varepsilon\right)\right)\cap L^\infty\left(0,T;H^1\left(\Omega^\varepsilon\right)\right)\cap L^\infty\left((0,T)\times\Omega^\varepsilon\right),$$

$$v_i^\varepsilon\in H^1\left(0,T;L^2\left(\Gamma^\varepsilon\right)\right)\cap L^\infty\left((0,T)\times\Gamma^\varepsilon\right).$$

Furthermore, this triplet $\left(\theta^\varepsilon,u_i^\varepsilon,v_i^\varepsilon\right)$ *is positive and the following energy estimates hold*

$$\kappa_{\min}\left\|\nabla\theta^\varepsilon(t)\right\|^2_{L^2(\Omega^\varepsilon)}+\int_0^t\left\|\partial_t\theta^\varepsilon(t)\right\|^2_{L^2(\Omega^\varepsilon)}dt\le C,$$

$$\left\|\nabla u_i^\varepsilon(t)\right\|^2_{L^2(\Omega^\varepsilon)}+\int_0^T\left(\left\|\partial_t u_i^\varepsilon(t)\right\|^2_{L^2(\Omega^\varepsilon)}+\left\|\partial_t v_i^\varepsilon(t)\right\|^2_{L^2(\Gamma^\varepsilon)}\right)dt\le C\quad \text{for a.e. } t\in(0,T].$$

We denote by $\left(P^0\right)$ the strong formulation of the macroscopic (limit) problem. We introduce below the limit problem whose precise structure has been obtained via a two-scale convergence procedure in [74]. When doing so, the effective constants are defined, as follows: For $i\in\{1,...,N\}$ and $j,k\in\{1,...,d\}$,

$$K_0:=\frac{1}{|Y_1|}\int_{Y_1}\kappa(y)dy,\quad K_{ij}:=\frac{1}{|Y_1|}\int_{Y_1}\kappa(y)\frac{\partial\bar\theta^j}{\partial y_i}dy, \tag{4.2.14}$$

$$T_0^i:=\frac{1}{|Y_1|}\int_{Y_1}\tau_i(y)dy,\quad T_{jk}^i:=\frac{1}{|Y_1|}\int_{Y_1}\tau_i(y)\frac{\partial\bar\theta^j}{\partial y_i}dy, \tag{4.2.15}$$

$$D_i:=\frac{1}{|Y_1|}\int_{Y_1}d_i(y)dy,\quad \mathbb{D}_0^i:=\left(\frac{1}{|Y_1|}\int_{Y_1}d_i(y)\frac{\partial\bar u_i^j}{\partial y_k}dy\right)_{jk}, \tag{4.2.16}$$

$$F_i := \frac{1}{|Y_1|}\int_{Y_1} \rho_i(y)\,dy, \quad \mathbb{F}^i := \left(\frac{1}{|Y_1|}\int_{Y_1} \rho_i(y)\frac{\partial \bar{u}_i^j}{\partial y_k}dy\right)_{jk}, \tag{4.2.17}$$

$$A_i := \frac{1}{|Y_1|}\int_{\partial Y_0} a_i dy, \quad B_i := \frac{1}{|Y_1|}\int_{\partial Y_0} b_i dy. \tag{4.2.18}$$

The reader can find in [74] the precise arguments behind the derivation of these effective coefficients.

Theorem 4.2.5. Strong formulation of the macroscopic problem – (P^0)
Assume (A_1)-(A_2). *For* $i \in \{1,...,N\}$, *the triplet* $\left(\theta^0, u_i^0, v_i^0\right)$ *of limit solutions* $\left(\theta^\varepsilon, u_i^\varepsilon, v_i^\varepsilon\right)$ *to* (P^ε) *in the sense of Definition 5.3.1 satisfies the following macroscopic system*

$$\partial_t \theta^0 + \nabla\cdot\left(-\mathbb{K}\nabla\theta^0\right) + g_0\frac{|\Gamma_R|}{|Y_1|}\theta^0 = \sum_{i=1}^N \left(\mathbb{T}^i\nabla^\delta u_i^0\right)\cdot\nabla\theta^0 \quad in\ Q_T, \tag{4.2.19}$$

$$\partial_t u_i^0 + \nabla\cdot\left(-\mathbb{D}^i\nabla u_i^0\right) + A_i u_i^0 - B_i v_i^0 = \left(\mathbb{F}^i\nabla u_i^0\right)\cdot\nabla^\delta\theta^0 + R_i\left(u^0\right) \quad in\ Q_T, \tag{4.2.20}$$

subject to the boundary conditions

$$-\mathbb{K}\nabla\theta^0\cdot n = 0 \quad on\ (0,T)\times\partial\Omega, \tag{4.2.21}$$

$$-\mathbb{D}^i\nabla u_i^0\cdot n = 0 \quad on\ (0,T)\times\partial\Omega, \tag{4.2.22}$$

and associated with the ordinary differential equations

$$\partial_t v_i^0 = A_i u_i^0 - B_i v_i^0 \quad in\ Q_T, \tag{4.2.23}$$

where we have denoted by $\mathbb{K} = K_0\mathbb{I} + \left(K_{ij}\right)_{ij}$, $\mathbb{T}^i = T_0^i\mathbb{I} + \left(T_{jk}^i\right)_{jk}$, $\mathbb{D}^i = D_i\mathbb{I} + \mathbb{D}_0^i$, $\mathbb{F}^i = F_i\mathbb{I} + \mathbb{F}_0^i$ *for* $j,k \in \{1,...,d\}$ *with* $\mathbb{I}$ *standing for the identity matrix and the quantities* K_0, K_{ij}, T_0^i, T_{jk}^i, D_i, $\mathbb{D}_0^i$, F_i, $\mathbb{F}^i$, A_i, B_i *being effective constants corresponding, respectively, to the oscillating coefficients and defined in* (4.2.14)-(4.2.18).
Furthermore, the initial conditions are provided by

$$\theta^0(t=0) = \theta^{0,0} \quad in\ \overline{\Omega}, \tag{4.2.24}$$

$$u_i^0(t=0) = u_i^{0,0} \quad in\ \overline{\Omega}, \tag{4.2.25}$$

$$v_i^0(t=0) = v_i^{0,0} \quad on\ \Gamma. \tag{4.2.26}$$

Theorem 4.2.6. The weak formulation of the macroscopic problem (P^0)
Assume (A_1)-(A_2) *and take* $i \in \{1,...,N\}$, *the triplet* $\left(\theta^0, u_i^0, v_i^0\right)$ *satifying*

$$\theta^0, u_i^0 \in H^1\left(0,T;L^2(\Omega)\right) \cap L^2\left(0,T;H^1(\Omega)\right) \cap L^\infty\left((0,T)\times\Omega\right),$$

$$v_i^0 \in H^1\left(0,T;L^2(\Omega)\right) \cap L^\infty\left((0,T)\times\Omega\right),$$

is a weak solution to (P^0) *provided that*

$$\begin{cases} \int_\Omega \partial_t \theta^0 \varphi dx + \int_\Omega \mathbb{K}\nabla\theta^0 \cdot \nabla\varphi dx + g_0 \frac{|\Gamma_R|}{|Y_1|} \int_\Omega \theta^0 \varphi dx = \int_\Omega \sum_{i=1}^N \left(\mathbb{T}^i \nabla^\delta u_i^0\right) \cdot \nabla\theta^0 \varphi dx, \\ \int_\Omega \partial_t u_i^0 \phi_i dx + \int_\Omega \mathbb{D}^i \nabla u_i^0 \cdot \nabla\phi_i dx + \int_\Omega \left(A_i u_i^0 - B_i v_i^0\right) \phi_i dx \\ \qquad\qquad = \int_\Omega \left(\mathbb{F}^i \nabla u_i^0\right) \cdot \nabla^\delta \theta^0 \phi_i dx + \int_\Omega R_i\left(u^0\right) \phi_i dx, \\ \int_\Omega \partial_t v_i^0 \psi_i dx = \int_\Omega \left(A_i u_i^0 - B_i v_i^0\right) \psi_i dx, \end{cases} \tag{4.2.27}$$

hold for all $(\varphi, \phi_i, \psi_i) \in C^\infty(\Omega) \times C^\infty(\Omega) \times C^\infty(\Omega)$.

Hereby, the functions $\bar{\theta}$ and $\bar{u}_i$ linearly formulate the limit functions θ^1 and u_i^1 by $\theta^1 := \bar{\theta} \cdot \nabla_x \theta^0 = \sum_{j=1}^d \partial_{x_j} \theta^0 \bar{\theta}^j$ and $u_i^1 := \bar{u}_i \cdot \nabla_x u_i^0 = \sum_{j=1}^d \partial_{x_j} u_i^0 \bar{u}_i^j$ for $i \in \{1, ..., N\}$. Moreover, they solve, respectively, the cell problems introduced in the following Theorem.

Theorem 4.2.7. The cell problems
Assume (A_1) *holds. The limit functions* θ^1 *and* u_i^1 *defined as above solve the following cell problems:*

$$\begin{cases} \nabla_y \cdot \left(-\kappa(y) \nabla_y \bar{\theta}^j(x,y)\right) = \nabla_y \cdot (\kappa n_j) & \text{in } Y_1, \\ -\kappa(y) \nabla_y \bar{\theta}^j \cdot n = \kappa n_j & \text{on } \partial Y_0, \\ \bar{\theta}^j \text{ is } Y\text{-periodic}, \end{cases} \tag{4.2.28}$$

$$\begin{cases} \nabla_y \cdot \left(-d_i(y) \nabla_y \bar{u}_i^j(x,y)\right) = \nabla_y \cdot (d_i n_j) & \text{in } Y_1, \\ -d_i(y) \nabla_y \bar{u}_i^j \cdot n = d_i n_j & \text{on } \partial Y_0, \\ \bar{u}_i^j \text{ is } Y\text{-periodic}, \end{cases} \tag{4.2.29}$$

where n_j *is the* j*th unit vector of* $\mathbb{R}^d$ *and* $i \in \{1, ..., N\}, j \in \{1, ..., d\}$. *Furthermore,*

1. If $\kappa, d_i \in [H^1(\bar{Y}_1)]^{d^2}$ are Lipschitz continuous, the system (4.2.28)-(4.2.29) admits a unique solution $\left(\bar{\theta}^j, \bar{u}_i^j\right) \in H^2_{loc}(Y_1) \times H^2_{loc}(Y_1)$;

2. If $k, d_i \in [H^1(Y_1)]^{d^2} \cap [H^{-\frac{1}{2}+s}(\partial Y_0)]^{d^2}$ for every $s \in \left(-\frac{1}{2}, \frac{1}{2}\right)$ are Lipschitz continuous, the system (4.2.28)-(4.2.29) admits a unique solution $\left(\bar{\theta}^j, \bar{u}_i^j\right) \in H^{1+s}(Y_1) \times H^{1+s}(Y_1)$.

The weak solvability of the cell problems (4.2.28) and (4.2.29) shall be further discussed in the proof of Theorem 4.3.1 (see Section 4.3). To derive the corrector estimate (4.1.1), we need a number of elementary inequalities.

- For all $1 \le p \le \infty$, the following estimates hold:

$$\left\|\nabla^\delta f \cdot g\right\|_{L^p(\Omega^\varepsilon)} \le C_\delta \|f\|_{L^\infty(\Omega^\varepsilon)} \|g\|_{[L^p(\Omega^\varepsilon)]^d} \text{ for } f \in L^\infty(\Omega^\varepsilon), g \in [L^p(\Omega^\varepsilon)]^d, \tag{4.2.30}$$

$$\left\|\nabla^\delta f\right\|_{L^p(\Omega^\varepsilon)} \le C_\delta \|f\|_{L^2(\Omega^\varepsilon)} \text{ for } f \in L^2(\Omega^\varepsilon), \tag{4.2.31}$$

  where $C_\delta > 0$ depends only on δ. See [74], e.g., for a proof of (4.2.30) and (4.2.31).

- To estimate the correctors for both the temperature θ^ε and colloidal concentrations u_i^ε, we consider the real-valued cut-off function $m^\varepsilon \in C_0^1(\Omega)$ satisfying $0 \le m^\varepsilon \le 1$, $\varepsilon |\nabla m^\varepsilon| \le C$, and $m^\varepsilon = 1$ on $\{x \in \Omega : \operatorname{dist}(x, \Gamma) \ge \varepsilon\}$. Furthermore, one can prove that

$$\|1 - m^\varepsilon\|_{L^2(\Omega^\varepsilon)} \le C\varepsilon^{1/2}, \quad \varepsilon \|\nabla m^\varepsilon\|_{L^2(\Omega^\varepsilon)} \le C\varepsilon^{1/2}. \tag{4.2.32}$$

Theorem 4.2.8. Existence and uniqueness results for (P^0)
Assume (A_1)-(A_2). For $i \in \{1, ..., N\}$, the macroscopic problem $\left(P^0\right)$ admits a unique (local) weak solution in $L^2((0,T) \times \Omega)$.

Proof. Due to the homogenization limit results in [74, Lemma 4.3], the existence of the triplet $\left(\theta^0, u_i^0, v_i^0\right)$ in Theorem 4.2.6 is guaranteed. The contraction of these functions in a closed subspace of $[L^2((0,T)\times\Omega)]^{N+2}$ can be proved concisely by a contraction argument. The proof can be sketched as follows: We define

$$K_1(M,T) := \left\{z \in L^2((0,T) \times \Omega) : |z| \le M \text{ a.e. in } Q_T\right\}.$$

For $i \in \{1, ..., N\}$, let $\theta^{0,1}, u_i^{0,1}, v_i^{0,1} \in K_1(M_1, T_1)$ and $\theta^{0,2}, u_i^{0,2}, v_i^{0,2} \in K_1(M_2, T_2)$ be two pairs of (weak) solutions of the macroscopic system. By choosing $T = \min\{T_1, T_2\}$ and $M = 2\max\{M_1, M_2\}$ and suitable test functions φ, ϕ_i, ψ_i in (4.2.27), we get $d\left(\theta^0\right) := \theta^{0,1} - \theta^{0,2}, d\left(u_i^0\right) := u_i^{0,1} - u_i^{0,2}, d\left(v_i^0\right) := v_i^{0,1} - v_i^{0,2} \in K_1(M,T)$, which satisfy the following equalities:

$$\begin{aligned}
&\frac{1}{2}\partial_t \left\|d\left(\theta^0\right)\right\|_{L^2(\Omega)}^2 + \mathbb{K}\left\|\nabla d\left(\theta^0\right)\right\|_{L^2(\Omega)}^2 + g_0 \frac{|\Gamma_R|}{|Y_1|}\left\|d\left(\theta^0\right)\right\|_{L^2(\Omega)}^2 \\
&\qquad = \int_\Omega \sum_{i=1}^N \left(\left(\mathbb{T}^i \nabla^\delta u_i^{0,1}\right) \cdot \nabla\theta^{0,1} - \left(\mathbb{T}^i \nabla^\delta u_i^{0,2}\right) \cdot \nabla\theta^{0,2}\right) d\left(\theta^0\right) dx,
\end{aligned}$$

$$\begin{aligned}
&\frac{1}{2}\partial_t \left\|d\left(u_i^0\right)\right\|_{L^2(\Omega)}^2 + \mathbb{D}^i \left\|\nabla d\left(u_i^0\right)\right\|_{L^2(\Omega)}^2 + A_i \left\|d\left(u_i^0\right)\right\|_{L^2(\Omega)}^2 - \int_\Omega B_i d\left(v_i^0\right) d\left(u_i^0\right) dx \\
&\qquad = \int_\Omega \left(\left(\mathbb{F}^i \nabla u_i^{0,1}\right) \cdot \nabla^\delta \theta^{0,1} - \left(\mathbb{F}^i \nabla u_i^{0,2}\right) \cdot \nabla^\delta \theta^{0,2}\right) d\left(u_i^0\right) dx \\
&\qquad + \int_\Omega \left(R_i\left(u_i^{0,1}\right) - R_i\left(u_i^{0,2}\right)\right) d\left(u_i^0\right) dx,
\end{aligned}$$

$$\frac{1}{2}\partial_t \left\|d\left(v_i^0\right)\right\|_{L^2(\Omega)}^2 + B_i \left\|d\left(v_i^0\right)\right\|_{L^2(\Omega)}^2 = \int_\Omega A_i d\left(u_i^0\right) d\left(v_i^0\right) dx.$$

Here, the contraction is obtained for $t < T_0$, where T_0 is small enough. For $n \in \mathbb{N}$, we can construct an approximation scheme $\left(\theta^{0,n}, u_i^{0,n}, v_i^{0,n}\right)$ for $n \in \mathbb{N}$ for the macroscopic system involving only linear terms. Based on the contraction argument, we can prove that $\left\{\theta^{0,n}\right\}_{n\in\mathbb{N}}$, $\left\{u_i^{0,n}\right\}_{n\in\mathbb{N}}$ and $\left\{v_i^{0,n}\right\}_{n\in\mathbb{N}}$ are Cauchy sequences in $K_1(M, T_0)$. Thus, the local existence and uniqueness of solutions in $[L^2((0,T)\times\Omega)]^{N+2}$ to $\left(P^0\right)$ is guaranteed. □

4.3 Corrector estimates

The main result of this chapter is stated in the next Theorem whose applicability is delimited by the assumptions (A_1)-(A_2), extra regularity and ε-control of the initial data. Note

that the involved macroscopic reconstructions $\theta_0^\varepsilon, u_{i,0}^\varepsilon, v_{i,0}^\varepsilon$ for $i \in \{1,...,N\}$ are introduced in Subsection 4.3.1.

Theorem 4.3.1. *Assume* (A_1)-(A_2). *Let* $\left(\theta^\varepsilon, u_i^\varepsilon, v_i^\varepsilon\right)$ *and* $\left(\theta^0, u_i^0, v_i^0\right)$ *for* $i \in \{1,...,N\}$ *be weak solutions to* (P^ε) *and* (P^0) *in the sense of Definition 5.3.1 and Theorem* 4.2.6*, respectively. Let* $\bar{\theta}, \bar{u}_i$ *be the cell functions solving the cell problems* (4.2.28)-(4.2.29) *and satisfying*

$$\bar{\theta}, \bar{u}_i \in L^\infty\left(\Omega^\varepsilon; W_\#^{1+s,2}(Y_1)\right) \cap H^1\left(\Omega^\varepsilon; W_\#^{s,2}(Y_1)\right) \quad \text{for } s > d/2.$$

For every $t \in (0,T]$*, we also assume that* $\theta^0(t,\cdot), u_i^0(t,\cdot) \in W^{1,\infty}(\Omega^\varepsilon) \cap H^2(\Omega^\varepsilon)$ *for* $i \in \{1,...,N\}$*. On top of that, we assume*

$$\left\|\theta^{\varepsilon,0} - \theta^{0,0}\right\|_{L^2(\Omega^\varepsilon)}^2 + \sum_{i=1}^N \left\|u_i^{\varepsilon,0} - u_i^{0,0}\right\|_{L^2(\Omega^\varepsilon)}^2 + \sum_{i=1}^N \left\|v_i^{\varepsilon,0} - v_i^{0,0}\right\|_{L^2(\Gamma^\varepsilon)}^2 \leq \varepsilon^\gamma,$$

for some $\gamma \in \mathbb{R}_+$*. Then the following corrector estimate holds*

$$\begin{aligned}
&\left\|\theta^\varepsilon - \theta^0\right\|_{L^2((0,T)\times\Omega^\varepsilon)}^2 + \sum_{i=1}^N \left\|u_i^\varepsilon - u_i^0\right\|_{L^2((0,T)\times\Omega^\varepsilon)}^2 \\
&+ \left\|\nabla\left(\theta^\varepsilon - \theta_1^\varepsilon\right)\right\|_{L^2\left(0,T;[L^2(\Omega^\varepsilon)]^d\right)}^2 + \sum_{i=1}^N \left\|\nabla\left(u_i^\varepsilon - u_{i,1}^\varepsilon\right)\right\|_{L^2\left(0,T;[L^2(\Omega^\varepsilon)]^d\right)}^2 \leq C \max\left\{\varepsilon, \varepsilon^\gamma\right\}.
\end{aligned}$$

Furthermore, if $\gamma \geq 1$*, then we obtain*

$$\varepsilon \sum_{i=1}^N \left\|v_i^\varepsilon - v_i^0\right\|_{L^2((0,T)\times\Gamma^\varepsilon)}^2 \leq C\varepsilon.$$

4.3.1 Macroscopic reconstruction

To derive correctors estimates for our problem, we use the concept of the macroscopic reconstruction. We borrow this terminology from [40], but note that it is also connected to similar concepts in the *a posteriori* numerical analysis of PDEs (see e.g. [76]). It turns out that we derive operators that could bring us the link between the strong formulations (P^ε) and $\left(P^0\right)$. For a.e. $t \in [0,T]$ and $x \in \Omega^\varepsilon$ we provide that

$$\theta_0^\varepsilon(t,x) := \theta^0(t,x), \tag{4.3.1}$$

$$u_{i,0}^\varepsilon(t,x) := u_i^0(t,x), \tag{4.3.2}$$

$$v_{i,0}^\varepsilon(t,x) := v_i^0(t,x). \tag{4.3.3}$$

Henceforward, we obtain the system of macroscopic reconstruction whose expression is similar to the strong formulations $\left(P^0\right)$, but acting on $x \in \Omega^\varepsilon$. We accordingly subtract this system from the microscopic system (P^ε) equation-by-equation and gain the difference system over Ω^ε. Then we proceed to the correctors justification by the following choice of test functions:

$$\varphi(t,x) := \theta^\varepsilon(t,x) - \left(\theta_0^\varepsilon(t,x) + \varepsilon m^\varepsilon(x)\bar{\theta}\left(x, \frac{x}{\varepsilon}\right) \cdot \nabla_x \theta^0(t,x)\right), \tag{4.3.4}$$

$$\phi_i(t,x) := u_i^\varepsilon(t,x) - \left(u_{i,0}^\varepsilon(t,x) + \varepsilon m^\varepsilon(x)\bar{u}_i\left(x, \frac{x}{\varepsilon}\right) \cdot \nabla_x u_i^0(t,x)\right), \tag{4.3.5}$$

where m^ε is a cut-off function with the properties (4.2.32).
Multiplying the difference system by the test functions $\varphi, \phi_i \in H^1(\Omega^\varepsilon)$ and integrating the resulting equations over Ω^ε, we obtain the system, denoted by $\left(\bar{\mathbb{P}}^\varepsilon\right)$, as follows:

$$\int_{\Omega_0^\varepsilon} \partial_t \left(\theta^\varepsilon - \theta_0^\varepsilon\right) \varphi dx + \int_{\Omega^\varepsilon} \left(\kappa^\varepsilon \nabla \theta^\varepsilon - \mathbb{K} \nabla \theta_0^\varepsilon\right) \cdot \nabla \varphi dx + \varepsilon \int_{\Gamma_R^\varepsilon} g_0 \theta^\varepsilon \varphi dS_\varepsilon - g_0 \frac{|\Gamma_R|}{|Y_1|} \int_{\Omega^\varepsilon} \theta_0^\varepsilon \varphi dx$$
$$= \int_{\Omega^\varepsilon} \left(\tau^\varepsilon \sum_{i=1}^N \nabla^\delta u_i^\varepsilon \cdot \nabla \theta^\varepsilon - \sum_{i=1}^N \left(\mathbb{T}^i \nabla^\delta u_{i,0}^\varepsilon\right) \cdot \nabla \theta_0^\varepsilon \right) \varphi dx,$$

$$\int_{\Omega^\varepsilon} \partial_t \left(u_i^\varepsilon - u_{i,0}^\varepsilon\right) \phi_i dx + \int_{\Omega^\varepsilon} \left(d_i^\varepsilon \nabla u_i^\varepsilon - \mathbb{D}^i \nabla u_{i,0}^\varepsilon\right) \cdot \nabla \phi_i dx$$
$$+ \varepsilon \int_{\Gamma^\varepsilon} \left(a_i^\varepsilon u_i^\varepsilon - b_i^\varepsilon v_i^\varepsilon\right) \phi_i dS_\varepsilon - \int_{\Omega^\varepsilon} \left(A_i u_{i,0}^\varepsilon - B_i v_{i,0}^\varepsilon\right) \phi_i dx$$
$$= \int_{\Omega^\varepsilon} \left(\rho_i^\varepsilon \nabla^\delta \theta^\varepsilon \cdot \nabla u_i^\varepsilon - \left(\mathbb{F}^i \nabla u_{i,0}^\varepsilon\right) \cdot \nabla^\delta \theta_0^\varepsilon\right) \phi_i dx + \int_{\Omega^\varepsilon} \left(R_i\left(u^\varepsilon\right) - R_i\left(u_0^\varepsilon\right)\right) \phi_i dx,$$

According to the system $\left(\bar{\mathbb{P}}^\varepsilon\right)$, we denote the following terms:

$$\mathscr{I}_1 := \int_{\Omega^\varepsilon} \partial_t \left(\theta^\varepsilon - \theta_0^\varepsilon\right) \varphi dx, \tag{4.3.6}$$

$$\mathscr{I}_2 := \int_{\Omega^\varepsilon} \left(\kappa^\varepsilon \nabla \theta^\varepsilon - \mathbb{K} \nabla \theta_0^\varepsilon\right) \cdot \nabla \varphi dx, \tag{4.3.7}$$

$$\mathscr{I}_3 := \varepsilon \int_{\Gamma_R^\varepsilon} g_0 \theta^\varepsilon \varphi dS_\varepsilon - g_0 \frac{|\Gamma_R|}{|Y_1|} \int_{\Omega^\varepsilon} \theta_0^\varepsilon \varphi dx, \tag{4.3.8}$$

$$\mathscr{I}_4 := \int_{\Omega^\varepsilon} \left(\tau^\varepsilon \sum_{i=1}^N \nabla^\delta u_i^\varepsilon \cdot \nabla \theta^\varepsilon - \sum_{i=1}^N \left(\mathbb{T}^i \nabla^\delta u_i^0\right) \cdot \nabla \theta_0^\varepsilon \right) \varphi dx, \tag{4.3.9}$$

$$\mathscr{J}_1^i := \int_{\Omega^\varepsilon} \partial_t \left(u_i^\varepsilon - u_{i,0}^\varepsilon\right) \phi_i dx, \tag{4.3.10}$$

$$\mathscr{J}_2^i := \int_{\Omega^\varepsilon} \left(d_i^\varepsilon \nabla u_i^\varepsilon - \mathbb{D}^i \nabla u_{i,0}^\varepsilon\right) \cdot \nabla \phi_i dx, \tag{4.3.11}$$

$$\mathscr{J}_3^i := \varepsilon \int_{\Gamma^\varepsilon} \left(a_i^\varepsilon u_i^\varepsilon - b_i^\varepsilon v_i^\varepsilon\right) \phi_i dS_\varepsilon - \int_{\Omega^\varepsilon} \left(A_i u_{i,0}^\varepsilon - B_i v_{i,0}^\varepsilon\right) \phi_i dx, \tag{4.3.12}$$

$$\mathscr{J}_4^i := \int_{\Omega^\varepsilon} \left(\rho_i^\varepsilon \nabla^\delta \theta^\varepsilon \cdot \nabla u_i^\varepsilon - \left(\mathbb{F}^i \nabla u_{i,0}^\varepsilon\right) \cdot \nabla^\delta \theta_0^\varepsilon\right) \phi_i dx + \int_{\Omega^\varepsilon} \left(R_i\left(u^\varepsilon\right) - R_i\left(u_0^\varepsilon\right)\right) \phi_i dx. \tag{4.3.13}$$

We introduce, in the same spirit as for (4.3.1) and (4.3.2), another macroscopic reconstruction $\theta_1^\varepsilon(t,x)$ and $u_{i,1}^\varepsilon(t,x)$ defined as follows:

$$\theta_1^\varepsilon(t,x) := \theta_0^\varepsilon(t,x) + \varepsilon \bar{\theta}\left(x, \frac{x}{\varepsilon}\right) \cdot \nabla_x \theta^0(t,x),$$
$$u_{i,1}^\varepsilon(t,x) := u_{i,0}^\varepsilon(t,x) + \varepsilon \bar{u}_i\left(x, \frac{x}{\varepsilon}\right) \cdot \nabla_x u_i^0(t,x),$$

where $\bar{\theta}$ and $\bar{u}_i$ are the cell functions introduced in Theorem 4.2.7 as weak solutions to the problems (4.2.28) and (4.2.29), respectively.
By definitions (4.3.1)-(4.3.2), the macroscopic reconstructions $\theta_0^\varepsilon(t,x)$ and $u_{i,0}^\varepsilon(t,x)$ are interchangeable, respectively, in notation with the limit functions $\theta^0(t,x)$ and $u_i^0(t,x)$ in Theorem 4.3.1.

4.3.2 Integral estimates

Remark 4.3.2. *From Lemma 4.3.3, one can apply directly the L^2-estimate between the space-dependent physical parameters of the microscopic problem (e.g. κ^ε, τ^ε) and their averages, even if the parameters in discussion are actually tensors. To this end, these estimates are controlled as $\|p^\varepsilon - \bar{p}\|_{L^2(\Omega^\varepsilon)} \leq C\varepsilon^{1/2}$, where p^ε refers to the oscillating coefficient and $\bar{p}$ denotes its average.*

Lemma 4.3.3. *Let Y_1 as defined in Subsection 4.2.1. Let $p^\varepsilon(x) := p(x/\varepsilon)$ belong to $H^1(\Omega^\varepsilon)$ satisfying*

$$\bar{p} := \frac{1}{|Y_1|}\int_{Y_1} p(y)\,dy.$$

Then the following estimate holds

$$\|p^\varepsilon - \bar{p}\|_{L^2(\Omega^\varepsilon)} \leq C\varepsilon^{1/2}\|p^\varepsilon\|_{H^1(\Omega^\varepsilon)}.$$

Proof. We consider the periodic geometry described in Figure 4.1 in Subsection 4.2.1. For a fixed test function $\phi \in H^1(\Omega^\varepsilon)$, we see that

$$\int_{\Omega^\varepsilon}(p^\varepsilon - \bar{p})\phi\,dx = \sum_{k\in\mathbb{Z}^d}\int_{\varepsilon Y_1^k}(p^\varepsilon - \bar{p})\phi\,dx \leq C\varepsilon^{-d}\int_{\varepsilon Y_1}(p^\varepsilon - \bar{p})\phi\,dx.$$

By changing the variable $x = \varepsilon y$, the relations

$$\int_{\varepsilon Y_1} p\left(\frac{x}{\varepsilon}\right)\phi(x)\,dx = \varepsilon^d\int_{Y_1} p(y)\phi(\varepsilon y)\,dy,$$
$$\int_{\varepsilon Y_1}\int_{Y_1} p(y)\phi(x)\,dy\,dx = \varepsilon^d\int_{Y_1}\int_{Y_1} p(y)\phi(\varepsilon z)\,dy\,dz,$$

enable us to write:

$$\int_{\varepsilon Y_1}(p^\varepsilon - \bar{p})\phi\,dx = \varepsilon^d|Y_1|^{-1}\int_{Y_1}\int_{Y_1}(p(y)\phi(\varepsilon y) - p(y)\phi(\varepsilon z))\,dz\,dy. \tag{4.3.14}$$

Since $\partial\Omega_0^\varepsilon \in C^{0,1}$ and a smooth path with finite length avoiding perforations can be taken, one can get

$$|\phi(\varepsilon y) - \phi(\varepsilon z)| \leq \varepsilon\bar{c}\int_0^1 |\nabla\phi(t\varepsilon y + (1-t)\varepsilon z)\cdot(y-z)|\,dt,$$

with $\xi = ty + (1-t)z$, $\eta = y - z$ and $\bar{c}$ independent of ε, then (4.3.14) can be bounded from above by

$$\left|\int_{\varepsilon Y_1}(p^\varepsilon - \bar{p})\phi\,dx\right| \leq \varepsilon^{d+1}|Y_1|^{-1}\left(\int_{Y_1}\int_{Y_2}|\nabla\phi(\varepsilon\xi)\cdot\eta|^2\,d\eta\,d\xi\right)^{1/2}\left(\int_{Y_1}\int_{Y_1}|p(y)|^2\,dy\,dz\right)^{1/2}. \tag{4.3.15}$$

In (4.3.15), we have denoted $Y_2 := \{y - z : \text{ for } y, z \in Y_1\}$. Also, (4.3.15) leads to

$$\int_{\Omega^\varepsilon}(p^\varepsilon - \bar{p})\phi\,dx \leq C\varepsilon\|p^\varepsilon\|_{L^2(\Omega^\varepsilon)}\|\nabla\phi\|_{L^2(\Omega^\varepsilon)},$$

and with $\phi = p^\varepsilon - \bar{p}$ and (A.0.1), (4.3.15) becomes $\|p^\varepsilon - \bar{p}\|^2_{L^2(\Omega^\varepsilon)} \leq C\varepsilon \left(\|p^\varepsilon\|^2_{L^2(\Omega^\varepsilon)} + \|\nabla p^\varepsilon\|^2_{L^2(\Omega^\varepsilon)} \right)$ and hence, we finally get

$$\|p^\varepsilon - \bar{p}\|_{L^2(\Omega^\varepsilon)} \leq C\varepsilon^{1/2} \|p^\varepsilon\|_{H^1(\Omega^\varepsilon)}.$$

This completes the proof of the lemma. □

We define the following function spaces playing a role in Lemma 4.3.4:

$$H^1\left(\Gamma_N^\varepsilon\right) := \left\{ v \in H^1(\Gamma^\varepsilon) \,|\, -\kappa^\varepsilon \nabla v^\varepsilon \cdot \mathrm{n} = 0 \text{ on } \Gamma_N^\varepsilon \right\},$$

which is a closed subspace of $H^1(\Gamma^\varepsilon)$, and

$$H_+^1(D) := \left\{ v \in H^1(D) \,|\, v \geq 0 \text{ in } D \right\},$$
$$L_+^\infty(D) := \{ v \in L^\infty(D) \,|\, v \geq 0 \text{ in } D \},$$

where D is a suitably measurable set e.g. Ω^ε or Γ^ε.

Lemma 4.3.4. *Let $\theta^\varepsilon \in L^2\left(0,T;H^1\left(\Gamma_N^\varepsilon\right)\right)$ and $\theta^0 \in L^2\left(0,T;H^1(\Omega^\varepsilon)\right)$. For any*

$$f_1 \in C\left([0,T]; H_+^1(\Omega^\varepsilon) \cap L_+^\infty(\Omega^\varepsilon)\right),$$

$$f_2 \in C\left([0,T]; H_+^1(\Gamma^\varepsilon) \cap L_+^\infty(\Gamma^\varepsilon)\right),$$

suppose that there exists $f_3 \in C[0,T]$ such that

$$\int_{\Omega^\varepsilon} f_1 \theta^0 dx = \int_{\Gamma_R^\varepsilon} f_2 \theta^\varepsilon dS_\varepsilon + \varepsilon f_3.$$

Then, it exists a $C > 0$ such that

$$\left| \int_{\Omega^\varepsilon} f_1 \theta^0 \varphi dx - \varepsilon \int_{\Gamma_R^\varepsilon} (f_2 \theta^\varepsilon + \varepsilon f_3) \varphi dS_\varepsilon \right| \leq \varepsilon C \|\varphi\|_{H^1(\Omega^\varepsilon)},$$

for any $\varphi \in H^1(\Omega^\varepsilon)$.

Proof. We adapt Lemma 5.2 from [86] to our context. The proof of the lemma is based on the following auxiliary problem: Given $f_1, f_2, \theta^\varepsilon, \theta^0$ as in the hypothesis of Lemma 4.3.4 and $\tilde{f} \in C[0,T]$, find Ψ such that

$$\begin{cases} \Delta_y \Psi(\cdot, x, y)|_{y=\frac{x}{\varepsilon}} = f_1 \theta^0 & \text{for } x \in \Omega^\varepsilon, \\ \nabla_y \Psi(\cdot, x, y) \cdot \mathrm{n} = f_2 \theta^\varepsilon + \varepsilon \tilde{f} & \text{for } (x,y) \in \Gamma_R^\varepsilon, \\ \nabla_y \Psi \cdot \mathrm{n} = 0 & \text{at } \Gamma_N^\varepsilon. \end{cases} \tag{4.3.16}$$

By [93, Lemma 2.1] and also [30], the problem (4.3.16) has a (weak) Y-periodic solution

$$\Psi(\cdot, x, y)|_{y=\frac{x}{\varepsilon}} \in L^2\left(0,T;H^1(\Omega^\varepsilon)\right)$$

satisfying the integral equality

$$\int_{\Omega^\varepsilon} f_1 \theta^0 dx = \int_{\Gamma^\varepsilon} \left(f_2 \theta^\varepsilon + \varepsilon \tilde{f}\right) dS_\varepsilon = \int_{\Gamma_R^\varepsilon} f_2 \theta^\varepsilon S_\varepsilon + \varepsilon f_3,$$

with f_3 being $\left|\Gamma_R^\varepsilon\right|^{-1}\tilde{f}$. Moreover, that solution is unique up to an additive constant.
Multiplying the first equation in (4.3.16) by $\varphi \in H^1(\Omega^\varepsilon)$ and then integrating the resulting equation over Ω^ε, we arrive at

$$\begin{aligned}
&\left|\int_{\Omega^\varepsilon} f_1\theta^0\varphi dx - \varepsilon\int_{\Gamma_R^\varepsilon}\left(f_2\theta^\varepsilon + \varepsilon\tilde{f}\right)\varphi dS_\varepsilon\right| \\
&\qquad = \left|\int_{\Omega^\varepsilon}\Delta_y\,\Psi(\cdot,x,y)|_{y=\frac{x}{\varepsilon}}\,\varphi dx - \varepsilon\int_{\Gamma_R^\varepsilon} f_2\theta^\varepsilon\varphi dS_\varepsilon - \varepsilon^2\int_{\Gamma_R^\varepsilon}\tilde{f}\varphi dS_\varepsilon\right| \\
&\qquad = \left|\int_{\Omega^\varepsilon}\varepsilon\left(\nabla_x\left[\nabla_y\,\Psi(\cdot,x,y)|_{y=\frac{x}{\varepsilon}}\right] - \nabla_x\nabla_y\,\Psi(\cdot,x,y)|_{y=\frac{x}{\varepsilon}}\right)\varphi\right. \\
&\qquad \left. - \varepsilon\int_{\Gamma_R^\varepsilon} f_2\theta^\varepsilon\varphi dS_\varepsilon - \varepsilon^2\left|\Gamma_R^\varepsilon\right|^{-1}\int_{\Gamma_R^\varepsilon} f_3\varphi dS_\varepsilon\right| \\
&\qquad = \left|\varepsilon\int_{\Gamma^\varepsilon}\left(\nabla_y\,\Psi(\cdot,x,y)|_{y=\frac{x}{\varepsilon}}\cdot \mathrm{n}\varphi dS_\varepsilon - \varepsilon\int_{\Omega^\varepsilon}\nabla_y\,\Psi(\cdot,x,y)|_{y=\frac{x}{\varepsilon}}\,\nabla_x\varphi dx\right)\right. \\
&\qquad - \varepsilon\int_{\Omega^\varepsilon}\nabla_x\nabla_y\,\Psi(\cdot,x,y)|_{y=\frac{x}{\varepsilon}}\,\varphi dx - \varepsilon\int_{\Gamma_R^\varepsilon} f_2\theta^\varepsilon\varphi dS_\varepsilon \\
&\qquad \left. - \varepsilon^2\left|\Gamma_R^\varepsilon\right|^{-1}\int_{\Gamma_R^\varepsilon} f_3\varphi dS_\varepsilon\right|. \qquad (4.3.17)
\end{aligned}$$

Since $\Gamma^\varepsilon = \Gamma_R^\varepsilon \cup \Gamma_N^\varepsilon$, the choice of boundary conditions in (4.3.16) allows the boundary integrals in (4.3.17) to disappear. It follows from the triangle inequality and the Hölder inequality that

$$\begin{aligned}
\left|\int_{\Omega^\varepsilon} f_1\theta^0\varphi dx - \varepsilon\int_{\Gamma_R^\varepsilon}\left(f_2\theta^\varepsilon + \varepsilon\tilde{f}\right)\varphi dS_\varepsilon\right| &\le \varepsilon\left(\left|\int_{\Omega^\varepsilon}\nabla_y\,\Psi(\cdot,x,y)|_{y=\frac{x}{\varepsilon}}\,\nabla_x\varphi dx\right|\right. \\
&\quad \left. + \left|\int_{\Omega^\varepsilon}\nabla_x\nabla_y\,\Psi(\cdot,x,y)|_{y=\frac{x}{\varepsilon}}\,\varphi dx\right|\right) \\
&\le C\varepsilon\,\|\varphi\|_{H^1(\Omega^\varepsilon)}.
\end{aligned}$$

This completes the proof of the lemma. □

4.3.3 Proof of Theorem 4.3.1

The proof of Theorem 4.3.1 relies on a fine control of the ε-dependence needed to estimate each term in (4.3.6)-(4.3.13), following the line of arguments indicated in [40]. At first, the term $\mathscr{I}_1$ can be rewritten as:

$$\begin{aligned}
&\int_{\Omega^\varepsilon}\partial_t\left(\theta^\varepsilon - \theta^0\right)\left(\theta^\varepsilon - \theta^0 - \varepsilon m^\varepsilon\bar{\theta}\left(x,\frac{x}{\varepsilon}\right)\cdot\nabla_x\theta^0\right) \\
&= \frac{1}{2}\frac{d}{dt}\left\|\theta^\varepsilon(t) - \theta^0(t)\right\|^2_{L^2(\Omega^\varepsilon)} - \varepsilon\int_{\Omega^\varepsilon}\partial_t\left(\theta^\varepsilon - \theta^0\right)m^\varepsilon\bar{\theta}\left(x,\frac{x}{\varepsilon}\right)\cdot\nabla_x\theta^0 dx. \qquad (4.3.18)
\end{aligned}$$

Similarly, we proceed to estimate $\mathscr{I}_1^i$ as follows:

$$\int_{\Omega^\varepsilon} \partial_t \left(u_i^\varepsilon - u_i^0\right)\left(u_i^\varepsilon - u_i^0 - \varepsilon m^\varepsilon \bar{u}_i\left(x, \frac{x}{\varepsilon}\right) \cdot \nabla_x u_i^0\right)$$
$$= \frac{1}{2}\frac{d}{dt}\left\|u_i^\varepsilon(t) - u_i^0(t)\right\|_{L^2(\Omega^\varepsilon)}^2 - \varepsilon \int_{\Omega^\varepsilon} \partial_t \left(u_i^\varepsilon - u_i^0\right) m^\varepsilon \bar{u}_i\left(x, \frac{x}{\varepsilon}\right) \cdot \nabla_x u_i^0 dx. \tag{4.3.19}$$

Using the decomposition

$$\kappa^\varepsilon \nabla \theta^\varepsilon - \mathbb{K}\nabla\theta^0 = \kappa^\varepsilon \nabla\left(\theta^\varepsilon - \theta_1^\varepsilon\right) + \kappa^\varepsilon \nabla \theta_1^\varepsilon - \mathbb{K}\nabla\theta^0,$$

the term $\mathscr{I}_2$ thus becomes

$$\mathscr{I}_2 = \int_{\Omega^\varepsilon} \kappa^\varepsilon \nabla\left(\theta^\varepsilon - \theta_1^\varepsilon\right) \cdot \nabla\varphi dx + \int_{\Omega^\varepsilon} \left(\kappa^\varepsilon \nabla\theta_1^\varepsilon - \mathbb{K}\nabla\theta^0\right) \cdot \nabla\varphi dx. \tag{4.3.20}$$

Concerning the first term on the right-hand side of (4.3.20), we get

$$\int_{\Omega^\varepsilon} \kappa^\varepsilon \nabla\left(\theta^\varepsilon - \theta_1^\varepsilon\right) \cdot \nabla\varphi dx \geq \frac{\kappa_{\min}}{2}\left\|\nabla\left(\theta^\varepsilon - \theta_1^\varepsilon\right)(t)\right\|_{L^2(\Omega^\varepsilon)}^2$$
$$- C\varepsilon^2 \left\|\nabla\left((1-m^\varepsilon)\bar{\theta}^\varepsilon \cdot \nabla_x \theta^0(t)\right)\right\|_{L^2(\Omega^\varepsilon)}^2.$$

It is worth pointing out that the cell problems (4.2.28) and (4.2.29) require more regularity on the heat conductivity κ and the diffusion coefficient d_i, namely we need $\kappa, d_i \in H^1(\bar{Y}_1)$. On the other side, since these cell problems are elliptic problems on a non-convex polygon, it is well-known that the cell functions $\bar{\theta}$ and $\bar{u}_i$ usually do not belong to $H^2(Y_1)$ in y regardless how smooth the right-hand sides of (4.2.28) and (4.2.29) are (cf. [61]). Due to the extra regularity on κ and d_i leading to their Lipschitz property in space and due to the Lipschitz boundary of the microstructure, the solutions can be at most in $H^2_{loc}(\bar{Y}_1)$ (see, e.g. [61, Theorem 2.2.2.3]). Notably, that result will not change even if the microstructure boundary is very smooth as in this case. We also emphasize that when investigating problems on domains without holes, the cell problems are then considered to hold in the unit cell Y and, by the convexity of the cell, one obtains the $H^2(Y)$ regularity of the cell functions.

It follows from [103, Theorem 4] that the cell problems (4.2.28)-(4.2.29) admit a unique solution $(\bar{\theta}, \bar{u}_i) \in H_\#^{1+s}(Y_1) \times H_\#^{1+r}(Y_1)$ for some $s, r \in (-\frac{1}{2}, \frac{1}{2})$. Essentially, this hinders us when dealing with the term $\varepsilon\left\|\nabla\left((1-m^\varepsilon)\bar{\theta}^\varepsilon \cdot \nabla_x\theta^0(t)\right)\right\|_{L^2(\Omega^\varepsilon)}$. In fact, we need $\bar{\theta} \in L^\infty(\Omega^\varepsilon; C_\#^1(\bar{Y}_1))$, whereas its maximal regularity only gives $L^\infty(\Omega^\varepsilon; H_\#^{1+s}(Y_1))$ (a similar situation holds for $\bar{u}_i$). Recall the Sobolev embedding $W^{j+s,p}(Y_1) \subset C^j(\bar{Y}_1)$ for $sp > d$ (cf. [2]). Our Hilbertian framework, i.e. $p = 2, j = 1$, requires $s > d/2 \geq 1/2$ which leads to the impossibility of getting $C_\#^1(\bar{Y}_1)$ from $H_\#^{1+s}(Y_1)$. Obviously, one of the possibilities is to working with the domain without holes in one-dimensional, i.e. $d = 1$ and $s = 1$. The fact that $(\bar{\theta}, \bar{u}_i) \in [L^\infty(\Omega^\varepsilon; W_\#^{1+s,2}(Y_1))]^2$ for $s > d/2$ is strictly needed to obtain $(\bar{\theta}, \bar{u}_i) \in [L^\infty(\Omega^\varepsilon; C_\#^1(\bar{Y}_1))]^2$. Then, with the assumption $\theta^0(t,\cdot) \in W^{1,\infty}(\Omega^\varepsilon) \cap H^2(\Omega^\varepsilon)$ and the extra

regularity $\bar{\theta} \in H^1(\Omega^\varepsilon; W^{s,2}_\#(Y_1))$ providing $\bar{\theta} \in H^1(\Omega^\varepsilon; C_\#(\bar{Y}_1))$, we estimate that

$$\begin{aligned}
\varepsilon \left\| \nabla \left((1-m^\varepsilon)\, \bar{\theta}^\varepsilon \cdot \nabla_x \theta^0(t) \right) \right\|_{L^2(\Omega^\varepsilon)} &\leq \varepsilon \left\| \nabla m^\varepsilon \right\|_{L^2(\Omega^\varepsilon)} \left\| \bar{\theta} \right\|_{L^\infty\left(\Omega^\varepsilon; C\left(\bar{Y}_1\right)\right)} \left\| \theta^0(t) \right\|_{W^{1,\infty}(\Omega^\varepsilon)} \\
&\quad + \varepsilon \left\| \nabla_x \bar{\theta} \right\|_{L^2\left(\Omega^\varepsilon; C\left(\bar{Y}_1\right)\right)} \left\| \theta^0(t) \right\|_{W^{1,\infty}(\Omega^\varepsilon)} \\
&\quad + \left\| 1-m^\varepsilon \right\|_{L^2(\Omega^\varepsilon)} \left\| \nabla_y \bar{\theta} \right\|_{L^\infty\left(\Omega^\varepsilon; C\left(\bar{Y}_1\right)\right)} \left\| \theta^0(t) \right\|_{W^{1,\infty}(\Omega^\varepsilon)} \\
&\quad + \varepsilon \left\| \bar{\theta} \right\|_{L^\infty\left(\Omega^\varepsilon; C\left(\bar{Y}_1\right)\right)} \left\| \theta^0(t) \right\|_{H^2(\Omega^\varepsilon)} \\
&\leq C\left(\varepsilon + \varepsilon^{1/2}\right),
\end{aligned}$$

where we use the inequalities (4.2.32) together with the relation $\nabla = \nabla_x + \varepsilon^{-1}\nabla_y$. Observe that

$$\nabla \theta_1^\varepsilon = \nabla_x \theta^0 + \left(\nabla_y \bar{\theta}\right)^\varepsilon \nabla_x \theta^0 + \varepsilon \bar{\theta}^\varepsilon \nabla_x \nabla \theta^0 + \varepsilon \left(\nabla_x \bar{\theta}\right)^\varepsilon \nabla_x \theta^0. \tag{4.3.21}$$

Hence, we get

$$\begin{aligned}
\kappa^\varepsilon \nabla \theta_1^\varepsilon - \mathbb{K} \nabla \theta^0 &= \kappa^\varepsilon \left(\nabla \theta^0 + \left(\nabla_y \bar{\theta}\right)^\varepsilon \nabla_x \theta^0 \right) - \mathbb{K} \nabla \theta^0 \\
&\quad + \kappa^\varepsilon \varepsilon \left(\bar{\theta}^\varepsilon \nabla_x \nabla \theta^0 + \left(\nabla_x \bar{\theta}\right)^\varepsilon \nabla_x \theta^0 \right).
\end{aligned} \tag{4.3.22}$$

We note that the L^2-norm of the second term on the right-hand side of (4.3.22) is bounded from above by

$$\begin{aligned}
\varepsilon \left\| \kappa^\varepsilon \left(\bar{\theta}^\varepsilon \nabla_x \nabla \theta^0 + \left(\nabla_x \bar{\theta}\right)^\varepsilon \nabla_x \theta^0 \right) \right\|_{L^2(\Omega^\varepsilon)} &\leq C\varepsilon \left\| \bar{\theta} \right\|_{L^\infty\left(\Omega^\varepsilon; C\left(\bar{Y}_1\right)\right)} \left\| \theta^0 \right\|_{H^2(\Omega^\varepsilon)} \\
&\quad + C\varepsilon \left\| \nabla_x \bar{\theta} \right\|_{L^2\left(\Omega^\varepsilon; C\left(\bar{Y}_1\right)\right)} \left\| \theta^0 \right\|_{W^{1,\infty}(\Omega^\varepsilon)}.
\end{aligned}$$

Let us handle now the remaining quantity $\kappa^\varepsilon \left(\nabla \theta^0 + \left(\nabla_y \bar{\theta}\right)^\varepsilon \nabla_x \theta^0 \right) - \mathbb{K} \nabla \theta^0$. In fact, recall that $\mathscr{G} := \kappa(\mathbb{I} + \nabla_y \bar{\theta}) - \mathbb{K}$ is divergence-free with respect to $y \in Y_1$ due to the structure of the cell problems in Theorem 4.2.7. Moreover, we know that its average also vanishes, i.e.

$$\int_{Y_1} \mathscr{G} dy = 0,$$

by virtue of the definition of the homogenized heat conductivity $\mathbb{K}$ in Theorem 4.2.5.
As a consequence, $\mathscr{G}$ possesses a vector potential $\mathbf{V}$ and this vector potential is skew-symmetric such that $\mathscr{G} = \nabla_y \mathbf{V}$. In general, the selection of the vector potential is non-unique. However, we can choose $\mathbf{V}$ to solve the Poisson equation $\Delta_y \mathbf{V} = \eta(x,y) \nabla_y \mathscr{G}$ for some function η just depending on the dimensions. Using this equation together with the periodic boundary conditions at ∂Y_0 and the vanishing cell average, we can determine this vector potential $\mathbf{V}$ uniquely. Now, we formulate the quantity $\mathscr{G}^\varepsilon \nabla \theta^0 = \kappa^\varepsilon \left(\nabla \theta^0 + \left(\nabla_y \bar{\theta}\right)^\varepsilon \nabla_x \theta^0 \right) - \mathbb{K} \nabla \theta^0$ in terms of this vector potential. Using the relation $\nabla_y = \varepsilon \nabla - \varepsilon \nabla_x$, we have

$$\mathscr{G}^\varepsilon \nabla \theta^0 = \varepsilon \nabla \cdot (\mathbf{V}^\varepsilon \nabla \theta^0) - \varepsilon \mathbf{V}^\varepsilon \Delta \theta^0 - \varepsilon (\nabla_x \mathbf{V})^\varepsilon \nabla \theta^0. \tag{4.3.23}$$

Due to the skew-symmetry of $\mathbf{V}$ (and also that of $\mathbf{V}^\varepsilon$), the first term on the right-hand side of (4.3.23) is divergence-free, indicating the boundedness in $L^2(\Omega^\varepsilon)$ with the order of $\mathscr{O}(\varepsilon)$. In addition, combining $\bar{\theta} \in L^\infty(\Omega^\varepsilon; W^{1+s,2}_\#(Y_1)) \cap H^1(\Omega^\varepsilon; W^{s,2}_\#(Y_1))$ with the above Poisson equation $\Delta_y \mathbf{V} = \eta(x,y) \nabla_y \mathscr{G}$ subject to the periodic boundary condition yields

$$\left\| \mathbf{V} \right\|_{W^{1+s,2}(Y_1)} \leq C \left\| \mathscr{G} \right\|_{W^{s,2}(Y_1)}.$$

By the compact embedding $W^{s,2}(Y_1) \hookrightarrow\hookrightarrow C(\bar{Y}_1)$ for $s > d/2 \geq 1$, we thus get

$$\mathbf{V} \in L^\infty\left(\Omega^\varepsilon; C_\#\left(\bar{Y}_1\right)\right) \cap H^1\left(\Omega^\varepsilon; C_\#\left(\bar{Y}_1\right)\right).$$

As a consequence, the boundedness in $L^2(\Omega^\varepsilon)$ of the second and third terms on the right-hand side of (4.3.23) is given by

$$\begin{aligned}\varepsilon \left\|\mathbf{V}^\varepsilon \Delta\theta^0 + (\nabla_x \mathbf{V})^\varepsilon \nabla\theta^0\right\|_{L^2(\Omega^\varepsilon)} \leq{}& \varepsilon \left\|\mathbf{V}\right\|_{L^\infty\left(\Omega^\varepsilon; C\left(\bar{Y}_1\right)\right)} \left\|\theta^0\right\|_{H^2(\Omega^\varepsilon)} \\ &+ \varepsilon \left\|\mathbf{V}\right\|_{H^1\left(\Omega^\varepsilon; C\left(\bar{Y}_1\right)\right)} \left\|\theta^0\right\|_{W^{1,\infty}(\Omega^\varepsilon)}.\end{aligned}$$

Therefore, with the help of the Hölder inequality, we note that

$$\int_{\Omega^\varepsilon} \left(\kappa^\varepsilon \nabla\theta_1^\varepsilon - \mathbb{K}\nabla\theta^0\right) \cdot \nabla\varphi \, dx \leq C\varepsilon,$$

which completes the estimates for $\mathscr{I}_2$.
Consequently, we can write

$$\mathscr{I}_2 \geq C \left\|\nabla\left(\theta^\varepsilon - \theta_1^\varepsilon\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d} - C\left(\varepsilon^2 + \varepsilon\right). \tag{4.3.24}$$

Similarly, estimating the term $\mathscr{J}_2^i$ leads to

$$\mathscr{J}_2^i \geq C \left\|\nabla\left(u_i^\varepsilon - u_{i,1}^\varepsilon\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d} - C\left(\varepsilon^2 + \varepsilon\right). \tag{4.3.25}$$

Concerning the estimate of the term $\mathscr{I}_3$, we note the following: Thanks to the compatibility constraint (Theorem 4.3.4) with the choice $\varphi = \theta^\varepsilon - \theta^0$, we get that

$$\begin{aligned}\mathscr{I}_3 &\leq C\varepsilon \left\|\varphi\right\|_{H^1(\Omega^\varepsilon)} \\ &\leq C\varepsilon\left(\left\|\theta^\varepsilon - \theta^0\right\|_{L^2(\Omega^\varepsilon)} + \left\|\nabla\left(\theta^\varepsilon - \theta_1^\varepsilon\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + \left\|\nabla\left(\theta_1^\varepsilon - \theta^0\right)\right\|_{[L^2(\Omega^\varepsilon)]^d}\right) \\ &\leq C\varepsilon\left(\left\|\theta^\varepsilon - \theta^0\right\|_{L^2(\Omega^\varepsilon)} + \left\|\nabla\left(\theta^\varepsilon - \theta_1^\varepsilon\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + C(1+\varepsilon)\right),\end{aligned} \tag{4.3.26}$$

where we use again the difference relation (4.3.21) and get the following bound from above

$$\begin{aligned}\left\|\nabla\left(\theta_1^\varepsilon - \theta^0\right)\right\|_{L^2(\Omega^\varepsilon)} \leq{}& \left\|\nabla_y \bar{\theta}\right\|_{L^\infty\left(\Omega^\varepsilon; C\left(\bar{Y}_1\right)\right)} \left\|\theta^0\right\|_{W^{1,\infty}(\Omega^\varepsilon)} \\ &+ \varepsilon\left(\left\|\bar{\theta}\right\|_{L^\infty\left(\Omega^\varepsilon; C\left(\bar{Y}_1\right)\right)} \left\|\theta^0\right\|_{H^2(\Omega^\varepsilon)} + \left\|\nabla_x \bar{\theta}\right\|_{L^2\left(\Omega^\varepsilon; C\left(\bar{Y}_1\right)\right)} \left\|\theta^0\right\|_{W^{1,\infty}(\Omega^\varepsilon)}\right).\end{aligned}$$

Similarly, the term $\mathscr{J}_3^i$ is bounded from above by

$$\mathscr{J}_3^i \leq C\varepsilon\left(\left\|u_i^\varepsilon - u_i^0\right\|_{L^2(\Omega^\varepsilon)} + \left\|\nabla\left(u_i^\varepsilon - u_{i,1}^\varepsilon\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + C(1+\varepsilon)\right). \tag{4.3.27}$$

Note the elementary decomposition:

$$\begin{aligned}\tau^\varepsilon \nabla^\delta u_i^\varepsilon \cdot \nabla\theta^\varepsilon - \left(\mathbb{T}^i \nabla^\delta u_i^0\right) \cdot \nabla\theta^0 ={}& \left(\tau^\varepsilon - \mathbb{T}^i\right) \nabla^\delta u_i^\varepsilon \cdot \nabla\theta^\varepsilon \\ &+ \mathbb{T}^i\left(\nabla^\delta u_i^\varepsilon - \nabla^\delta u_i^0\right) \cdot \nabla\theta^\varepsilon + \mathbb{T}^i\left(\nabla\theta^\varepsilon - \nabla\theta^0\right) \cdot \nabla^\delta u_i^0.\end{aligned}$$

Multiplying the above equation by the test function φ, we arrive at

$$\begin{aligned}\left(\tau^\varepsilon \nabla^\delta u_i^\varepsilon \cdot \nabla\theta^\varepsilon - \left(\mathbb{T}^i \nabla^\delta u_i^0\right)\cdot\nabla\theta^0\right)\varphi &= \left(\tau^\varepsilon - \mathbb{T}^i\right)\nabla^\delta u_i^\varepsilon \cdot \nabla\theta^\varepsilon\left(\theta^\varepsilon - \theta^0\right)\\ &\quad - \varepsilon\left(\tau^\varepsilon - \mathbb{T}^i\right)\nabla^\delta u_i^\varepsilon \cdot \nabla\theta^\varepsilon m^\varepsilon \bar{\theta}^\varepsilon \cdot \nabla_x\theta^0\\ &\quad + \mathbb{T}^i\left(\nabla^\delta u_i^\varepsilon - \nabla^\delta u_i^0\right)\cdot\nabla\theta^\varepsilon\left(\theta^\varepsilon - \theta^0\right)\\ &\quad - \varepsilon\mathbb{T}^i\left(\nabla^\delta u_i^\varepsilon - \nabla^\delta u_i^0\right)\cdot\nabla\theta^\varepsilon m^\varepsilon \bar{\theta}^\varepsilon \cdot \nabla_x\theta^0\\ &\quad + \mathbb{T}^i\left(\nabla\theta^\varepsilon - \nabla\theta^0\right)\cdot\nabla^\delta u_i^0\left(\theta^\varepsilon - \theta^0\right)\\ &\quad - \varepsilon\mathbb{T}^i\left(\nabla\theta^\varepsilon - \nabla\theta^0\right)\cdot\nabla^\delta u_i^0 m^\varepsilon \bar{\theta}^\varepsilon \cdot \nabla_x\theta^0\\ &= \sum_{k=1}^{6}\mathscr{I}_4^k.\end{aligned}$$

To be able to estimate $\mathscr{I}_4$, we need to ensure the boundedness of each of the terms $\int_{\Omega^\varepsilon}\mathscr{I}_4^{k_i}$ for $k_i \in \{1,\dots,6\}$ and $i \in \{1,\dots,N\}$. We obtain:

$$\begin{aligned}\int_{\Omega^\varepsilon}\left|\mathscr{I}_4^2\right|dx &\le \varepsilon\left\|\nabla^\delta u_i^\varepsilon\cdot\nabla\theta^\varepsilon\right\|_{L^2(\Omega^\varepsilon)}\left\|\left(\tau^\varepsilon - \mathbb{T}^i\right)m^\varepsilon\bar{\theta}\left(\frac{x}{\varepsilon}\right)\cdot\nabla_x\theta^0\right\|_{L^2(\Omega^\varepsilon)}\\ &\le \varepsilon\left\|u_i^\varepsilon\right\|_{L^\infty(\Omega^\varepsilon)}\|\nabla\theta^\varepsilon\|_{[L^2(\Omega^\varepsilon)]^d}\left\|\bar{\theta}\right\|_{L^\infty(\Omega^\varepsilon;C(Y_1))}\left\|\theta^0\right\|_{W^{1,\infty}(\Omega^\varepsilon)}\left\|\tau^\varepsilon - \mathbb{T}^i\right\|_{L^2(\Omega^\varepsilon)},\end{aligned}\tag{4.3.28}$$

and

$$\begin{aligned}\int_{\Omega^\varepsilon}\left|\mathscr{I}_4^4\right|dx &\le \frac{\varepsilon}{2}\left|\mathbb{T}^i\right|\left\|\left(\nabla^\delta u_i^\varepsilon - \nabla^\delta u_i^0\right)\cdot\nabla\theta^\varepsilon\right\|_{L^2(\Omega^\varepsilon)}\left\|m^\varepsilon\bar{\theta}\left(\frac{x}{\varepsilon}\right)\cdot\nabla_x\theta^0\right\|_{L^2(\Omega^\varepsilon)}\\ &\le \frac{\varepsilon}{2}\left|\mathbb{T}^i\right|C_\delta^2\left\|u_i^\varepsilon - u_i^0\right\|_{L^2(\Omega^\varepsilon)}\|\nabla\theta^\varepsilon\|_{[L^2(\Omega^\varepsilon)]^d}\left\|\bar{\theta}\right\|_{L^\infty(\Omega^\varepsilon;C(Y_1))}\left\|\theta^0\right\|_{W^{1,\infty}(\Omega^\varepsilon)}.\end{aligned}\tag{4.3.29}$$

Furthermore, we estimate

$$\begin{aligned}\int_{\Omega^\varepsilon}\left|\mathscr{I}_4^1\right|dx &\le \left\|\tau^\varepsilon - \mathbb{T}^i\right\|_{L^2(\Omega^\varepsilon)}\left\|\nabla^\delta u_i^\varepsilon\cdot\nabla\theta^\varepsilon\right\|_{L^2(\Omega^\varepsilon)}\left\|\theta^\varepsilon - \theta^0\right\|_{L^\infty(\Omega^\varepsilon)}\\ &\le C_\delta\left\|\tau^\varepsilon - \mathbb{T}^i\right\|_{L^2(\Omega^\varepsilon)}\left\|u_i^\varepsilon\right\|_{L^\infty(\Omega^\varepsilon)}\|\nabla\theta^\varepsilon\|_{[L^2(\Omega^\varepsilon)]^d}\left(\|\theta^\varepsilon\|_{L^\infty(\Omega^\varepsilon)} + \left\|\theta^0\right\|_{W^{1,\infty}(\Omega^\varepsilon)}\right),\end{aligned}\tag{4.3.30}$$

and by Young's inequality (cf. Lemma A.0.7), it yields

$$\begin{aligned}\int_{\Omega^\varepsilon}\left|\mathscr{I}_4^3\right|dx &\le \frac{\left|\mathbb{T}^i\right|^2}{2}C_\delta^2\left\|\nabla^\delta u_i^\varepsilon - \nabla^\delta u_i^0\right\|_{L^\infty(\Omega^\varepsilon)}^2\|\nabla\theta^\varepsilon\|_{[L^2(\Omega^\varepsilon)]^d}^2 + \frac{1}{2}\left\|\theta^\varepsilon - \theta^0\right\|_{L^2(\Omega^\varepsilon)}^2\\ &\le \frac{\left|\mathbb{T}^i\right|^2}{2}C_\delta^4\|\nabla\theta^\varepsilon\|_{[L^2(\Omega^\varepsilon)]^d}^2\left\|u_i^\varepsilon - u_i^0\right\|_{L^2(\Omega^\varepsilon)}^2 + \frac{1}{2}\left\|\theta^\varepsilon - \theta^0\right\|_{L^2(\Omega^\varepsilon)}^2,\end{aligned}\tag{4.3.31}$$

and

$$\begin{aligned}\int_{\Omega^\varepsilon}\left|\mathscr{I}_4^5\right|dx &\le \frac{|\mathbb{T}_i|^2}{2}\left\|\left(\nabla\theta^\varepsilon - \nabla\theta^0\right)\cdot\nabla^\delta u_i^0\right\|_{L^2(\Omega^\varepsilon)}^2 + \frac{1}{2}\left\|\theta^\varepsilon - \theta^0\right\|_{L^2(\Omega^\varepsilon)}^2\\ &\le \frac{|\mathbb{T}_i|^2}{2}C_\delta^2\left\|u_i^0\right\|_{L^\infty(\Omega^\varepsilon)}^2\left\|\nabla\theta^\varepsilon - \nabla\theta^0\right\|_{[L^2(\Omega^\varepsilon)]^d}^2 + \frac{1}{2}\left\|\theta^\varepsilon - \theta^0\right\|_{L^2(\Omega^\varepsilon)}^2,\end{aligned}\tag{4.3.32}$$

$$\int_{\Omega^\varepsilon}\left|\mathscr{I}_4^6\right|dx \le \frac{\varepsilon\,|\mathbb{T}_i|^2}{2}\left\|u_i^0\right\|_{L^\infty(\Omega^\varepsilon)}^2\left\|\nabla\theta^\varepsilon - \nabla\theta^0\right\|_{[L^2(\Omega^\varepsilon)]^d}^2 + \frac{\varepsilon}{2}\left\|\bar{\theta}\right\|_{L^\infty\left(\Omega^\varepsilon;C(\bar{Y}_1)\right)}^2\left\|\theta^0\right\|_{W^{1,\infty}(\Omega^\varepsilon)}^2.\tag{4.3.33}$$

Remark that the first integral in $\mathscr{J}_4^i$ can be estimated similarly. On top of that, observe that we can find constants $C_{R_i} > 0$ (independent of ε) such that

$$\left\|R_i\left(u^\varepsilon\right)-R_i\left(u^0\right)\right\|_{L^2(\Omega^\varepsilon)} \leq C_{R_i}\sum_{j=1}^{N}\left\|u_j^\varepsilon-u_j^0\right\|_{L^2(\Omega^\varepsilon)} \quad \text{for } i\in\{1,\ldots,N\},$$

in which the constants C_{R_i} depend on the L^∞-bounds of the concentrations u^ε, u^0 as discussed in [69, Section 5].

The estimate on the second integral of $\mathscr{J}_4^i$ can be computed directly. Note that for $i \in \{1,\ldots,N\}$, we have:

$$\begin{aligned}\left(R_i\left(u^\varepsilon\right)-R_i\left(u^0\right)\right)\phi_i &= \left(R_i\left(u^\varepsilon\right)-R_i\left(u^0\right)\right)\left(u_i^\varepsilon-u_i^0\right)\\ &\quad -\varepsilon\left(R_i\left(u^\varepsilon\right)-R_i\left(u^0\right)\right)m^\varepsilon\bar{u}_i\left(\frac{x}{\varepsilon}\right)\cdot\nabla_x u_i^0.\end{aligned}$$

This gives

$$\begin{aligned}\int_{\Omega^\varepsilon}\left(R_i\left(u^\varepsilon\right)-R_i\left(u^0\right)\right)\phi_i dx &\leq C_{R_i}\sum_{j=1}^{N}\left\|u_j^\varepsilon-u_j^0\right\|_{L^2(\Omega^\varepsilon)}\Big(\left\|u_i^\varepsilon-u_i^0\right\|_{L^2(\Omega^\varepsilon)}\\ &\quad +\varepsilon\left\|\bar{u}_i\right\|_{L^\infty\left(\Omega^\varepsilon;C(\bar{Y}_1)\right)}\left\|u_i^0\right\|_{W^{1,\infty}(\Omega^\varepsilon)}\Big).\end{aligned} \tag{4.3.34}$$

Collecting the estimates (4.3.24), (4.3.25), (4.3.26), (4.3.27), (4.3.28)-(4.3.33) and (4.3.34), we obtain:

$$\begin{aligned}&\left\|\nabla\left(\theta^\varepsilon-\theta_1^\varepsilon\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}+\sum_{i=1}^{N}\left\|\nabla\left(u_i^\varepsilon-u_{i,1}^\varepsilon\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}\\ &\leq C\left(\varepsilon^2+\varepsilon\right)+C\varepsilon\left(\left\|\theta^\varepsilon(t)-\theta^0(t)\right\|_{L^2(\Omega^\varepsilon)}+\left\|\nabla\left(\theta^\varepsilon-\theta_1^\varepsilon\right)(t)\right\|_{[L^2(\Omega^\varepsilon)]^d}+C(1+\varepsilon)\right)\\ &+C\varepsilon\sum_{i=1}^{N}\left(\left\|u_i^\varepsilon(t)-u_i^0(t)\right\|_{L^2(\Omega^\varepsilon)}+\left\|\nabla\left(u_i^\varepsilon-u_{i,1}^\varepsilon\right)(t)\right\|_{[L^2(\Omega^\varepsilon)]^d}+C(1+\varepsilon)\right)\\ &+C\left(\left\|\tau^\varepsilon-\mathbb{T}^i\right\|_{L^2(\Omega^\varepsilon)}\left\|\theta^\varepsilon(t)-\theta^0(t)\right\|_{L^2(\Omega^\varepsilon)}+\sum_{i=1}^{N}\left\|\rho_i^\varepsilon-\mathbb{F}^i\right\|_{L^2(\Omega^\varepsilon)}\left\|u_i^\varepsilon(t)-u_i^0(t)\right\|_{L^2(\Omega^\varepsilon)}\right)\\ &+C\varepsilon\left(\sum_{i=1}^{N}\left\|u_i^\varepsilon(t)-u_i^0(t)\right\|_{L^2(\Omega^\varepsilon)}+\left\|\theta^\varepsilon(t)-\theta^0(t)\right\|_{L^2(\Omega^\varepsilon)}\right)\\ &+C\left(\sum_{i=1}^{N}\left\|u_i^\varepsilon(t)-u_i^0(t)\right\|^2_{L^2(\Omega^\varepsilon)}+\left\|\theta^\varepsilon(t)-\theta^0(t)\right\|^2_{L^2(\Omega^\varepsilon)}\right)\\ &+C\varepsilon\left(\left\|\nabla\left(\theta^\varepsilon-\theta^0\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}+\sum_{i=1}^{N}\left\|\nabla\left(u_i^\varepsilon-u_i^0\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}\right)+C\varepsilon.\end{aligned}$$

Notably, Theorem 4.3.3 provides us that the L^2-error estimates between the Soret and Dufour coefficients and their homogenized (averaged) versions, i.e. $\left\|\tau^\varepsilon-\mathbb{T}^i\right\|_{L^2(\Omega^\varepsilon)}$ and $\left\|\rho_i^\varepsilon-\mathbb{F}^i\right\|_{L^2(\Omega^\varepsilon)}$

are of the order $\mathscr{O}(\varepsilon^{1/2})$. It thus yields that

$$
\begin{aligned}
&\left\|\nabla\left(\theta^{\varepsilon}-\theta_1^{\varepsilon}\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}+\sum_{i=1}^{N}\left\|\nabla\left(u_i^{\varepsilon}-u_{i,1}^{\varepsilon}\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}\\
&\leq C\left(\varepsilon^2+\varepsilon\right)+C\varepsilon\left(\left\|\theta^{\varepsilon}(t)-\theta^0(t)\right\|_{L^2(\Omega^\varepsilon)}+\left\|\nabla\left(\theta^{\varepsilon}-\theta_1^{\varepsilon}\right)(t)\right\|_{[L^2(\Omega^\varepsilon)]^d}\right)\\
&+C\varepsilon\sum_{i=1}^{N}\left(\left\|u_i^{\varepsilon}(t)-u_i^0(t)\right\|_{L^2(\Omega^\varepsilon)}+\left\|\nabla\left(u_i^{\varepsilon}-u_{i,1}^{\varepsilon}\right)(t)\right\|_{[L^2(\Omega^\varepsilon)]^d}\right)\\
&+C\varepsilon^{1/2}\left(\left\|\theta^{\varepsilon}(t)-\theta^0(t)\right\|_{L^2(\Omega^\varepsilon)}+\sum_{i=1}^{N}\left\|u_i^{\varepsilon}(t)-u_i^0(t)\right\|_{L^2(\Omega^\varepsilon)}\right)\\
&+C\left(\sum_{i=1}^{N}\left\|u_i^{\varepsilon}(t)-u_i^0(t)\right\|^2_{L^2(\Omega^\varepsilon)}+\left\|\theta^{\varepsilon}(t)-\theta^0(t)\right\|^2_{L^2(\Omega^\varepsilon)}\right)\\
&+C\varepsilon\left(\left\|\nabla\left(\theta^{\varepsilon}-\theta_1^{\varepsilon}\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}+\sum_{i=1}^{N}\left\|\nabla\left(u_i^{\varepsilon}-u_{i,1}^{\varepsilon}\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}\right).
\end{aligned}
\tag{4.3.35}
$$

It now remains to estimate the second term on the right-hand side of (4.3.18)-(4.3.19). In fact, integrating by parts gives

$$
\begin{aligned}
&\int_0^t\int_{\Omega^\varepsilon} m^{\varepsilon}\partial_t\left(u_i^{\varepsilon}-u_i^0\right)\bar{u}_i\left(\frac{x}{\varepsilon}\right)\cdot\nabla_x u_i^0(s,x)\,dxds\\
&\qquad=\int_{\Omega^\varepsilon} m^{\varepsilon}\left(u_i^{\varepsilon}-u_i^0\right)\bar{u}_i\left(\frac{x}{\varepsilon}\right)\cdot\nabla_x u_i^0(s,x)\,dx\Big|_{s=0}^{s=t}\\
&\qquad-\int_0^t\int_{\Omega^\varepsilon} m^{\varepsilon}\left(u_i^{\varepsilon}-u_i^0\right)\bar{u}_i\left(\frac{x}{\varepsilon}\right)\cdot\nabla_x\partial_t u_i^0(s,x)\,dxds.
\end{aligned}
$$

We then observe that

$$
\begin{aligned}
&\varepsilon\left|\int_{\Omega^\varepsilon} m^{\varepsilon}\left[\left(u_i^{\varepsilon}-u_i^0\right)-\left(u_i^{\varepsilon}(0)-u_i^0(0)\right)\right]\bar{u}_i^{\varepsilon}\cdot\nabla_x u_i^0(t,x)\,dx\right|\\
&\qquad\leq C\varepsilon\left(\left\|u_i^{\varepsilon}(t)-u_i^0(t)\right\|_{L^2(\Omega^\varepsilon)}+\left\|u_i^{\varepsilon,0}-u_i^{0,0}\right\|_{L^2(\Omega^\varepsilon)}\right),
\end{aligned}
$$

and hence,

$$
\begin{aligned}
&\varepsilon\left|\int_{\Omega^\varepsilon} m^{\varepsilon}\left[\left(\theta^{\varepsilon}-\theta^0\right)-\left(\theta^{\varepsilon}(0)-\theta^0(0)\right)\right]\bar{\theta}^{\varepsilon}\cdot\nabla_x\theta^0(t,x)\,dx\right|\\
&\qquad\leq C\varepsilon\left(\left\|\theta^{\varepsilon}(t)-\theta^0(t)\right\|_{L^2(\Omega^\varepsilon)}+\left\|\theta^{\varepsilon,0}-\theta^{0,0}\right\|_{L^2(\Omega^\varepsilon)}\right).
\end{aligned}
$$

For all $t\in(0,T]$, we set

$$
\begin{aligned}
w_1(t)&=\left\|\theta^{\varepsilon}(t)-\theta^0(t)\right\|^2_{L^2(\Omega^\varepsilon)}+\sum_{i=1}^{N}\left\|u_i^{\varepsilon}(t)-u_i^0(t)\right\|^2_{L^2(\Omega^\varepsilon)},\\
w_2(t)&=\left\|\nabla\left(\theta^{\varepsilon}-\theta_1^{\varepsilon}\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}+\sum_{i=1}^{N}\left\|\nabla\left(u_i^{\varepsilon}-u_{i,1}^{\varepsilon}\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d},\\
w_0&=\left\|\theta^{\varepsilon,0}-\theta^{0,0}\right\|^2_{L^2(\Omega^\varepsilon)}+\sum_{i=1}^{N}\left\|u_i^{\varepsilon,0}-u_i^{0,0}\right\|^2_{L^2(\Omega^\varepsilon)}.
\end{aligned}
$$

Then, when integrating (4.3.35) and (4.3.18)-(4.3.19) from 0 to t, we are led to the following Gronwall-like estimate

$$w_1(t)+\int_0^t w_2(s)\,ds \le C\left(\varepsilon^2+\varepsilon+(1+\varepsilon)w_0+\varepsilon\int_0^t w_1(s)\,ds\right),$$

which can be rewritten as

$$w_1(t)+\int_0^t w_2(s)\,ds \le C(\varepsilon+(1+\varepsilon)w_0)e^{C\varepsilon t} \quad \text{for } t\in[0,T]. \tag{4.3.36}$$

Finally, we turn our attention to the corrector estimate for v_i^ε. For $i\in\{1,...,N\}$ we consider the equation for the reconstruction $v_{i,0}^\varepsilon = v_i^0$, obtained from (4.2.23), with the test function $\psi_i\in L^2(\Gamma^\varepsilon)$ and integrate the resulting equation over Γ^ε to get

$$\varepsilon\int_{\Gamma^\varepsilon}\partial_t v_i^0\psi_i\,dS_\varepsilon = \varepsilon\int_{\Gamma^\varepsilon}\left(A_iu_i^0-B_iv_i^0\right)\psi_i\,dS_\varepsilon. \tag{4.3.37}$$

Then, we find the difference equation for the micro concentration v_i^ε and the reconstruction v_i^0 by subtracting the third equation of (4.2.13) and (4.3.37), provided that

$$\begin{aligned}\varepsilon\int_{\Gamma^\varepsilon}\partial_t\left(v_i^\varepsilon-v_i^0\right)\psi_i\,dS_\varepsilon &= \varepsilon\int_{\Gamma^\varepsilon}\left(a_i^\varepsilon u_i^\varepsilon-A_iu_i^0\right)\psi_i\,dS_\varepsilon-\varepsilon\int_{\Gamma^\varepsilon}\left(b_i^\varepsilon v_i^\varepsilon-B_iv_i^0\right)\psi_i\,dS_\varepsilon\\ &= \varepsilon\int_{\Gamma^\varepsilon}\left[a_i^\varepsilon\left(u_i^\varepsilon-u_i^0\right)+\left(a_i^\varepsilon-A_i\right)u_i^0\right]\psi_i\,dS_\varepsilon\\ &\quad-\varepsilon\int_{\Gamma^\varepsilon}\left[b_i^\varepsilon\left(v_i^\varepsilon-v_i^0\right)+\left(b_i^\varepsilon-B_i\right)v_i^0\right]\psi_i\,dS_\varepsilon.\end{aligned}$$

Hereby, we choose $\psi_i = v_i^\varepsilon - v_i^0$ to obtain the following estimate

$$\begin{aligned}\frac{\varepsilon}{2}\frac{d}{dt}\left\|v_i^\varepsilon-v_i^0\right\|^2_{L^2(\Gamma^\varepsilon)} &\le C\varepsilon\left(\left\|u_i^\varepsilon-u_i^0\right\|^2_{L^2(\Gamma^\varepsilon)}+\left\|v_i^\varepsilon-v_i^0\right\|^2_{L^2(\Gamma^\varepsilon)}\right)\\ &\quad+\varepsilon\int_{\Gamma^\varepsilon}\left|a_i^\varepsilon-A_i\right|\left|u_i^0\right|\left|v_i^\varepsilon-v_i^0\right|dS_\varepsilon\\ &\quad+\varepsilon\int_{\Gamma^\varepsilon}\left|b_i^\varepsilon-B_i\right|\left|v_i^0\right|\left|v_i^\varepsilon-v_i^0\right|dS_\varepsilon.\end{aligned} \tag{4.3.38}$$

Since Ω^ε is a Lipschitz domain, we recall the trace embedding $H^1(\Omega^\varepsilon)\subset L^q(\partial\Omega^\varepsilon)$ which holds for $1\le q\le 2^*_{\partial\Omega^\varepsilon}$ where $2^*_{\partial\Omega^\varepsilon}=2(d-1)/(d-2)$ if $d\ge 3$, and $2^*_{\partial\Omega^\varepsilon}=\infty$ if $d=2$ (cf. [44]). Therefore, if $d=2$, then we continue to estimate (4.3.38) as follows:

$$\begin{aligned}\frac{\varepsilon}{2}\frac{d}{dt}\sum_{i=1}^N\left\|v_i^\varepsilon-v_i^0\right\|^2_{L^2(\Gamma^\varepsilon)} &\le C\varepsilon\left(\sum_{i=1}^N\left\|u_i^\varepsilon-u_i^0\right\|^2_{L^2(\Gamma^\varepsilon)}+\sum_{i=1}^N\left\|v_i^\varepsilon-v_i^0\right\|^2_{L^2(\Gamma^\varepsilon)}\right)\\ &\quad+C\varepsilon\left(\sum_{i=1}^N\left\|a_i^\varepsilon-A_i\right\|^2_{L^2(\Gamma^\varepsilon)}+\sum_{i=1}^N\left\|b_i^\varepsilon-B_i\right\|^2_{L^2(\Gamma^\varepsilon)}\right).\end{aligned}$$

Using the trace inequality (A.0.2) for the difference norms $\left\|a_i^\varepsilon-A_i\right\|_{L^2(\Gamma^\varepsilon)}$, $\left\|b_i^\varepsilon-B_i\right\|_{L^2(\Gamma^\varepsilon)}$ and $\left\|u_i^\varepsilon-u_i^0\right\|_{L^2(\Gamma^\varepsilon)}$ together with Lemma 4.3.3 and (4.3.36) gives

$$\frac{\varepsilon}{2}\frac{d}{dt}\sum_{i=1}^N\left\|v_i^\varepsilon-v_i^0\right\|^2_{L^2(\Gamma^\varepsilon)} \le C\max\{\varepsilon,\varepsilon^\gamma\}+C\varepsilon\sum_{i=1}^N\left\|v_i^\varepsilon-v_i^0\right\|^2_{L^2(\Gamma^\varepsilon)}. \tag{4.3.39}$$

Note herein that the gradient norms are ignored when applying the trace inequality to the differences. It is simply because that they are of the order $\mathcal{O}(\varepsilon^2)$ by their own regularity. Henceforward, we apply the Gronwall inequality to (4.3.39) and obtain

$$\varepsilon \sum_{i=1}^{N} \left\| v_i^\varepsilon - v_i^0 \right\|_{L^2(\Gamma^\varepsilon)}^2 \leq C \max\{\varepsilon, \varepsilon^\gamma\} e^{C\varepsilon t}.$$

In the same manner, if $d \geq 3$, we can now bound in (4.3.38) the absolute differences $\left| a_i^\varepsilon - A_i \right|$ and $\left| b_i^\varepsilon - B_i \right|$ from above by a constant C independent of ε (by (A_1)) and then get back the estimate (4.3.39).
This completes the proof of Theorem 4.3.1.

4.4 Concluding remarks

In this work, we have presented corrector estimates for the homogenization limit for a thermo-diffusion system with Smoluchowski interactions coupled with a system of differential equations, posed in a perforated domain. This type of error-control justifies the formal homogenization asymptotics obtained in [75] and completes the convergence result in [74] by giving convergence rates. This is done using the concept of macroscopic reconstruction together with fine integral estimates on the solution and oscillating coefficients. Compared to Chapter 2 and Chapter 3, we see that the estimates are rather complicated when dealing with a more realistic model with several equations. The required regularity of the involved limit and cell functions is also different. However, in general we all need higher regularity to get strong convergences. Accordingly, that is the price as one can expect. Moreover, the speed of convergence is now affected by the choice of the initial value of reconstructions. This means that if the initial homogenization limit is large, there is no way to get a good approximation of the micro-concentrations in any time. Essentially, our working technique can be applied to a larger class of coupled nonlinear systems of partial differential equations posed in perforated media.

CHAPTER 5

Correctors justification for a Stokes-Nernst-Planck-Poisson model in perforated domains

5.1 Introduction

Colloidal dynamics is a relevant research topic of interest from both theoretical perspectives and modern industrial applications. Relevant technological applications include oil recovery and transport [110], drug-delivery design [82], motion of micro-organisms in biological suspensions [38], harvesting energy via solar cells [18], and also, sol-gel synthesis [23]. Typically, they all involve different phases of dispersed media (solid morphologies), which resemble at least remotely to homogeneous domains paved with arrays of contrasting microstructures that are distributed periodically. Mathematically, the interplay between populations of colloidal particles leads to work in the multiscale analysis of PDEs especially what concerns the Smoluchowski coagulation-fragmentation system and the Stokes-Nernst-Planck-Poisson system, which is our target here.

It is well known (cf. [35], e.g.) that many particles in colloidal chemistry are able to carry electrical charges (positive or negative) and, in some circumstances, they can be described using intensive quantities like the number density or ions concentration, say $c_\varepsilon^\pm$. Following [42], we consider such concentrations $c_\varepsilon^\pm$ of electrically charged colloidal particles to be involved as unknowns in the Nernst-Planck equations. These equations model the diffusion, deposition, convection and electrostatic interaction within a porous medium. The associated electrostatic potential, called here Φ_ε, is usually determined by a Poisson equation linearly coupled with the densities of charged species, describing the electric field formation inside the heterogeneous domain. Colloidal particles are always immersed in a background fluid. Here, we assume that the fluid velocity v_ε fulfills a suitable variant of the Stokes equations.

It is the aim of this chapter to explore mathematically the upscaling of such non-stationary Stokes-Nernst-Planck-Poisson (SNPP) systems posed in a porous medium $\Omega^\varepsilon \subset \mathbb{R}^d$, where $\varepsilon \in (0,1)$ represents the scale parameter relative to the perforation (pore sizes) of the domain. To be more precise, we wish to justify the homogenization asymptotics for a class of SNPP systems developed by the group of Prof. P. Knabner in Erlangen, Germany, that fit well to the motion of charged colloidal particles through saturated soils.

As starting point of the discussion, we consider the following microscopic Stokes-Nernst-

Planck-Poisson (SNPP) system:

$$-\varepsilon^2\Delta v_\varepsilon + \nabla p_\varepsilon = -\varepsilon^\beta\left(c_\varepsilon^+ - c_\varepsilon^-\right)\nabla\Phi_\varepsilon \text{ in } Q_T^\varepsilon := (0,T)\times\Omega^\varepsilon, \tag{5.1.1}$$

$$\nabla\cdot v_\varepsilon = 0 \text{ in } Q_T^\varepsilon, \tag{5.1.2}$$

$$v_\varepsilon = 0 \text{ on } (0,T)\times(\Gamma^\varepsilon\cup\partial\Omega), \tag{5.1.3}$$

$$-\varepsilon^\alpha\Delta\Phi_\varepsilon = c_\varepsilon^+ - c_\varepsilon^- \text{ in } Q_T^\varepsilon, \tag{5.1.4}$$

$$\varepsilon^\alpha\nabla\Phi_\varepsilon\cdot \mathrm{n} = 0 \text{ on } (0,T)\times\partial\Omega, \tag{5.1.5}$$

$$\partial_t c_\varepsilon^\pm + \nabla\cdot\left(v_\varepsilon c_\varepsilon^\pm - \nabla c_\varepsilon^\pm \mp \varepsilon^\gamma c_\varepsilon^\pm\nabla\Phi_\varepsilon\right) = R_\varepsilon^\pm\left(c_\varepsilon^+, c_\varepsilon^-\right) \text{ in } Q_T^\varepsilon, \tag{5.1.6}$$

$$-\left(v_\varepsilon c_\varepsilon^\pm - \nabla c_\varepsilon^\pm \mp \varepsilon^\gamma c_\varepsilon^\pm\nabla\Phi_\varepsilon\right)\cdot \mathrm{n} = 0 \text{ on } (0,T)\times(\Gamma^\varepsilon\cup\partial\Omega), \tag{5.1.7}$$

$$c_\varepsilon^\pm = c^{\pm,0} \text{ in } \{t=0\}\times\Omega^\varepsilon. \tag{5.1.8}$$

We refer to (5.1.1)-(5.1.8) as (P^ε). The system (5.1.1)-(5.1.8) is endowed either with

$$\varepsilon^\alpha\nabla\Phi_\varepsilon\cdot \mathrm{n} = \varepsilon\sigma \text{ on } (0,T)\times\Gamma_N^\varepsilon, \tag{5.1.9}$$

or with

$$\Phi_\varepsilon = \Phi_D \text{ on } (0,T)\times\Gamma_D^\varepsilon. \tag{5.1.10}$$

We deliberately use variable scaling parameters α,β,γ for the ratio of the magnitudes of differently incorporated physical processes to weigh the effect a certain heterogeneity (morphology) has on effective transport coefficients.

A few additional remarks are in order: The background fluid (solvent) is assumed to be isothermal, incompressible and electrically neutral. The movement of this liquid at low Reynolds numbers decides the momentum equation behind our Stokes flow (see in (5.1.1)-(5.1.3)). The Stokes equation further couples to the mass balance equations of the involved colloidal species as described by the Nernst-Planck equations in (5.1.6)-(5.1.8). The initial charged densities $c^{\pm,0}$ are present cf. (5.1.8). The Poisson-type equation points out an induced electric field acting on the liquid as well as on the charges carried by the colloidal species (see in (5.1.4)-(5.1.5)). The surface charge density σ of the porous medium is prescribed as in (5.1.9).

Although it can in principle introduce a boundary layer potentially interacting with the homogenization asymptotics, the magnitude of the ζ-potential Φ_D in (5.1.10) does not influence our theoretical results. Here, it only indicates the degree of electrostatic repulsion between charged colloidal particles within a dispersion. In fact, experiments provide that colloids with high ζ-potential (i.e. $\Phi_D \gg 1$ or $\Phi_D \ll -1$) are electrically stabilized while with low ζ-potential, they tend to coagulate or flocculate rapidly (see e.g. [59, 88] for a detailed calculation).

Specific scenarios for averaging Poisson-Nernst-Planck (PNP) systems as well as Stokes-Nernst-Planck-Poisson (SNPP) systems were discussed in a number of recent papers; see e.g. [106, 104, 50, 47, 54, 53]. The SNPP-type models are more difficult to handle mathematically mostly because of the oscillations introduced by the presence of the Stokes flow. The SNPP systems shown in [99, 51] are endowed with several scaling choices to cover various types of SNPP systems including Schmuck's work cf. [104] and the study of a stationary and linearized SNPP system by Allaire et al. cf. [7]. As main results, the global weak solvability of the respective models as well as their periodic homogenization limit procedures were obtained. We refer to reader to the *lit. cit.* also for the precise structure of the associated effective transport tensor parameters and upscaled equations. It is worth also mentioning that sometimes,

$v_\varepsilon : Q_T^\varepsilon \to \mathbb{R}$	velocity
$p_\varepsilon : Q_T^\varepsilon \to \mathbb{R}$	pressure
$\Phi_\varepsilon : Q_T^\varepsilon \to \mathbb{R}$	electrostatic potential
$c_\varepsilon^\pm : Q_T^\varepsilon \to \mathbb{R}$	number densities
$c^{\pm,0} : \Omega^\varepsilon \to \mathbb{R}$	initial charged densities
$\sigma \in \mathbb{R}$	surface charge density
$\Phi_D \in \mathbb{R}$	ζ-potential
$R_\varepsilon^\pm : \mathbb{R}^2 \to \mathbb{R}$	reaction rates
$\alpha, \beta, \gamma \in \mathbb{R}$	variable choices of scalings

Table 5.1: Physical unknowns and parameters arising in the microscopic problem (P^ε).

like e.g. in [106, 104, 105], a classification of the upscaling results is done depending on the choice of boundary conditions for the Poisson equation.

The main theme of this chapter is the derivation of corrector estimates quantifying the convergence rate of the periodic homogenization limit process leading to upscaled SNPP systems. This should be seen as a quantitative check of the quality of the two-scale averaging procedure. Getting grip on corrector estimates is a needed step in designing convergent multiscale finite element methods (see, e.g. [66]) and can play an important role also in studying multiscale inverse problems.

Our main results are reported in Theorem 5.4.2 in and Theorem 5.4.3. Here both the Neumann and Dirichlet boundary data for the electrostatic potential are considered. The two types of boundary conditions for the electrostatic potential will lead to different structures of the upscaled systems, and hence, also the structure of the correctors will be different. To obtain these corrector estimates, we rely on the energy method combined with integral estimates for periodically oscillating functions as well as with appropriate macroscopic reconstructions, regularity results on limit and cell functions as well as the smoothness assumptions for the microscopic boundaries and data. It is worth mentioning that the corrector estimate for the closest model to ours, i.e. for the PNP equations in [105, Theorem 2.3], reveals already a class of possible assumptions on the cell functions (taken in $W^{1,\infty}$) as well as on the smoothness of the interior and exterior boundaries (taken in C^∞). Also, we borrowed ideas from both linear elliptic theory [3] as well as from the techniques behind the previously obtained corrector estimates [31, 69, 70, 68] for periodically perforated media. Concerning the locally periodic case, we refer the reader to [86] and references cited therein or to Zhang et al. [118]. In the latter paper, the authors have studied the homogenization of a steady reaction-diffusion system in a chemical vapor infiltration (CVI) process and have also deduced the convergence rate for the homogenization limit.

The reader should bear in mind that our way of deriving corrector estimates does not extend to the stochastic homogenization setting, but can cover, involving only minimal technical modifications, the locally periodic homogenization setting.

The corrector estimates we claim are the following:

Case 1: If the electrostatic potential Φ_ε satisfies the homogeneous Neumann boundary condition, then it holds

$$\left\|\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0^\varepsilon\right\|_{L^2((0,T)\times\Omega^\varepsilon)} + \left\|c_\varepsilon^\pm - c_0^{\pm,\varepsilon}\right\|_{L^2((0,T)\times\Omega^\varepsilon)}$$
$$+ \left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d} \leq C \max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\}, \tag{5.1.11}$$
$$\left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d} \leq C \max\left\{\varepsilon^{\frac{1}{4}}, \varepsilon^{\frac{\mu}{2}}\right\}, \tag{5.1.12}$$
$$\left\|v_\varepsilon - |Y_l|^{-1}\,\mathbb{D}v_0^\varepsilon - \varepsilon\,|Y_l|^{-1}\,\mathbb{D}v_1^\varepsilon\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d}$$
$$+ \|p_\varepsilon - p_0\|_{L^2(\Omega)/\mathbb{R}} \leq C\left(\max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\} + \varepsilon^{\frac{\lambda}{2}} + \varepsilon^{1-\frac{3\lambda}{2}} + \varepsilon^{\frac{1}{2}-\lambda}\right), \tag{5.1.13}$$

where $\mu \in \mathbb{R}_+$ and $\lambda \in (0,1)$.

Case 2: If the electrostatic potential Φ_ε satisfies the homogeneous Dirichlet boundary condition, then it holds

$$\left\|\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0^\varepsilon\right\|_{L^2((0,T)\times\Omega^\varepsilon)} + \left\|c_\varepsilon^\pm - c_0^{\pm,\varepsilon}\right\|_{L^2((0,T)\times\Omega^\varepsilon)} + \left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0^\varepsilon\right)\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d}$$
$$+ \left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d} \leq C \max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\}, \tag{5.1.14}$$
$$\left\|v_\varepsilon - |Y_l|^{-1}\,\mathbb{D}v_0^\varepsilon - \varepsilon\,|Y_l|^{-1}\,\mathbb{D}v_1^\varepsilon\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d}$$
$$+ \|p_\varepsilon - p_0\|_{L^2(\Omega)/\mathbb{R}} \leq C\left(\max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\} + \varepsilon^{\frac{\lambda}{2}} + \varepsilon^{1-\frac{3\lambda}{2}} + \varepsilon^{\frac{1}{2}-\lambda}\right). \tag{5.1.15}$$

The chapter is organized as follows. In Section 5.2, the geometry of our perforated domains is introduced together with some notation and conventions. The list of assumptions on the data is also reported here. In Section 5.3, we provide the weak and strong formulations of all systems of PDEs mentioned in this framework (including the microscopic and macroscopic evolution systems, the cell problems). Section 5.4 is devoted to the statement of our main results and to the corresponding proofs. The remarks from Section 5.5 conclude the chapter.

5.2 Technical preliminaries

5.2.1 A geometrical interpretation of porous media

Let Ω be a bounded and open domain in $\mathbb{R}^d$ with $\partial\Omega \in C^{0,1}$. Without loss of generality, we reduce ourselves to consider Ω as the parallelepiped $(0,a_1)\times\ldots\times(0,a_d)$ for $a_i > 0, i \in \{1,\ldots,d\}$.
Let Y be the unit cell defined by

$$Y := \left\{\sum_{i=1}^d \lambda_i \vec{e}_i : 0 < \lambda_i < 1\right\},$$

where $\vec{e}_i$ denotes the ith unit vector in $\mathbb{R}^d$. We suppose that Y consists of two open sets Y_l and Y_s which respectively represent the liquid part (the pore) and the solid part (the skeleton) such that $\bar{Y}_l \cup \bar{Y}_s = \bar{Y}$ and $Y_l \cap Y_s = \emptyset$, while $\bar{Y}_l \cap \bar{Y}_s = \Gamma$ has a non-zero $(d-1)$-dimensional Hausdorff measure. Additionally, we do not allow the solid part Y_s to touch the outer boundary ∂Y of the unit cell. As a consequence, the fluid part is connected (see Figure 5.1).

Let $Z \subset \mathbb{R}^d$ be a hypercube. For $X \subset Z$ we denote by X^k the shifted subset

$$X^k := X + \sum_{i=1}^{d} k_i \vec{e}_i,$$

where $k = (k_1, ..., k_d) \in \mathbb{Z}^d$ is a vector of indices.
Let $\varepsilon > 0$ be a given scale factor. We assume that Ω is completely covered by a regular array of ε-scaled shifted cells. In porous media terminology, the solid part/pore skeleton is defined as the union of cell regions εY_s^k, i.e.

$$\Omega_0^\varepsilon := \bigcup_{k \in \mathbb{Z}^d} \varepsilon Y_s^k,$$

while the fluid part, which is filling up the total space, is represented by

$$\Omega^\varepsilon := \bigcup_{k \in \mathbb{Z}^d} \varepsilon Y_l^k.$$

We denote the total pore surface of the skeleton by $\Gamma^\varepsilon := \partial \Omega_0^\varepsilon$. This description indicates that the porous medium we have in mind is saturated with the fluid.
Note that we use the subscripts N and D in (5.1.9)-(5.1.10) to distinguish, respectively, the case when the Neumann and Dirichlet conditions are applied across the pore surface. Furthermore, the assumption $\partial \Omega \cap \Gamma^\varepsilon = \emptyset$ holds.
In Figure 5.1, we show an admissible geometry mimicking a porous meidum with periodic microstructures. We let $\mathrm{n}_\varepsilon := (n_1, ..., n_d)$ be the unit outward normal vector on the boundary Γ^ε. The representation of the periodic geometries is in line with [65, 69, 99] and references cited therein.
We denote by $x \in \Omega^\varepsilon$ the macroscopic variable and by $y = x/\varepsilon$ the microscopic variable representing fast variations at the microscopic geometry. In the following, the upper index ε thus denotes the corresponding quantity evaluated at $y = x/\varepsilon$. Suppose that our total pore space Ω^ε is bounded, connected and possesses $C^{0,1}$-boundary.
In the sequel, all the constants C are independent of the homogenization parameter ε, but their precise values may differ from line to line and may change even within a single chain of estimates. Throughout this chapter, we use the superscript ε to emphasize the dependence on the heterogeneity of the material characterized by the homogenization parameter. In the following, we use dS_ε to indicate the surface measure of oscillating surfaces (boundary of microstructures). In addition, depending on the context, by $|\cdot|$ we denote either the volume measure of a domain or the absolute value of a function domain.
When writing the superscript $\pm$ or $\mp$ in e.g. $c_\varepsilon^\pm$, we mean both the positive c_ε^+ and negative densities c_ε^-.
Due to our choice of microstructures, the interior extension from $H^1(\Omega^\varepsilon)$ into $H^1(\Omega)$ exists and the extension constant is independent of ε (see [65, Lemma 5]).

5.2.2 Assumptions on the data

To ensure the weak solvability of our SNPP system, we need essentially several assumptions on the involved data and parameters.

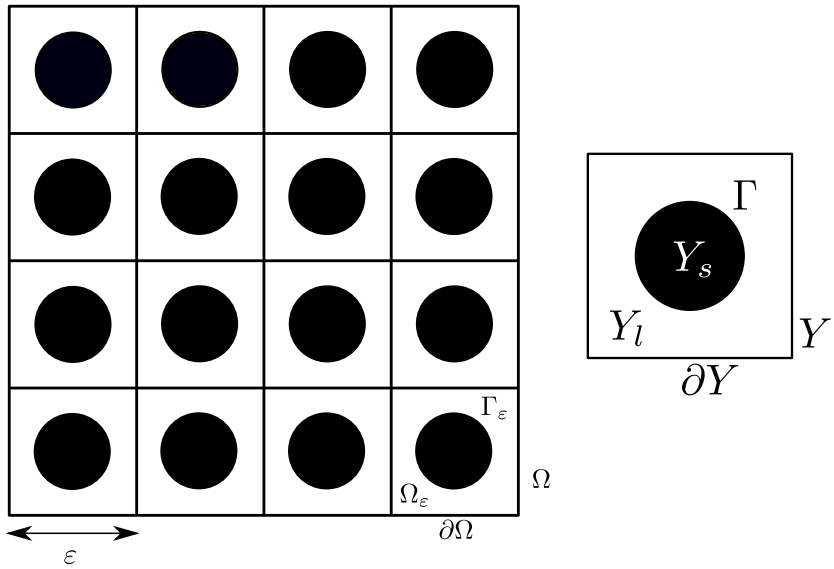

Figure 5.1: An admissible perforated domain. The perforations are referred here as microstructures.

(A_1) The initial data of charged densities are non-negative and bounded independently of ε, i.e. there exists an ε-independent constant $C_0 > 0$ such that

$$0 \leq c^{\pm,0}(x) \leq C_0 \quad \text{for a.e. } x \in \Omega.$$

(A_2) The initial data of charged densities satisfy the compatibility condition:

$$\int_{\Omega^\varepsilon} \left(c^{+,0} - c^{-,0}\right) dx = \int_{\Gamma^\varepsilon} \sigma dS_\varepsilon.$$

(A_3) The chemical reaction rates are structured as $R_\varepsilon^\pm\left(c_\varepsilon^+, c_\varepsilon^-\right) = \mp\left(c_\varepsilon^+ - c_\varepsilon^-\right)$.
(A_4) The surface charge density σ and ζ-potential Φ_D are constants.
(A_5) The electrostatic potential Φ_ε has zero mean value in the fluid part, i.e. it satisfies

$$\int_{\Omega^\varepsilon} \Phi_\varepsilon dx = 0.$$

(A_6) The pressure p_ε has zero mean value in the fluid part, i.e. it satisfies

$$\int_{\Omega^\varepsilon} p_\varepsilon(t,x) dx = 0 \quad \text{for all } \ t \geq 0.$$

Remark 5.2.1. *Assumption (A_1) implies that at the initial moment, our charged colloidal particles are either neutral or positive in the macroscopic domain and their maximum voltage is known. Based on (A_2), if the surface charge density is static (i.e. $\sigma = 0$), then we obtain the so-called global charge neutrality which means that the charge density of our colloidal particles $c_\varepsilon^\pm$ is initially in neutrality. This global electroneutrality condition is particularly helpful in the analysis work (well-posedness, upscaling approach and numerical scheme) of related systems as stated in e.g. [101, 106, 99]. Nevertheless, it is not used in the derivation of the corrector estimates in this work. Cf. (A_3), the reaction rates are linear and ensure the conservation of mass for the concentration fields.*

5.3 Weak settings of SNPP models

5.3.1 Preliminary results

In this subsection, we recall the results on the weak solvability and periodic homogenization of the problem (P^ε), which are derived rigorously in [97, 99], e.g.

Definition 5.3.1. Weak formulation of (P^ε)
A pair of functions $\left(v_\varepsilon, p_\varepsilon, \Phi_\varepsilon, c_\varepsilon^\pm\right)$ satisfying

$$v_\varepsilon \in L^\infty\left(0,T;H_0^1(\Omega^\varepsilon)\right), p_\varepsilon \in L^\infty\left(0,T;L^2(\Omega^\varepsilon)\right), \Phi_\varepsilon \in L^\infty\left(0,T;H^1(\Omega^\varepsilon)\right),$$

$$c_\varepsilon^\pm \in L^\infty\left(0,T;L^2(\Omega^\varepsilon)\right) \cap L^2\left(0,T;H^1(\Omega^\varepsilon)\right), \partial_t c_\varepsilon^\pm \in L^2\left(0,T;\left(H^1(\Omega^\varepsilon)\right)'\right),$$

is a weak solution to (P^ε) provided that

$$\begin{aligned}
&\int_{\Omega^\varepsilon}\left(\varepsilon^2\nabla v_\varepsilon\cdot\nabla\varphi_1 - p_\varepsilon\nabla\cdot\varphi_1\right)dx = -\int_{\Omega^\varepsilon}\varepsilon^\beta\left(c_\varepsilon^+ - c_\varepsilon^-\right)\nabla\Phi_\varepsilon\cdot\varphi_1 dx,\\
&\int_{\Omega^\varepsilon} v_\varepsilon\cdot\nabla\psi dx = 0,\\
&\int_{\Omega^\varepsilon}\varepsilon^\alpha\nabla\Phi_\varepsilon\cdot\nabla\varphi_2 dx - \int_{\Gamma^\varepsilon}\varepsilon^\alpha\nabla\Phi_\varepsilon\cdot \mathrm{n}\varphi_2 dS_\varepsilon = \int_{\Omega^\varepsilon}\left(c_\varepsilon^+ - c_\varepsilon^-\right)\varphi_2 dx,\\
&\left\langle\partial_t c_\varepsilon^\pm, \varphi_3\right\rangle_{(H^1(\Omega^\varepsilon))',H^1(\Omega^\varepsilon)} + \int_{\Omega^\varepsilon}\left(-v_\varepsilon c_\varepsilon^\pm + \nabla c_\varepsilon^\pm \pm \varepsilon^\gamma c_\varepsilon^\pm\nabla\Phi_\varepsilon\right)\cdot\nabla\varphi_3 dx\\
&\qquad = \int_{\Omega^\varepsilon} R_\varepsilon^\pm\left(c_\varepsilon^+, c_\varepsilon^-\right)\varphi_3 dx.
\end{aligned}$$

for all $(\varphi_1,\varphi_2,\varphi_3,\psi) \in \left[H_0^1(\Omega^\varepsilon)\right]^d \times H^1(\Omega^\varepsilon)\times H^1(\Omega^\varepsilon)\times H^1(\Omega^\varepsilon)$.

Theorem 5.3.2. Existence and Uniqueness of solution
Assume (A_1)-(A_6). For each $\varepsilon > 0$, the microscopic problem (P^ε) admits a unique weak solution $\left(v_\varepsilon, p_\varepsilon, \Phi_\varepsilon, c_\varepsilon^\pm\right)$ in the sense of Definition 5.3.1.

The proof of Theorem 5.3.2 can be found in [99] (see Theorem 3.7) and [97].

Theorem 5.3.3. Averaged tensors and Cell problems
The averaged macroscopic permittivity/diffusion tensor $\mathbb{D} = \left(D_{ij}\right)_{1\le i,j\le d}$ is defined by

$$D_{ij} := \int_{Y_l}\left(\delta_{ij} + \partial_{y_i}\varphi_j(y)\right)dy,$$

where $\varphi_j = \varphi_j(y)$ for $1 \le j \le d$ are unique weak solutions in $H^1(Y_l)$ of the following family of cell problems

$$\begin{cases} -\Delta_y\varphi_j(y) = 0 & \text{in } Y_l,\\ \nabla_y\varphi_j(y)\cdot n = -e_j\cdot n & \text{on } \Gamma,\\ \varphi_j \text{ periodic in } y. \end{cases} \tag{5.3.1}$$

Furthermore, the averaged macroscopic permeability tensor $\mathbb{K} = \left(K_{ij}\right)_{1\le i,j\le d}$ is defined by

$$K_{ij} := \int_{Y_l} w_j^i dy,$$

where $w_j = w_j(y)$ together with $\pi_j = \pi_j(y)$ for $1 \le j \le d$ are unique weak solutions, respectively, in $H^1(Y_l)$ and $L^2(Y_l)$ of the following family of cell problems

$$\begin{cases} -\Delta_y w_j + \nabla_y \pi_j = e_j & \text{in } Y_l, \\ \nabla_y \cdot w_j = 0 & \text{in } Y_l, \\ w_j = 0 & \text{in } \Gamma, \\ w_j, \pi_j \text{ periodic in } y. \end{cases} \tag{5.3.2}$$

Also, we define the following cell problem

$$\begin{cases} -\Delta_y \varphi(y) = 1 & \text{in } Y_l, \\ \varphi(y) = 0 & \text{on } \Gamma, \\ \varphi \text{ periodic in } y, \end{cases} \tag{5.3.3}$$

which admits a unique weak solution in $H^1(Y_l)$.
Note that δ_{ij} denotes the Kronecker symbol and e_j is the jth unit vector of $\mathbb{R}^d$.

The proof of Theorem 5.3.3 can be found in [99] (see Definition 4.4) and [97].

Remark 5.3.4. *Fundamental results for elliptic equations provide that the problems* (5.3.1) *and* (5.3.3) *admit a unique weak solution in $H^1(Y_l)$. Similarly, the solutions w_j^i and π_j $(1 \le i, j \le d)$ of* (5.3.2) *are in $H^1(Y_l)$ and $L^2(Y_l)$, respectively. Particularly, for every $s \in \left(-\frac{1}{2}, \frac{1}{2}\right)$ it follows from Theorem 4 and Theorem 7 in [103] that for $1 \le i, j \le d$,*

$$\varphi_j^i \in H^{1+s}(Y_l) \text{ and } w_j^i \in H^{1+s}(Y_l), \pi_j \in H^s(Y_l)$$

are unique weak solution uniquely to (5.3.1) *and* (5.3.2)*, respectively.*
The permeability tensor $\mathbb{K}$ is symmetric and positive definite (cf. [102, Proposition 2.2,Chapter 7]), whilst the same properties of the permittivity tensor $\mathbb{D}$ are proven in [31].

5.3.2 Neumann condition for the electrostatic potential

Theorem 5.3.5. Positivity and Boundedness of solution
Assume (A_1)-(A_4). Let $\left(v_\varepsilon, p_\varepsilon, \Phi_\varepsilon, c_\varepsilon^\pm\right)$ be a weak solution of the microscopic problem (P^ε) with the Neumann condition (5.1.9) *in the sense of Definition 5.3.1. Then the concentration fields $c_\varepsilon^\pm$ are non-negative and essentially bounded from above uniformly in ε.*

The proof of Theorem 5.3.5 can be found in [99] (see Theorems 3.3 and 3.4) and [97].

Theorem 5.3.6. *A priori* estimates
Assume (A_1)-(A_6). The following a priori *estimates hold:*
For the electrostatic potential, we have

$$\varepsilon^\alpha \|\Phi_\varepsilon\|_{L^2(0,T;H^1(\Omega^\varepsilon))} \le C. \tag{5.3.4}$$

If $\beta \ge \alpha$, it holds

$$\|v_\varepsilon\|_{L^2((0,T)\times\Omega^\varepsilon)} + \varepsilon \|\nabla v_\varepsilon\|_{L^2((0,T)\times\Omega^\varepsilon)} \le C, \tag{5.3.5}$$

and additionally if $\gamma \geq \alpha$, it holds

$$\max_{t\in[0,T]} \left\|c_\varepsilon^-\right\|_{L^2(\Omega^\varepsilon)} + \max_{t\in[0,T]} \left\|c_\varepsilon^+\right\|_{L^2(\Omega^\varepsilon)} + \left\|\nabla c_\varepsilon^-\right\|_{L^2((0,T)\times\Omega^\varepsilon)} + \left\|\nabla c_\varepsilon^+\right\|_{L^2((0,T)\times\Omega^\varepsilon)}$$
$$+ \left\|\partial_t c_\varepsilon^-\right\|_{L^2\left(0,T;(H^1(\Omega^\varepsilon))'\right)} + \left\|\partial_t c_\varepsilon^+\right\|_{L^2\left(0,T;(H^1(\Omega^\varepsilon))'\right)} \leq C. \tag{5.3.6}$$

The proof of Theorem 5.3.6 can be found in [99] (see Theorem 3.5) and [97].

Theorem 5.3.7. Homogenization of (P_N^ε)
Let the a priori *estimates* (5.3.4)-(5.3.6) *of Theorem 5.3.13 be valid. Taking $\tilde{\Phi}_\varepsilon := \varepsilon^\alpha \Phi_\varepsilon$, there exist functions $\tilde{\Phi}_0 \in L^2\left(0,T;H^1(\Omega)\right)$ and $\tilde{\Phi}_1 \in L^2\left((0,T)\times\Omega;H^1_\#(Y)\right)$ such that, up to a subsequence, we have*

$$\tilde{\Phi}_\varepsilon \overset{2}{\rightharpoonup} \tilde{\Phi}_0,$$
$$\nabla\tilde{\Phi}_\varepsilon \overset{2}{\rightharpoonup} \nabla_x\tilde{\Phi}_0 + \nabla_y\tilde{\Phi}_1.$$

If $\beta \geq \alpha$, then there exist functions $v_0 \in L^2\left((0,T)\times\Omega;H^1_\#(Y)\right)$ and $p_0(t,x,y) \in L^2((0,T)\times\Omega\times Y)$ such that, up to a subsequence, we have

$$v_\varepsilon \overset{2}{\rightharpoonup} v_0,$$
$$\varepsilon\nabla v_\varepsilon \overset{2}{\rightharpoonup} \nabla_y v_0,$$
$$p_\varepsilon \overset{2}{\rightharpoonup} p_0.$$

Moreover, the convergence for the pressure is strong in $L^2(\Omega)/\mathbb{R}$.
If $\gamma \geq \alpha$, then there exist functions $c_0^\pm \in L^2\left(0,T;H^1(\Omega)\right)$ and $c_1^\pm \in L^2\left((0,T)\times\Omega;H^1_\#(Y)\right)$ such that, up to a subsequence, we have

$$c_\varepsilon^\pm \to c_0^\pm \text{ strongly in } L^2((0,T)\times\Omega),$$
$$\nabla c_\varepsilon^\pm \overset{2}{\rightharpoonup} \nabla_x c_0^\pm + \nabla_y c_1^\pm.$$

Theorem 5.3.8. Strong formulation of the macroscopic problem in the Neuman case - (P_N^0)
Let $\left(v_\varepsilon, p_\varepsilon, \Phi_\varepsilon, c_\varepsilon^\pm\right)$ be a weak solution of (P^ε) in the sense of Definition 5.3.1 with Neumann boundary conditions. According to Theorem 5.3.7, we have the following results:
Let $\tilde{\Phi}_0$ be the two-scale limit of the electrostatic potential $\tilde{\Phi}_\varepsilon$, it then satisfies the following macroscopic system:

$$\begin{cases} -\nabla_x\cdot\left(\mathbb{D}\nabla_x\tilde{\Phi}_0(t,x)\right) = \bar{\sigma} + |Y_l|\left(c_0^+(t,x) - c_0^-(t,x)\right) & \text{in } (0,T)\times\Omega, \\ \mathbb{D}\nabla_x\tilde{\Phi}_0(t,x)\cdot n = 0 & \text{on } (0,T)\times\partial\Omega, \end{cases}$$

where $\bar{\sigma} := \int_\Gamma \sigma dS_y$ and the permittivity/diffusion tensor $\mathbb{D}$ is defined in Theorem 5.3.3.
Let v_0 be the two-scale limit of the velocity field v_ε. With additionally $\beta \geq \alpha$, it then satisfies the following macroscopic system:

$$\begin{cases} \bar{v}_0(t,x) + \mathbb{K}\nabla_x p_0(t,x) & \\ = -\mathbb{K}\left(c_0^+(t,x) - c_0^-(t,x)\right)\nabla_x\tilde{\Phi}_0(t,x) & \text{in } (0,T)\times\Omega, \text{ if } \beta = \alpha, \\ \bar{v}_0(t,x) + \mathbb{K}\nabla_x p_0(t,x) = 0 & \text{in } (0,T)\times\Omega, \text{ if } \beta > \alpha, \\ \nabla_x\cdot\bar{v}_0(t,x) = 0 & \text{in } (0,T)\times\Omega, \\ \bar{v}_0(t,x)\cdot n = 0 & \text{on } (0,T)\times\partial\Omega, \end{cases}$$

where $\bar{v}_0(t,x) = \int_{Y_l} v_0(t,x,y)\,dy$ *and the permeability tensor* $\mathbb{K}$ *is defined in Theorem 5.3.3.*

Let $c_0^{\pm}$ *be the two-scale limits of the concentration fields* $c_\varepsilon^{\pm}$*. With* $\gamma = \alpha$*, they satisfy the following macroscopic system:*

$$\begin{cases} |Y_l|\,\partial_t c_0^{\pm}(t,x) + \nabla_x \cdot \left[c_0^{\pm}(t,x)\,\bar{v}_0(t,x) - \mathbb{D}\nabla_x c_0^{\pm}(t,x)\right] \\ \mp \nabla_x \cdot \left(c_0^{\pm}(t,x)\,\mathbb{D}\nabla_x \tilde{\Phi}_0(t,x)\right) = |Y_l| R_0^{\pm}\left(c_0^{+}(t,x), c_0^{-}(t,x)\right) & \text{in } (0,T)\times\Omega, \\ \left(c_0^{\pm}(t,x)\left(\bar{v}_0(t,x) \mp \mathbb{D}\nabla_x \tilde{\Phi}_0(t,x)\right) - \mathbb{D}\nabla_x c_0^{\pm}(t,x)\right)\cdot n = 0 & \text{on } (0,T)\times\partial\Omega, \end{cases}$$

while with $\gamma > \alpha$*, they satisfy*

$$\begin{cases} |Y_l|\,\partial_t c_0^{\pm}(t,x) + \nabla_x \cdot \left[c_0^{\pm}(t,x)\,\bar{v}_0(t,x) - \mathbb{D}\nabla_x c_0^{\pm}(t,x)\right] \\ = |Y_l| R_0^{\pm}\left(c_0^{+}(t,x), c_0^{-}(t,x)\right) & \text{in } (0,T)\times\Omega, \\ \left(c_0^{\pm}(t,x)\,\bar{v}_0(t,x) - \mathbb{D}\nabla_x c_0^{\pm}(t,x)\right)\cdot n = 0 & \text{on } (0,T)\times\partial\Omega. \end{cases}$$

Remark 5.3.9. *Due to the* a priori *estimate for the electrostatic potential in Theorem 5.3.13,* Φ_ε *and its gradient* $\nabla\Phi_\varepsilon$ *converge to zero when* $\alpha < 0$*. In Theorem 5.3.8, the number densities* $c_0^{\pm}$ *in the macroscopic Poisson equations with permittivity tensor* $\mathbb{D}$ *positions itself as forcing terms. Similarly, the forcing terms in the macroscopic Stokes equations with the case* $\beta = \alpha$ *dwell in the part of the electrostatic potential* $\tilde{\Phi}_0$ *and the distribution of the number densities* $c_0^{\pm}$*. Clearly, the macroscopic Nernst-Planck equations in the case* $\gamma = \alpha$ *yield the fully coupled system of partial differential equations, whilst with* $\gamma > \alpha$ *it reduces to a convection-diffusion-reaction system due to also the structure of the reaction terms* $R_0^{\pm}$*.*

Let us define the function space

$$H_N^1(\Omega) := \left\{v \in H^1(\Omega) : -\mathbb{D}\nabla_x u \cdot \mathrm{n} = 0 \ \text{ on } \partial\Omega\right\},$$

which is a closed subspace of $H^1(\Omega)$. This Hilbert space plays a role when writing the weak formulation of the macroscopic systems in Theorem 5.3.10 and Theorem 5.3.17.

Theorem 5.3.10. Weak formulation of (P_N^0)

Let a pair of functions $\left(v_0, p_0, \tilde{\Phi}_0, c_0^{\pm}\right)$ *be defined as in Theorem 5.3.8. Then, it satisfies*

$$\begin{aligned} &\bar{v}_0 \in L^2((0,T)\times\Omega), p_0 \in L^2((0,T)\times\Omega), \\ &\tilde{\Phi}_0 \in L^2\left(0,T;H^1(\Omega)\right), c_0^{\pm} \in L^2\left(0,T;H^1(\Omega)\right), \partial_t c_0^{\pm} \in L^2\left(0,T;\left(H^1(\Omega)\right)'\right) \end{aligned}$$

and becomes a weak solution to $\left(P_N^0\right)$ *provided that*

$$\int_\Omega (\bar{v}_0\varphi_1 - \mathbb{K}p_0\nabla\cdot\varphi_1)\,dx = -\mathbb{K}\int_\Omega \left(c_0^+ - c_0^-\right)\nabla\tilde{\Phi}_0\cdot\varphi_1 dx \text{ if } \beta=\alpha,$$
$$\int_\Omega (\bar{v}_0\varphi_1 - \mathbb{K}p_0\nabla\cdot\varphi_1)\,dx = 0 \text{ if } \beta>\alpha,$$
$$\int_\Omega \bar{v}_0\cdot\nabla\psi dx = 0,$$
$$\int_\Omega |Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0\cdot\nabla\varphi_2 dx - |Y_l|^{-1}\,\bar{\sigma}\int_\Omega \varphi_2 dx = \int_\Omega \left(c_0^+ - c_0^-\right)\varphi_2 dx,$$
$$\left\langle \partial_t c_0^\pm, \varphi_3\right\rangle_{(H^1)',H^1} + \int_\Omega |Y_l|^{-1}\left(-c_0^\pm\left(\bar{v}_0 \mp \mathbb{D}\nabla\tilde{\Phi}_0\right) + \mathbb{D}\nabla c_0^\pm\right)\cdot\nabla\varphi_3 dx$$
$$= \int_\Omega R_0^\pm\left(c_0^+, c_0^-\right)\varphi_3 dx \text{ if } \gamma=\alpha,$$
$$\left\langle \partial_t c_0^\pm, \varphi_3\right\rangle_{(H^1)',H^1} + \int_\Omega |Y_l|^{-1}\left(-c_0^\pm\bar{v}_0 + \mathbb{D}\nabla c_0^\pm\right)\cdot\nabla\varphi_3 dx = \int_\Omega R_0^\pm\left(c_0^+, c_0^-\right)\varphi_3 dx \text{ if } \gamma>\alpha,$$

for all $(\varphi_1,\varphi_2,\varphi_3,\psi)\in\left[H_0^1(\Omega)\right]^d\times H_N^1(\Omega)\times H^1(\Omega)\times H^1(\Omega)$.

The proof of Theorems 5.3.7, 5.3.8 and 5.3.10 are collected from Theorems 4.5-4.10 in [99] and can also be found in [97].

5.3.3 Dirichlet condition for the electrostatic potential

Remark 5.3.11. *In Theorem 5.3.5, the proof (as mentioned in [99, Theorem 3.3, Theorem 3.4]) consists in suitable choices of test functions, based on the energy-estimates arguments. Nevertheless, for the problem where the Dirichlet boundary condition* (5.1.10) *is prescribed, the volume additivity constraint* $c_\varepsilon^+ + c_\varepsilon^- = 1$ *is required to guarantee the* ε*-independent boundedness of the concentration fields.*

Definition 5.3.12. Assume (A_1)-(A_4). Let Φ_ε be a solution of the microscopic problem (P^ε) in the sense of Definition 5.3.1. Then the transformed electrostatic potential $\Phi_\varepsilon^{\mathrm{hom}} := \Phi_\varepsilon - \Phi_D$ satifies the following system:

$$-\varepsilon^\alpha\Delta\Phi_\varepsilon^{\mathrm{hom}} = c_\varepsilon^+ - c_\varepsilon^- \text{ in } Q_T^\varepsilon,$$
$$\Phi_\varepsilon^{\mathrm{hom}} = 0 \text{ in } (0,T)\times\Gamma_D^\varepsilon,$$
$$\varepsilon^\alpha\nabla\Phi_\varepsilon^{\mathrm{hom}}\cdot\mathrm{n} = 0 \text{ in } (0,T)\times\partial\Omega.$$

Theorem 5.3.13. ***A priori* estimates**
Assume (A_1)-(A_4). *The following* a priori *estimates hold:*
For the electrostatic potential, we have

$$\varepsilon^{\alpha-2}\left\|\Phi_\varepsilon^{hom}\right\|_{L^2((0,T)\times\Omega^\varepsilon)} + \varepsilon^{\alpha-1}\left\|\nabla\Phi_\varepsilon^{hom}\right\|_{L^2((0,T)\times\Omega^\varepsilon)} \le C.$$

If $\beta\ge\alpha-1$, *it holds*

$$\|v_\varepsilon\|_{L^2((0,T)\times\Omega^\varepsilon)} + \varepsilon\,\|\nabla v_\varepsilon\|_{L^2((0,T)\times\Omega^\varepsilon)} \le C,$$

and additionally if $\gamma \geq \alpha - 1$, it holds

$$\max_{t\in[0,T]} \left\|c_\varepsilon^-\right\|_{L^2(\Omega^\varepsilon)} + \max_{t\in[0,T]} \left\|c_\varepsilon^+\right\|_{L^2(\Omega^\varepsilon)} + \left\|\nabla c_\varepsilon^-\right\|_{L^2((0,T)\times\Omega^\varepsilon)} + \left\|\nabla c_\varepsilon^+\right\|_{L^2((0,T)\times\Omega^\varepsilon)}$$
$$+ \left\|\partial_t c_\varepsilon^-\right\|_{L^2\left(0,T;(H^1(\Omega^\varepsilon))'\right)} + \left\|\partial_t c_\varepsilon^+\right\|_{L^2\left(0,T;(H^1(\Omega^\varepsilon))'\right)} \leq C.$$

The proof of Theorem 5.3.13 can be found in [99] (see Theorem 3.6) and [97].

Theorem 5.3.14. Homogenization of (P_D^ε)
Let the a priori *estimates of Theorem 5.3.13 be valid. Let Φ_ε^{hom} be as defined in Definition 5.3.12. Taking $\tilde{\Phi}_\varepsilon := \varepsilon^{\alpha-2}\Phi_\varepsilon^{\text{hom}}$, then it satisfies the following system:*

$$\begin{aligned}
&-\varepsilon^2\Delta\tilde{\Phi}_\varepsilon = c_\varepsilon^+ - c_\varepsilon^- \text{ in } Q_T^\varepsilon,\\
&\tilde{\Phi}_\varepsilon = 0 \text{ in } (0,T)\times\Gamma_\varepsilon,\\
&\varepsilon^2\nabla\tilde{\Phi}_\varepsilon\cdot n = 0 \text{ in } (0,T)\times\partial\Omega.
\end{aligned}$$

Therefore, we can find a function $\tilde{\Phi}_0 \in L^2\left((0,T)\times\Omega; H_\#^1(Y)\right)$ such that, up to a subsequence,

$$\begin{aligned}
&\tilde{\Phi}_\varepsilon \overset{2}{\rightharpoonup} \tilde{\Phi}_0,\\
&\varepsilon\nabla\tilde{\Phi}_\varepsilon \overset{2}{\rightharpoonup} \nabla_y\tilde{\Phi}_0.
\end{aligned}$$

If additionally $\beta \geq \alpha-1$, then there exist functions $v_0 \in L^2\left((0,T)\times\Omega; H_\#^1(Y)\right)$ and $p_0(t,x,y) \in L^2((0,T)\times\Omega\times Y)$ such that, up to a subsequence, we have

$$\begin{aligned}
&v_\varepsilon \overset{2}{\rightharpoonup} v_0,\\
&\varepsilon\nabla v_\varepsilon \overset{2}{\rightharpoonup} \nabla_y v_0,\\
&p_\varepsilon \overset{2}{\rightharpoonup} p_0.
\end{aligned}$$

Furthermore, there exist functions $c_0^\pm \in L^2\left(0,T;H^1(\Omega)\right)$ and $c_1^\pm \in L^2\left((0,T)\times\Omega; H_\#^1(Y)\right)$ such that, up to a subsequence, we have

$$\begin{aligned}
&c_\varepsilon^\pm \to c_0^\pm \text{ strongly in } L^2((0,T)\times\Omega),\\
&\nabla c_\varepsilon^\pm \overset{2}{\rightharpoonup} \nabla_x c_0^\pm + \nabla_y c_1^\pm.
\end{aligned}$$

Theorem 5.3.15. Strong formulation of the macroscopic problem in the Dirichlet case - (P_D^0)
Let $\left(v_\varepsilon, p_\varepsilon, \Phi_\varepsilon, c_\varepsilon^\pm\right)$ be a weak solution of (P^ε) in the sense of Definition 5.3.1. According to Theorem 5.3.14, we have the following results:
Let $\tilde{\Phi}_0$ be the two-scale limit of the electrostatic potential $\tilde{\Phi}_\varepsilon$, it then satisfies the following macroscopic equation:

$$\overline{\tilde{\Phi}}_0(t,x) = \left(\int_{Y_l} \varphi(y)\,dy\right)\left(c_0^+(t,x) - c_0^-(t,x)\right),$$

where $\overline{\tilde{\Phi}}_0(t,x) = \int_{Y_l}\tilde{\Phi}_0(t,x,y)\,dy$ and φ is the solution of the cell problem (5.3.3).
Let v_0 be the two-scale limit of the velocity field v_ε. With $\beta \geq \alpha-1$, it then satisfies the following macroscopic system:

$$\begin{cases}
\bar{v}_0(t,x) + \mathbb{K}\nabla_x p_0(t,x) = 0 & \text{in } (0,T)\times\Omega,\\
\nabla_x\cdot\bar{v}_0(t,x) = 0 & \text{in } (0,T)\times\Omega,\\
\bar{v}_0(t,x)\cdot n = 0 & \text{on } (0,T)\times\partial\Omega,
\end{cases}$$

where $\bar{v}_0(t,x) = \int_{Y_l} v_0(t,x,y)\,dy$ *and the permeability tensor* $\mathbb{K}$ *is defined in Theorem 5.3.3. Let* $c_0^{\pm}$ *be the two-scale limits of the concentration fields* $c_\varepsilon^{\pm}$*. With* $\gamma \geq \alpha - 1$*, they satisfy the following macroscopic system:*

$$\begin{cases} |Y_l|\,\partial_t c_0^{\pm}(t,x) + \nabla_x \cdot \left[c_0^{\pm}(t,x)\,\bar{v}_0(t,x) - \mathbb{D}\nabla_x c_0^{\pm}(t,x)\right] & \\ = |Y_l| R_0^{\pm}\left(c_0^{+}(t,x), c_0^{-}(t,x)\right) & \text{in } (0,T)\times\Omega, \\ \left(c_0^{\pm}(t,x)\,\bar{v}_0(t,x) - \mathbb{D}\nabla_x c_0^{\pm}(t,x)\right)\cdot n = 0 & \text{on } (0,T)\times\partial\Omega. \end{cases}$$

where the permittivity/diffusion tensor $\mathbb{D}$ *is defined in Theorem 5.3.3.*

Remark 5.3.16. *Due to the* a priori *estimate for the electrostatic potential in Theorem 5.3.13,* Φ_ε *converges to* Φ_D *as* $\alpha < 2$*. Moreover, in the case* $\alpha < 1$ *we obtain the convergence of* Φ_ε *and its gradient* $\nabla\Phi_\varepsilon$ *to the* ζ*-potential* Φ_D *and zero, respectively. When* $\alpha = 2$*, then* $\tilde{\Phi}_\varepsilon = \Phi_\varepsilon^{hom} := \Phi_\varepsilon - \Phi_D$ *holds, we compute that*

$$\bar{\Phi}_0(t,x) = \int_{Y_l}\left(\Phi_0^{hom}(t,x,y) + \Phi_D\right)dy = \left(\int_{Y_l}\varphi(y)\,dy\right)\left(c_0^{+}(t,x) - c_0^{-}(t,x)\right) + |Y_l|\,\Phi_D. \tag{5.3.7}$$

In Theorem 5.3.15, we see that in contrast to Theorem 5.3.8, the electrostatic potential is not present in the macroscopic Stokes and Nernst-Planck equations. In addition, the macroscopic Poisson system for the electrostatic potential reduces from the partial differential equations in the Neumann case to the macroscopic "representation" in the Dirichlet case. Both cases are all coupled with the concentration fields $c_0^{\pm}$*. Note that in both Neumann and Dirichlet cases, we need the strong convergence of the concentration fields, i.e.* $c_\varepsilon^{\pm} \to c_0^{\pm}$ *in* $L^2((0,T)\times\Omega)$*, to derive the macroscopic systems for the electrostatic potential, the fluid flow as well as for the pressure, respectively.*

Theorem 5.3.17. Weak formulation of (P_D^0)
Let the quadruple of functions $\left(v_0, p_0, \tilde{\Phi}_0, c_0^{\pm}\right)$ *be defined as in Theorem 5.3.15. Then, it satisfies*

$$\begin{aligned} &\bar{v}_0 \in L^2((0,T)\times\Omega),\, p_0 \in L^2((0,T)\times\Omega), \\ &\tilde{\Phi}_0 \in L^2((0,T)\times\Omega),\, c_0^{\pm} \in L^2\left(0,T;H^1(\Omega)\right),\, \partial_t c_0^{\pm} \in L^2\left(0,T;\left(H^1(\Omega)\right)'\right) \end{aligned}$$

and is a weak solution to $\left(P_N^0\right)$ *provided that*

$$\begin{aligned} &\int_\Omega \left(\bar{v}_0\varphi_1 - \mathbb{K}p_0\nabla\cdot\varphi_1\right)dx = 0, \\ &\int_\Omega \bar{v}_0\cdot\nabla\psi\,dx = 0, \\ &\int_\Omega \bar{\tilde{\Phi}}_0\varphi_2\,dx = \left(\int_{Y_l}\varphi(y)\,dy\right)\int_\Omega\left(c_0^{+} - c_0^{-}\right)\varphi_2\,dx, \\ &\left\langle \partial_t c_0^{\pm}, \varphi_3\right\rangle_{(H^1)',H^1} + \int_\Omega |Y_l|^{-1}\left(-c_0^{\pm}\bar{v}_0 + \mathbb{D}\nabla c_0^{\pm}\right)\cdot\nabla\varphi_3\,dx = \int_\Omega R_0^{\pm}\left(c_0^{+}, c_0^{-}\right)\varphi_3\,dx, \end{aligned}$$

for all $(\varphi_1,\varphi_2,\varphi_3,\psi) \in \left[H_0^1(\Omega)\right]^d \times H_N^1(\Omega)\times H^1(\Omega)\times H^1(\Omega)$*.*

The proof of Theorems 5.3.14, 5.3.15 and 5.3.17 are collected from Theorems 4.11-4.16 in [99] and can also be found in [97].

5.3.4 Discussions

According to proofs of the macroscopic systems in Theorems 4.6, 4.8, 4.10, 4.12, 4.14 and 4.16 cf. [97], we formulate here the first-order limit functions of the systems (P_N^0) and (P_D^0), respectively.
When the electric potential satisfies the Neumann condition on the micro-surface, we deduce that $\tilde{\Phi}_1$ can be formulated by

$$\tilde{\Phi}_1(t,x,y) = \sum_{j=1}^{d} \varphi_j(y)\,\partial_{x_j}\tilde{\Phi}_0(t,x),$$

with φ_j being solutions of the cell problems (5.3.1). We also remark that the limit function p_0 for the pressure is proved to be independent of y, i.e. $p_0(t,x,y) = p_0(t,x)$, due to the structure of the Stokes equation, see Theorem 5.3.7. Accordingly, the representation of the limit function v_0 for the fluid flow is given by

$$v_0(t,x,y) = \begin{cases} -\sum_{j=1}^{d} w_j(y)\Big[\big(c_0^+(t,x) - c_0^-(t,x)\big)\,\partial_{x_j}\tilde{\Phi}_0(t,x) + \partial_{x_j}p_0(t,x)\Big] & \text{if } \beta = \alpha, \\ -\sum_{j=1}^{d} w_j(y)\,\partial_{x_j}p_0(t,x) & \text{if } \beta > \alpha, \end{cases}$$

where $w_j = w_j(y)$ for $1 \le j \le d$ are the solutions of the cell problems (5.3.2). We are able to determine the (extended) macroscopic Darcy's law by the following pressure:

$$\tilde{p}_1(t,x,y) = p_1(t,x,y) + \big(c_0^+(t,x) - c_0^-(t,x)\big)\tilde{\Phi}_1(t,x,y),$$

where with $\pi_j = \pi_j(y)$ for $1 \le j \le d$ are the solutions of the cell problems (5.3.2), we compute that

$$p_1(t,x,y) = \begin{cases} -\sum_{j=1}^{d} \pi_j(y)\Big[\big(c_0^+(t,x) - c_0^-(t,x)\big)\,\partial_{x_j}\tilde{\Phi}_0(t,x) + \partial_{x_j}p_0(t,x)\Big] & \text{if } \beta = \alpha, \\ -\sum_{j=1}^{d} \pi_j(y)\,\partial_{x_j}p_0(t,x) & \text{if } \beta > \alpha. \end{cases}$$

On the other hand, the representation of the first-order functions $c_1^{\pm}$ is

$$c_1^{\pm}(t,x,y) = \begin{cases} \sum_{j=1}^{d}\Big(\varphi_j(y)\,\partial_{x_j}c_0^{\pm}(t,x) \mp c_0^{\pm}(t,x)\,\partial_{x_j}\tilde{\Phi}_0(t,x)\Big) & \text{if } \gamma = \alpha, \\ \sum_{j=1}^{d}\varphi_j(y)\,\partial_{x_j}c_0^{\pm}(t,x) & \text{if } \gamma > \alpha, \end{cases}$$

where $\varphi_j = \varphi_j(y)$ for $1 \le j \le d$ are the solutions of the cell problems (5.3.1).
When the electric potential satisfies the Dirichlet condition on the micro-surface, we obtain a different scenario. In fact, the macroscopic electrostatic potential $\tilde{\Phi}_0$ in this case is dependent of y and it can be computed by the averaged-like term $\overline{\tilde{\Phi}}_0$ (see Theorem 5.3.15 and the special case in (5.3.7)). We obtain the same manner with the macroscopic velocity v_0 in Theorem

5.3.15. However, the limit function p_0 for the pressure remains independent of y. As a consequence, the representation of the first-order functions $c_1^{\pm}$ is

$$c_1^{\pm}(t,x,y)=\begin{cases}\displaystyle\sum_{j=1}^{d}\Big(\varphi_j(y)\,\partial_{x_j}c_0^{\pm}(t,x)\mp c_0^{\pm}(t,x)\,\tilde{\Phi}_0(t,x)\Big) & \text{if } \gamma=\alpha-1,\\ \displaystyle\sum_{j=1}^{d}\varphi_j(y)\,\partial_{x_j}c_0^{\pm}(t,x) & \text{if } \gamma>\alpha-1,\end{cases}$$

where $\varphi_j=\varphi_j(y)$ for $1\le j\le d$ are the solutions of the cell problems (5.3.1).
It is worth mentioning that upscaling the microscopic system (P^{ε}) is done by the two-scale convergence method. This approach, which aims to derive the limit system, does not require the derivation of the first-order macroscopic velocity, denoted by v_1 herein. To gain the corrector for the oscillating pressure arising in the Stokes equation, we use the same procedures as in [80], and thus, we need the structure of v_1.
Following [102], we have in the Neumann case for the electrostatic potential that

$$v_1\left(t,x,\frac{x}{\varepsilon}\right)=\begin{cases}\displaystyle-\sum_{i,j=1}^{d}r_{ij}\left(\frac{x}{\varepsilon}\right)\partial_{x_i}\Big(\big(c_0^{+}-c_0^{-}\big)\,\partial_{x_j}\tilde{\Phi}_0(t,x)+\partial_{x_j}p_0(t,x)\Big) & \text{if } \beta=\alpha,\\ \displaystyle-\sum_{i,j=1}^{d}r_{ij}\left(\frac{x}{\varepsilon}\right)\partial^2_{x_ix_j}p_0(t,x) & \text{if } \beta>\alpha,\end{cases}$$

where $r_{ij}\in H^1(Y_l)$ for $1\le i,j\le d$ is the solution for the following cell problem

$$\begin{cases}\nabla_y\cdot r_{ij}+w_j^i=|Y_l|^{-1}K_{ij} & \text{in } Y_l,\\ r_{ij}=0 & \text{on } \Gamma,\\ r_{ij}\ \text{ periodic in } y.\end{cases}\tag{5.3.8}$$

It holds

$$v_1\left(t,x,\frac{x}{\varepsilon}\right)=-\sum_{i,j=1}^{d}r_{ij}\left(\frac{x}{\varepsilon}\right)\partial^2_{x_ix_j}p_0(t,x),$$

provided the electrostatic potential satisfies the Dirichlet boundary data on the micro-surfaces.

5.3.5 Auxiliary estimates

Here, we let Y_l and Ω^{ε} as defined in Subsubsection 5.2.1.

Lemma 5.3.18. *(cf. [70]) Let $p^{\varepsilon}(x):=p(x/\varepsilon)\in H^1(\Omega^{\varepsilon})$ satisfy*

$$\bar{p}:=\frac{1}{|Y_l|}\int_{Y_l}p(y)\,dy,$$

then the following estimate holds:

$$\|p^{\varepsilon}-\bar{p}\|_{L^2(\Omega^{\varepsilon})}\le C\varepsilon^{\frac{1}{2}}\,\|p^{\varepsilon}\|_{H^1(\Omega^{\varepsilon})}.$$

Lemma 5.3.19. *(cf. [80]) Assume $\partial\Omega \in C^k$ for $k \geq 4$ holds. Then, there exists $\delta_0 > 0$ and a function $\eta^\delta \in \left[C^{k-1}\left(\bar{\Omega}\right)\right]^d$ such that $\eta^\delta = \bar{v}_0$ on $\partial\Omega$ with $\bar{v}_0$ being the averaged macroscopic velocity defined in Theorem 5.3.8, $\nabla_x \cdot \eta^\delta = 0$ in Ω and for any $1 \leq q \leq \infty$ and $0 \leq \ell \leq k-1$, the following estimate holds:*

$$\left\|\nabla^\ell \eta^\delta\right\|_{L^q(\Omega)} \leq C\delta^{\frac{1}{q}-\ell} \quad \text{for } \delta \in (0, \delta_0]. \tag{5.3.9}$$

Proof. We adapt the notation from [80] (see Lemma 1) to our proof here. It is well known from [56, Lemma 14.16] that there exists an ε-independent $\gamma > 0$ such that the distance function $z(x) = \operatorname{dist}(x, \partial\Omega)$ belongs to $C^k\left(\mathscr{S}_\gamma\right)$ where

$$\mathscr{S}_\gamma := \left\{x \in \overline{\Omega} : \operatorname{dist}(x, \partial\Omega) \leq \gamma\right\}. \tag{5.3.10}$$

By definition, we have

$$\partial\Omega := \left\{x \in \mathbb{R}^d : z(x) = 0\right\} \text{ and } \mathrm{n} := -\frac{\nabla z}{|\nabla z|} \quad \text{for } x \in \mathscr{S}_\gamma.$$

If we define a function $V(z, \xi)$ by

$$V(z, \xi) := -\frac{\bar{v}_0(x)}{|\nabla z(x)|} \quad \text{for } x = x(z, \xi) \in \mathscr{S}_\gamma \tag{5.3.11}$$

where ξ is the tangential component of z along $\partial\Omega$. We observe that $|\nabla z| > 0$ for $x \in \mathscr{S}_\gamma$ and the trace $V(0, \xi)$ is well-defined as a function in $C^k\left(\mathscr{S}_\gamma\right)$.
Following the same spirit of the argument as in [112] in e.g. Proposition 2.3, we aim to take η^δ as $\operatorname{curl}\psi$, where ψ is chosen in such a way that

$$\frac{\partial\psi}{\partial\tau} = 0 \quad \text{on } \partial\Omega,$$

where we denote by τ the tangential component of ψ, and

$$\nabla\psi \cdot \mathrm{n} = \bar{v}_0 \cdot \tau \quad \text{on } \partial\Omega.$$

Note from the structure of the macroscopic Stokes system (cf. Theorem 5.3.8 and Theorem 5.3.15) that $\bar{v}_0 \cdot \mathrm{n} = 0$ on $\partial\Omega$ and from the fact that the tangential component is different from 0 in principle. We aim to choose $\psi = 0$ on $\partial\Omega$. Based on the function $V(z, \xi)$, defined in (5.3.11), we choose

$$\psi(x) = z(x)\exp\left(-\frac{z(x)}{\delta}\right)V(0, \xi) \cdot \tau(x).$$

Due to the presence of z, it is clear that $\psi = 0$ on $\partial\Omega$. Furthermore, we can check that

$$\nabla\psi \cdot \mathrm{n} = -\frac{\nabla z}{|\nabla z|} \cdot \left(\nabla z \frac{\partial\psi}{\partial z}\right) = -|\nabla z|\left(1 - \frac{z}{\delta}\right)\exp\left(-\frac{z}{\delta}\right)V(0, \xi) \cdot \tau(x) = \bar{v}_0 \cdot \tau$$

holds on $\partial\Omega$.
Therefore, we are now allowed to take $\eta^\delta = \operatorname{curl}\psi$ in $\mathscr{S}_\gamma$.
We can now complete the proof of the lemma. Indeed, we estimate that

$$\begin{aligned}\|\nabla\psi\|^q_{L^q(\mathscr{S}_\gamma)} &\leq C\int_{\mathscr{S}_\gamma}\left(\left|\left(1 - \frac{z}{\delta}\right)\exp\left(-\frac{z}{\delta}\right)V(0, \xi)\right|^2 + \left|z\exp\left(-\frac{z}{\delta}\right)\frac{\partial V}{\partial\xi}(0, \xi)\right|^2\right)^{\frac{q}{2}} dx \\ &\leq C\delta.\end{aligned}$$

Owning to the C^k-smoothness of $\partial\Omega$, we can proceed as above to obtain the following high-order estimate:

$$\left\|\nabla^{\ell+1}\psi\right\|_{L^q(\mathscr{S}_\gamma)} \leq C\delta^{\frac{1}{q}-\ell} \quad \text{for } 0 \leq \ell \leq k-1.$$

Hence, for $\delta \ll \gamma$ the function ψ is exponentially small at $\bar{\mathscr{S}}_\gamma = \left\{x \in \overline{\Omega} : \operatorname{dist}(x, \partial\Omega) = \gamma\right\}$ and we can extend it to a function, which is denoted again by ψ, in $C^k\left(\overline{\Omega}\right)$ such that it satisfies $\eta^\delta = \operatorname{curl}\psi$ and thus the estimate (5.3.9). □

By Lemma 5.3.19, we can introduce a cut-off function $m^\varepsilon \in \mathscr{D}\left(\overline{\Omega}\right)$ corresponding to $\partial\Omega$, satisfying

$$m^\varepsilon(x) = \begin{cases} 0 & \text{if } \operatorname{dist}(x, \partial\Omega) \leq \varepsilon, \\ 1 & \text{if } \operatorname{dist}(x, \partial\Omega) \geq 2\varepsilon, \end{cases} \quad \text{and} \quad \left\|\nabla^\ell m^\varepsilon\right\|_{L^\infty(\Omega)} \leq C\varepsilon^{-\ell} \text{ for } \ell \in [0,2].$$

As a consequence, one can also show that

$$\|1 - m^\varepsilon\|_{L^2(\Omega^\varepsilon)} \leq C\varepsilon^{\frac{1}{2}}, \quad \varepsilon\|\nabla m^\varepsilon\|_{L^2(\Omega^\varepsilon)} \leq C\varepsilon^{\frac{1}{2}}. \tag{5.3.12}$$

Lemma 5.3.20. *(cf. [102, Lemma 1, Appendix]) For any $u \in H_0^1(\Omega^\varepsilon)$, it holds*

$$\|u\|_{L^2(\Omega^\varepsilon)} \leq C\varepsilon\|\nabla u\|_{[L^2(\Omega^\varepsilon)]^d}.$$

5.4 Macroscopic reconstructions and corrector estimates

In this section, we begin by introducing the so-called macroscopic reconstructions and provide supplementary estimates needed for the proof of our main results stated in Theorem 5.4.2 and Theorem 5.4.3. Our working methodology was used in [40] and successfully applied to derive the corrector estimates for a thermo-diffusion system in a uniformly periodic medium (cf. [70]) and an advection-diffusion-reaction system in a locally-periodic medium (cf. [86]). In principle, the asymptotic expansion can be justified by estimating the differences of the solutions of the micro model (P^ε) and macroscopic reconstructions which can be defined from the macroscopic models $\left(P_N^0\right)$ and $\left(P_D^0\right)$.
Our main results correspond to two cases:

Case 1: The electric potential satisfies the Neumann boundary condition at the boundary of the perforations

Case 2: The electric potential satisfies the Dirichlet boundary condition at the boundary of the perforations

Remark 5.4.1. *To gain the corrector estimates, we require more regularity assumptions on the involved functions as well as the smoothness of the boundaries of the macroscopic domain; compare to the assumptions obtained when upscaling (P^ε). In fact, it is worth pointing out that in Theorem 5.4.2 and Theorem 5.4.3 we assume the regularity properties on the limit functions, postulated in Theorem 5.3.10 for Case 1 and in Theorem 5.3.17 for Case 2, as follows:*

$$\tilde{\Phi}_0, c_0^\pm \in W^{1,\infty}(\Omega^\varepsilon) \cap H^2(\Omega^\varepsilon), \bar{v}_0 \in L^\infty(\Omega^\varepsilon). \tag{5.4.1}$$

The cell functions φ_j for $1 \le j \le d$ solving the family of cell problems (5.3.1) *are supposed to fulfill*

$$\varphi_j \in W^{1+s,2}(Y_l) \text{ for } s > d/2. \tag{5.4.2}$$

Moreover, the cell functions w_j^i, π_j and r_{ij} for $1 \le i, j \le d$ solving the cell problems (5.3.2) *and* (5.3.8)*, respectively, satisfy*

$$w_j^i \in W^{2+s,2}(Y_l), \pi_j \in W^{1+s,2}(Y_l) \text{ and } r_{ij} \in W^{1+s,2}(Y_l) \text{ for } s > d/2. \tag{5.4.3}$$

In addition, we stress that the corrector estimates for the Stokes equation can be gained if we take $\partial\Omega \in C^4$. This assumption is only needed to handle Lemma 5.3.19.

5.4.1 Main results

Theorem 5.4.2. Corrector estimates for Case 1
Assume $(A_1)-(A_6)$. Let the quadruples $\left(v_\varepsilon, p_\varepsilon, \Phi_\varepsilon, c_\varepsilon^\pm\right)$ and $\left(v_0, p_0, \Phi_0, c_0^\pm\right)$ be weak solutions to (P^ε) and $\left(P_N^0\right)$ in the sense of Definition 5.3.1 and Theorem 5.3.10, respectively. Furthermore, we assume that the limit solutions satisfy the regularity property (5.4.1)*. Let φ_j for $1 \le j \le d$ be the cell functions solving the family of cell problems* (5.3.1) *and satisfy* (5.4.2)*. Assume that the initial homogenization limit is of the rate*

$$\left\|c_\varepsilon^{\pm,0} - c_0^{\pm,0}\right\|_{L^2(\Omega^\varepsilon)}^2 \le C\varepsilon^\mu \quad \text{for some } \mu \in \mathbb{R}_+.$$

Then the following corrector estimates hold:

$$\begin{aligned}
&\left\|v_\varepsilon - \bar{v}_0^\varepsilon\right\|_{L^2((0,T)\times\Omega^\varepsilon)} \le C\varepsilon^{\frac{1}{2}},\\
&\left\|\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0^\varepsilon\right\|_{L^2((0,T)\times\Omega^\varepsilon)} + \left\|c_\varepsilon^\pm - c_0^{\pm,\varepsilon}\right\|_{L^2((0,T)\times\Omega^\varepsilon)}\\
&+ \left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d} \le C\max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\},\\
&\left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d} \le C\max\left\{\varepsilon^{\frac{1}{4}}, \varepsilon^{\frac{\mu}{2}}\right\},
\end{aligned}$$

where $\bar{v}_0^\varepsilon$, Φ_0^ε, $c_0^{\pm,\varepsilon}$, $\tilde{\Phi}_1^\varepsilon$, $c_1^{\pm,\varepsilon}$ are the macroscopic reconstructions defined in (5.4.4)-(5.4.8)*.*
Let w_j^i, π_j and r_{ij} for $1 \le i, j \le d$ be the cell functions solving the cell problems (5.3.2) *and* (5.3.8)*, respectively, and satisfy* (5.4.3)*. If we further assume that*

$$\tilde{\Phi}_0 \in H^4(\Omega^\varepsilon), c_0^\pm \in W^{2,\infty}(\Omega^\varepsilon), p_0 \in H^4(\Omega^\varepsilon),$$

then for any $\lambda \in (0,1)$, the following corrector estimates hold:

$$\begin{aligned}
&\left\|v_\varepsilon - |Y_l|^{-1}\mathbb{D}v_0^\varepsilon - \varepsilon|Y_l|^{-1}\mathbb{D}v_1^\varepsilon\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d} \le C\left(\max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\} + \varepsilon^{\frac{\lambda}{2}} + \varepsilon^{1-\frac{3\lambda}{2}} + \varepsilon^{\frac{1}{2}-\lambda}\right),\\
&\|p_\varepsilon - p_0\|_{L^2(\Omega)/\mathbb{R}} \le C\left(\max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\} + \varepsilon^{\frac{\lambda}{2}} + \varepsilon^{1-\frac{3\lambda}{2}} + \varepsilon^{\frac{1}{2}-\lambda}\right),
\end{aligned}$$

where v_0^ε and v_1^ε are defined in (5.4.9) *and* (5.4.10)*, respectively.*

Theorem 5.4.3. *Assume $(A_1)-\left(A_4\right)$. Let the quadruples $\left(v_\varepsilon, p_\varepsilon, \Phi_\varepsilon, c_\varepsilon^\pm\right)$ and $\left(v_0, p_0, \Phi_0, c_0^\pm\right)$ be weak solutions to (P^ε) and $\left(P_D^0\right)$ in the sense of Definition 5.3.1 and Theorem 5.3.17, respectively. Furthermore, we assume that the limit solutions satisfy the regularity property* (5.4.1)*. Let φ_j*

for $1 \le j \le d$ *be the cell functions solving the family of cell problems* (5.3.1) *and satisfy* (5.4.2). *Assume that the initial homogenization limit is of the rate*

$$\left\| c_\varepsilon^{\pm,0} - c_0^{\pm,0} \right\|^2_{L^2(\Omega^\varepsilon)} \le C\varepsilon^\mu \quad \textit{for some } \mu \in \mathbb{R}_+.$$

Then the following corrector estimates hold:

$$\begin{aligned}
&\left\| \tilde{\Phi}_\varepsilon - \tilde{\Phi}_0^\varepsilon \right\|_{L^2((0,T)\times\Omega^\varepsilon)} + \left\| \nabla \left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0^\varepsilon \right) \right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d} + \left\| c_\varepsilon^\pm - c_0^{\pm,\varepsilon} \right\|_{L^2((0,T)\times\Omega^\varepsilon)} \\
&+ \left\| \nabla \left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon} \right) \right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d} + \left\| \tilde{\Phi}_\varepsilon - \overline{\tilde{\Phi}}_0^\varepsilon \right\|_{L^2((0,T)\times\Omega^\varepsilon)} \le C \max\left\{ \varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}} \right\},
\end{aligned}$$

where $c_0^{\pm,\varepsilon}$, $c_1^{\pm,\varepsilon}$, Φ_0^ε, $\overline{\tilde{\Phi}}_0^\varepsilon$ *are the macroscopic reconstructions defined in* (5.4.54)-(5.4.55) *and* (5.4.56)-(5.4.57).

Let w_j^i, π_j *and* r_{ij} *for* $1 \le i, j \le d$ *be the cell functions solving the cell problems* (5.3.2) *and* (5.3.8), *respectively, and satisfy* (5.4.3). *If we further assume that* $p_0 \in H^4(\Omega^\varepsilon)$, *then for any* $\lambda \in (0,1)$, *the following corrector estimates hold:*

$$\begin{aligned}
&\left\| v_\varepsilon - |Y_l|^{-1} \mathbb{D} v_0^\varepsilon - \varepsilon |Y_l|^{-1} \mathbb{D} v_1^\varepsilon \right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d} \le C \left(\max\left\{ \varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}} \right\} + \varepsilon^{\frac{\lambda}{2}} + \varepsilon^{1-\frac{3\lambda}{2}} + \varepsilon^{\frac{1}{2}-\lambda} \right), \\
&\| p_\varepsilon - p_0 \|_{L^2(\Omega)/\mathbb{R}} \le C \left(\max\left\{ \varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}} \right\} + \varepsilon^{\frac{\lambda}{2}} + \varepsilon^{1-\frac{3\lambda}{2}} + \varepsilon^{\frac{1}{2}-\lambda} \right),
\end{aligned}$$

where v_0^ε *and* v_1^ε *are defined in* (5.4.52) *and* (5.4.53), *respectively.*

5.4.2 Proof of Theorem 5.4.2

To study the homogenization limit, the existence of asymptotic expansions

$$\begin{aligned}
v_\varepsilon(t,x) &= v_0\left(t,x,\frac{x}{\varepsilon}\right) + \varepsilon v_1\left(t,x,\frac{x}{\varepsilon}\right) + \varepsilon^2 v_2\left(t,x,\frac{x}{\varepsilon}\right) + \dots \\
p_\varepsilon(t,x) &= p_0\left(t,x,\frac{x}{\varepsilon}\right) + \varepsilon p_1\left(t,x,\frac{x}{\varepsilon}\right) + \varepsilon^2 p_2\left(t,x,\frac{x}{\varepsilon}\right) + \dots \\
\tilde{\Phi}_\varepsilon(t,x) &= \tilde{\Phi}_0\left(t,x,\frac{x}{\varepsilon}\right) + \varepsilon \tilde{\Phi}_1\left(t,x,\frac{x}{\varepsilon}\right) + \varepsilon^2 \tilde{\Phi}_2\left(t,x,\frac{x}{\varepsilon}\right) + \dots \\
c_\varepsilon^\pm(t,x) &= c_0^\pm\left(t,x,\frac{x}{\varepsilon}\right) + \varepsilon c_1^\pm\left(t,x,\frac{x}{\varepsilon}\right) + \varepsilon^2 c_2^\pm\left(t,x,\frac{x}{\varepsilon}\right) + \dots,
\end{aligned}$$

is assumed and some terms (e.g. $v_0, p_0, \tilde{\Phi}_0, c_0^\pm$) have been determined in the previous section. Since the route to derive the corrector for Stokes' equation is different from the usual construction of corrector estimates for the other equations, we shall postpone for a moment the proof of the corrector for the pressure.

We define the macroscopic reconstructions, as follows:

$$\bar{v}_0^\varepsilon(t,x) := |Y_l|^{-1}\,\bar{v}_0(t,x), \tag{5.4.4}$$

$$\tilde{\Phi}_0^\varepsilon(t,x) := \tilde{\Phi}_0(t,x), \tag{5.4.5}$$

$$\tilde{\Phi}_1^\varepsilon(t,x) := \tilde{\Phi}_0^\varepsilon(t,x) + \varepsilon\sum_{j=1}^{d}\varphi_j\left(\frac{x}{\varepsilon}\right)\partial_{x_j}\tilde{\Phi}_0^\varepsilon(t,x), \tag{5.4.6}$$

$$c_0^{\pm,\varepsilon}(t,x) := c_0^{\pm}(t,x), \tag{5.4.7}$$

$$c_1^{\pm,\varepsilon}(t,x) := c_0^{\pm,\varepsilon}(t,x) + \varepsilon\sum_{j=1}^{d}\varphi_j\left(\frac{x}{\varepsilon}\right)\partial_{x_j}c_0^{\pm,\varepsilon}(t,x), \tag{5.4.8}$$

$$v_0^\varepsilon(t,x) := v_0\left(t,x,\frac{x}{\varepsilon}\right), \tag{5.4.9}$$

$$v_1^\varepsilon(t,x) := v_1\left(t,x,\frac{x}{\varepsilon}\right). \tag{5.4.10}$$

Lemma 5.3.18 ensures the following estimate:

$$\left\|v_\varepsilon - \bar{v}_0^\varepsilon\right\|_{L^2((0,T)\times\Omega^\varepsilon)} \le C\varepsilon^{\frac{1}{2}}, \tag{5.4.11}$$

where Definition 5.3.1 and Theorem 5.3.2 guarantee the regularity for v_ε.
Let us now consider the correctors for the electrostatic potential and the concentrations. We take the difference of the microscopic and macroscopic Poisson equations in Definition 5.3.1 and Theorem 5.3.8, respectively, with the test function $\varphi_2 \in H^1(\Omega^\varepsilon)$ and thus obtain

$$\begin{aligned}\int_{\Omega^\varepsilon}\left(\nabla\tilde{\Phi}_\varepsilon - |Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0\right)\cdot\nabla\varphi_2 dx + |Y_l|^{-1}\,\bar{\sigma}\int_{\Omega^\varepsilon}\varphi_2 dx - \varepsilon\int_{\Gamma^\varepsilon}\sigma\varphi_2 dS_\varepsilon \\ = \int_{\Omega^\varepsilon}\left(c_\varepsilon^+ - c_0^+ + c_0^- - c_\varepsilon^-\right)\varphi_2 dx,\end{aligned} \tag{5.4.12}$$

where we recall that $\tilde{\Phi}_\varepsilon = \varepsilon^\alpha\Phi_\varepsilon$ cf. Theorem 5.3.7.
Similarly, for $\varphi_3 \in H^1(\Omega^\varepsilon)$ we also find the difference equation for the Nernst-Planck equation, as follows:

$$\begin{aligned}\left\langle\partial_t\left(c_\varepsilon^\pm - c_0^\pm\right),\varphi_3\right\rangle_{(H^1)',H^1} + \int_{\Omega^\varepsilon}\left(\nabla c_\varepsilon^\pm - |Y_l|^{-1}\,\mathbb{D}\nabla c_0^\pm\right)\cdot\nabla\varphi_3 dx \\ + \int_{\Omega^\varepsilon}\left[|Y_l|^{-1}\,c_0^\pm\left(\bar{v}_0 \mp \mathbb{D}\nabla\tilde{\Phi}_0\right) - c_\varepsilon^\pm\left(v_\varepsilon \mp \nabla\tilde{\Phi}_\varepsilon\right)\right]\cdot\nabla\varphi_3 dx \\ = \int_{\Omega^\varepsilon}\left(R_\varepsilon^\pm\left(c_\varepsilon^+,c_\varepsilon^-\right) - R_0^\pm\left(c_0^+,c_0^-\right)\right)\varphi_3 dx.\end{aligned} \tag{5.4.13}$$

We start the investigation of these corrector justifications by the following choice of test functions:

$$\varphi_2(t,x) := \tilde{\Phi}_\varepsilon(t,x) - \left(\tilde{\Phi}_0^\varepsilon(t,x) + \varepsilon m^\varepsilon(x)\sum_{j=1}^{d}\varphi_j\left(\frac{x}{\varepsilon}\right)\partial_{x_j}\tilde{\Phi}_0(t,x)\right), \tag{5.4.14}$$

$$\varphi_3(t,x) := c_\varepsilon^\pm(t,x) - \left(c_0^{\pm,\varepsilon}(t,x) + \varepsilon m^\varepsilon(x)\sum_{j=1}^{d}\varphi_j\left(\frac{x}{\varepsilon}\right)\partial_{x_j}c_0^\pm(t,x)\right). \tag{5.4.15}$$

To get the estimates from (5.4.12) and (5.4.13), we denote the following terms just for ease of presentation:

$$
\begin{aligned}
\mathscr{J}_1 &:= \int_{\Omega^\varepsilon} \left(\nabla\tilde{\Phi}_\varepsilon - |Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0\right)\cdot\nabla\varphi_2 dx,\\
\mathscr{J}_2 &:= |Y_l|^{-1}\,\bar{\sigma}\int_{\Omega^\varepsilon}\varphi_2 dx - \varepsilon\int_{\Gamma^\varepsilon}\sigma\varphi_2 dS_\varepsilon,\\
\mathscr{J}_3 &:= \int_{\Omega^\varepsilon}\left(c_\varepsilon^+ - c_0^+ + c_0^- - c_\varepsilon^-\right)\varphi_2 dx,\\
\mathscr{K}_1 &:= \left\langle \partial_t\left(c_\varepsilon^\pm - c_0^\pm\right), \varphi_3\right\rangle_{(H^1)',H^1} = \int_{\Omega^\varepsilon}\partial_t\left(c_\varepsilon^\pm - c_0^\pm\right)\varphi_3 dx,\\
\mathscr{K}_2 &:= \int_{\Omega^\varepsilon}\left(\nabla c_\varepsilon^\pm - |Y_l|^{-1}\,\mathbb{D}\nabla c_0^\pm\right)\cdot\nabla\varphi_3 dx,\\
\mathscr{K}_3 &:= \int_{\Omega^\varepsilon}\left[|Y_l|^{-1}\,c_0^\pm\left(\bar{v}_0 \mp \mathbb{D}\nabla\tilde{\Phi}_0\right) - c_\varepsilon^\pm\left(v_\varepsilon \mp \nabla\tilde{\Phi}_\varepsilon\right)\right]\cdot\nabla\varphi_3 dx,\\
\mathscr{K}_4 &:= \int_{\Omega^\varepsilon}\left(R_\varepsilon^\pm\left(c_\varepsilon^+, c_\varepsilon^-\right) - R_0^\pm\left(c_0^+, c_0^-\right)\right)\varphi_3 dx.
\end{aligned}
$$

Using the representation

$$
\nabla\tilde{\Phi}_\varepsilon - |Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0 = \nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right) + \nabla\tilde{\Phi}_1^\varepsilon - |Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0,
$$

the term $\mathscr{J}_1$ thus becomes

$$
\mathscr{J}_1 = \int_{\Omega^\varepsilon}\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\cdot\nabla\varphi_2 dx + \int_{\Omega^\varepsilon}\left(\nabla\tilde{\Phi}_1^\varepsilon - |Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0\right)\cdot\nabla\varphi_2 dx.
$$

With the choice of φ_2 in (5.4.14), we have

$$
\begin{aligned}
\int_{\Omega^\varepsilon}\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\cdot\nabla\varphi_2 dx \geq{}& C\left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}\\
&- C\varepsilon^2\left\|\nabla\left((1-m^\varepsilon)\sum_{j=1}^d\varphi_j^\varepsilon\partial_{x_j}\tilde{\Phi}_0\right)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}.
\end{aligned}
\tag{5.4.16}
$$

To estimate the second term on the right-hand side of (5.4.16), we assume that $\tilde{\Phi}_0 \in W^{1,\infty}(\Omega^\varepsilon)\cap H^2(\Omega^\varepsilon)$ and $\varphi_j \in W^{1+s,2}(Y_l)$ for $s > d/2$ and $1 \leq j \leq d$. Using the Sobolev embedding $W^{1+s,2}(Y_l) \subset C^1\left(\bar{Y}_l\right)$ together with the inequalities in (5.3.12), we estimate that

$$
\begin{aligned}
\varepsilon\left\|\nabla\left((1-m^\varepsilon)\sum_{j=1}^d\varphi_j^\varepsilon\partial_{x_j}\tilde{\Phi}_0\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} &\leq \varepsilon\left\|\nabla m^\varepsilon\right\|_{[L^2(\Omega^\varepsilon)]^d}\left\|\tilde{\Phi}_0\right\|_{W^{1,\infty}(\Omega^\varepsilon)}\sum_{j=1}^d\left\|\varphi_j\right\|_{C\left(\bar{Y}_l\right)}\\
&\quad + \left\|1-m^\varepsilon\right\|_{L^2(\Omega^\varepsilon)}\left\|\tilde{\Phi}_0\right\|_{W^{1,\infty}(\Omega^\varepsilon)}\sum_{j=1}^d\left\|\nabla_y\varphi_j\right\|_{\left[C\left(\bar{Y}_l\right)\right]^d}\\
&\quad + \varepsilon\left\|\tilde{\Phi}_0\right\|_{H^2(\Omega^\varepsilon)}\sum_{j=1}^d\left\|\varphi_j\right\|_{C\left(\bar{Y}_l\right)}\\
&\leq C\left(\varepsilon + \varepsilon^{\frac{1}{2}}\right).
\end{aligned}
$$

Taking into account the explicit computation of $\nabla\tilde{\Phi}_1^\varepsilon$ which reads

$$\nabla\tilde{\Phi}_1^\varepsilon = \nabla_x\tilde{\Phi}_0 + \left(\nabla_y\bar{\varphi}\right)^\varepsilon \nabla_x\tilde{\Phi}_0 + \varepsilon\bar{\varphi}^\varepsilon\nabla_x\nabla\tilde{\Phi}_0 \quad \text{for } \bar{\varphi} = \left(\varphi_j\right)_{j=\overline{1,d}},$$

we can write

$$\nabla\tilde{\Phi}_1^\varepsilon - |Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0 = \nabla\tilde{\Phi}_0 + \left(\nabla_y\bar{\varphi}\right)^\varepsilon \nabla_x\tilde{\Phi}_0 - |Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0 + \varepsilon\bar{\varphi}^\varepsilon\nabla_x\nabla\tilde{\Phi}_0. \tag{5.4.17}$$

Due to the smoothness of the involved functions, the fourth term in (5.4.17) is bounded in L^2-norm by

$$\varepsilon\left\|\bar{\varphi}^\varepsilon\nabla_x\nabla\tilde{\Phi}_0\right\|_{[L^2(\Omega^\varepsilon)]^d} \le C\varepsilon\left\|\bar{\varphi}\right\|_{\left[C\left(\bar{Y}_l\right)\right]^d}\left\|\tilde{\Phi}_0\right\|_{H^2(\Omega^\varepsilon)}. \tag{5.4.18}$$

On the other hand, from the structure of the cell problem 5.3.1 we see that $\mathscr{G} := \mathbb{I} + \nabla_y\bar{\varphi} - |Y_l|^{-1}\,\mathbb{D}$ is divergence-free with respect to y. In parallel with that, its average also vanishes in the sense that

$$\int_{Y_l}\mathscr{G}dy = 0.$$

Consequently, the function $\mathscr{G}$ possesses a vector potential $\mathbf{V}$ which is skew-symmetric and satisfies $\mathscr{G} = \nabla_y\mathbf{V}$. Note that the choice of this potential is not unique in general, but $\mathbf{V}$ can be chosen in such a way that it solves a Poisson equation $\Delta_y\mathbf{V} = f\left(y\right)\nabla_y\mathscr{G}$ for some constant f only dependent of the cell's dimensions. Therefore, to determine $\mathbf{V}$ uniquely, we associate this Poisson equation with the periodic boundary condition at Γ and the vanishing cell average. Using the simple relation $\nabla_y = \varepsilon\nabla - \varepsilon\nabla_x$, we arrive at

$$\mathscr{G}^\varepsilon\nabla\tilde{\Phi}_0 = \varepsilon\nabla\cdot\left(\mathbf{V}^\varepsilon\nabla\tilde{\Phi}_0\right) - \varepsilon\mathbf{V}^\varepsilon\Delta\tilde{\Phi}_0. \tag{5.4.19}$$

Due to the skew-symmetry of $\mathbf{V}$, the first term on the right-hand side of (5.4.19) is divergence-free and its boundedness in $L^2\left(\Omega^\varepsilon\right)$ is thus with the order of ε. Since $\bar{\varphi}\in\left[W^{1+s,2}\left(Y_l\right)\right]^d$ for $s > d/2$ is assumed, it yields from the Poisson equation for $\mathbf{V}$ that

$$\left\|\mathbf{V}\right\|_{W^{1+s,2}(Y_l)} \le C\left\|\mathscr{G}\right\|_{W^{s,2}(Y_l)}.$$

Applying again the compact embedding $W^{s,2}\left(Y_l\right)\subset C\left(\bar{Y}_l\right)$ for $s > d/2$, we obtain $\mathbf{V}\in C\left(\bar{Y}_l\right)$ and it enables us to get the boundedness of the second term on the right-hand side of (5.4.19). In fact, it gives

$$\varepsilon\left\|\mathbf{V}^\varepsilon\Delta\tilde{\Phi}_0\right\|_{L^2(\Omega^\varepsilon)} \le \varepsilon\left\|\mathbf{V}\right\|_{C\left(\bar{Y}_l\right)}\left\|\tilde{\Phi}_0\right\|_{H^2(\Omega^\varepsilon)}.$$

Combining this with (5.4.17), (5.4.18) and using the Hölder's inequality, we conclude that

$$\int_{\Omega^\varepsilon}\left(\nabla\tilde{\Phi}_1^\varepsilon - |Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0\right)\cdot\nabla\varphi_2 dx \le C\varepsilon.$$

This step completes the estimates for $\mathscr{J}_1$. More precisely, we obtain

$$\mathscr{J}_1 \ge C\left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\right\|^2_{[L^2(\Omega^\varepsilon)]^d} - C\left(\varepsilon^2+\varepsilon\right). \tag{5.4.20}$$

In the same vein, we can estimate the term $\mathscr{K}_2$ with the aid of the *a priori* arguments $c_0^\pm\in W^{1,\infty}\left(\Omega^\varepsilon\right)\cap H^2\left(\Omega^\varepsilon\right)$ and $\varphi_j\in W^{1+s,2}\left(Y_l\right)$ for $s > d/2$ and $1\le j\le d$. We thus get

$$\mathscr{K}_2 \ge C\left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|^2_{[L^2(\Omega^\varepsilon)]^d} - C\left(\varepsilon^2+\varepsilon\right). \tag{5.4.21}$$

We now turn our attention to the estimates for $\mathscr{J}_2$ and $\mathscr{J}_3$. Noticing $\bar{\sigma} = \int_\Gamma \sigma dS_y$ which implies that

$$|Y_l|^{-1} \int_{Y_l} \bar{\sigma} dy = \int_\Gamma \sigma dS_y,$$

we then apply [86, Lemma 5.2] to gain

$$|\mathscr{J}_2| \leq C\varepsilon \|\varphi_2\|_{H^1(\Omega^\varepsilon)}.$$

Note that due to the choice of φ_2 in (5.4.14), we have

$$\begin{aligned}
\|\varphi_2\|_{H^1(\Omega^\varepsilon)} &\leq \left\|\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0\right\|_{L^2(\Omega^\varepsilon)} + \left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} \\
&\quad + \left\|\nabla\left(\tilde{\Phi}_1^\varepsilon - \tilde{\Phi}_0\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + \varepsilon \left\|m^\varepsilon \bar{\varphi} \cdot \nabla_x \tilde{\Phi}_0\right\|_{H^1(\Omega^\varepsilon)} \\
&\leq \left\|\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0\right\|_{L^2(\Omega^\varepsilon)} + \left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + C\left(1 + \varepsilon + \varepsilon^{\frac{1}{2}}\right),
\end{aligned} \tag{5.4.22}$$

where we use the inequalities (5.3.12) with the regularity assumptions on $\bar{\varphi}$ and $\tilde{\Phi}_0$, and the following bound:

$$\left\|\nabla\left(\tilde{\Phi}_1^\varepsilon - \tilde{\Phi}_0\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} \leq \left\|\nabla_y \bar{\varphi}\right\|_{C\left(\bar{Y}_l\right)} \left\|\tilde{\Phi}_0\right\|_{W^{1,\infty}(\Omega^\varepsilon)} + \varepsilon \|\bar{\varphi}\|_{C\left(\bar{Y}_l\right)} \left\|\tilde{\Phi}_0\right\|_{H^2(\Omega^\varepsilon)}.$$

Therefore, we can write that

$$|\mathscr{J}_2| \leq C\varepsilon\left(\left\|\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0\right\|_{L^2(\Omega^\varepsilon)} + \left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + 1\right). \tag{5.4.23}$$

The estimate for $\mathscr{J}_3$ can be derived by the Hölder inequality, which reads

$$|\mathscr{J}_3| \leq C\left(\left\|c_\varepsilon^+ - c_0^+\right\|_{L^2(\Omega^\varepsilon)} + \left\|c_\varepsilon^- - c_0^-\right\|_{L^2(\Omega^\varepsilon)}\right) \|\varphi_2\|_{L^2(\Omega^\varepsilon)},$$

and then leads to

$$|\mathscr{J}_3| \leq C\left(\left\|c_\varepsilon^+ - c_0^+\right\|_{L^2(\Omega^\varepsilon)} + \left\|c_\varepsilon^- - c_0^-\right\|_{L^2(\Omega^\varepsilon)}\right)\left(\left\|\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0\right\|_{L^2(\Omega^\varepsilon)} + 1\right). \tag{5.4.24}$$

Let us now consider the term $\mathscr{K}_1$ and $\mathscr{K}_4$. Note that $\mathscr{K}_1$ can be rewritten as

$$\begin{aligned}
&\int_{\Omega^\varepsilon} \partial_t\left(c_\varepsilon^\pm - c_0^\pm\right)\left[c_\varepsilon^\pm(t,x) - \left(c_0^{\pm,\varepsilon}(t,x) + \varepsilon m^\varepsilon \bar{\varphi}^\varepsilon \cdot \nabla_x c_0^\pm\right)\right] dx \\
&\qquad = \frac{1}{2}\frac{d}{dt}\left\|c_\varepsilon^\pm - c_0\right\|_{L^2(\Omega^\varepsilon)}^2 - \varepsilon \int_{\Omega^\varepsilon} \partial_t\left(c_\varepsilon^\pm - c_0^\pm\right) m^\varepsilon \bar{\varphi} \cdot \nabla_x c_0^\pm dx,
\end{aligned} \tag{5.4.25}$$

while from the structure of the reaction in (A_3), we have the similar result for $\mathscr{K}_4$ (to $\mathscr{J}_3$), i.e.

$$\left|\mathscr{K}_4\right| \leq C\left(\left\|c_\varepsilon^+ - c_0^+\right\|_{L^2(\Omega^\varepsilon)} + \left\|c_\varepsilon^- - c_0^-\right\|_{L^2(\Omega^\varepsilon)}\right)\left(\left\|c_\varepsilon^\pm - c_0^\pm\right\|_{L^2(\Omega^\varepsilon)} + 1\right). \tag{5.4.26}$$

The estimate for $\mathscr{K}_3$ relies on the following decomposition:

$$\begin{aligned}
|Y_l|^{-1} c_0^\pm\left(\bar{v}_0 \mp \mathbb{D}\nabla\tilde{\Phi}_0\right) - c_\varepsilon^\pm\left(v_\varepsilon \mp \nabla\tilde{\Phi}_\varepsilon\right) &= \left(c_0^\pm - c_\varepsilon^\pm\right)\left(|Y_l|^{-1}\bar{v}_0 \mp |Y_l|^{-1}\mathbb{D}\nabla\tilde{\Phi}_0\right) \\
&\quad + c_\varepsilon^\pm\left(|Y_l|^{-1}\bar{v}_0 - v_\varepsilon\right) \mp c_\varepsilon^\pm\left(|Y_l|^{-1}\mathbb{D}\nabla\tilde{\Phi}_0 - \nabla\tilde{\Phi}_\varepsilon\right).
\end{aligned}$$

Clearly, if $\bar{v}_0 \in L^\infty(\Omega^\varepsilon)$ and the fact already assumed that $\tilde{\Phi}_0 \in W^{1,\infty}(\Omega^\varepsilon) \cap H^2(\Omega^\varepsilon)$, one can estimate, by Hölder's inequality, that

$$\int_{\Omega^\varepsilon} \left(c_0^\pm - c_\varepsilon^\pm\right)\left(|Y_l|^{-1}\bar{v}_0 \mp |Y_l|^{-1}\mathbb{D}\nabla\tilde{\Phi}_0\right) \cdot \nabla\varphi_3 dx \leq C\left\|c_\varepsilon^\pm - c_0^\pm\right\|_{L^2(\Omega^\varepsilon)} \|\nabla\varphi_3\|_{[L^2(\Omega^\varepsilon)]^d}. \tag{5.4.27}$$

By using the same arguments in estimating the norm $\|\varphi_2\|_{H^1(\Omega^\varepsilon)}$ in (5.4.22), we get from (5.4.27) that

$$\int_{\Omega^\varepsilon} \left(c_0^\pm - c_\varepsilon^\pm\right)\left(|Y_l|^{-1}\,\bar{v}_0 \mp |Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0\right)\cdot\nabla\varphi_3 dx$$
$$\leq C\left\|c_\varepsilon^\pm - c_0^\pm\right\|_{L^2(\Omega^\varepsilon)}\left(\left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + 1\right). \tag{5.4.28}$$

Next, we observe that

$$\int_{\Omega^\varepsilon} c_\varepsilon^\pm\left(|Y_l|^{-1}\,\bar{v}_0 - v_\varepsilon\right)\cdot\nabla\varphi_3 dx$$
$$\leq C\left\|v_\varepsilon - \bar{v}_0^\varepsilon\right\|_{L^2(\Omega^\varepsilon)}\left(\left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + 1\right)$$
$$\leq C\varepsilon^{\frac{1}{2}}\left(\left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + 1\right), \tag{5.4.29}$$

which is a direct result from (5.4.11) and of the fact that all the microscopic solutions are bounded from above uniformly in the choice of ε (see Theorem 5.3.5).
Using again Theorem 5.3.5, we estimate that

$$\int_{\Omega^\varepsilon} c_\varepsilon^\pm\left(|Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0 - \nabla\tilde{\Phi}_\varepsilon\right)\cdot\nabla\varphi_3 dx$$
$$\leq C\left(\left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + \varepsilon\right)\left(\left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + 1\right), \tag{5.4.30}$$

which also completes the estimates for $\mathscr{K}_3$.
Combining (5.4.20), (5.4.21), (5.4.23), (5.4.24), (5.4.26), (5.4.28), (5.4.29) and (5.4.30), we obtain, after some rearrangements, that

$$\left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\right\|^2_{[L^2(\Omega^\varepsilon)]^d} + \varepsilon\left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}$$
$$\leq C\left(\varepsilon^2 + \varepsilon\right) + C\varepsilon^{\frac{3}{2}}\left(\left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + 1\right)$$
$$+ C\varepsilon\left(\left\|\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0\right\|_{L^2(\Omega^\varepsilon)} + \left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\right\|_{[L^2(\Omega^\varepsilon)]^d}\right)$$
$$+ C\left\|c_\varepsilon^\pm - c_0^\pm\right\|_{L^2(\Omega^\varepsilon)}\left(\left\|\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0\right\|_{L^2(\Omega^\varepsilon)} + 1\right)$$
$$+ C\varepsilon\left(\left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_1^\varepsilon\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + \varepsilon\right)\left(\left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + 1\right)$$
$$+ C\varepsilon\left\|c_\varepsilon^\pm - c_0^\pm\right\|_{L^2(\Omega^\varepsilon)}\left(\left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|_{[L^2(\Omega^\varepsilon)]^d} + 1\right). \tag{5.4.31}$$

It now remains to estimate the second term on the right-hand side of (5.4.25). In fact, integrating the right-hand side of (5.4.25) by parts gives

$$\int_0^t\int_{\Omega^\varepsilon} m^\varepsilon\,\partial_t\left(c_\varepsilon^\pm - c_0^\pm\right)\bar{\varphi}\cdot\nabla_x c_0^\pm dx ds = \int_{\Omega^\varepsilon} m^\varepsilon\left(c_\varepsilon^\pm - c_0^\pm\right)\bar{\varphi}\cdot\nabla_x c_0^\pm dx\Big|_{s=0}^{s=t}$$
$$- \int_0^t\int_{\Omega^\varepsilon} m^\varepsilon\left(c_\varepsilon^\pm - c_0^\pm\right)\bar{\varphi}\cdot\nabla_x\partial_t c_0^\pm dx ds,$$

and we also have

$$\varepsilon\left|\int_{\Omega^\varepsilon} m^\varepsilon\left[\left(c_\varepsilon^\pm - c_0^\pm\right) - \left(c_\varepsilon^\pm(0) - c_0^\pm(0)\right)\right]\bar{\varphi}\cdot\nabla_x c_0^\pm dx\right|$$
$$\leq C\varepsilon\left(\left\|c_\varepsilon^\pm - c_0^\pm\right\|_{L^2(\Omega^\varepsilon)} + \left\|c_\varepsilon^{\pm,0} - c_0^{\pm,0}\right\|_{L^2(\Omega^\varepsilon)}\right). \tag{5.4.32}$$

At this moment, if we set

$$\begin{aligned} w_1(t) &:= \left\|\tilde{\Phi}_\varepsilon(t)-\tilde{\Phi}_0(t)\right\|^2_{L^2(\Omega^\varepsilon)} + \left\|c^\pm_\varepsilon(t)-c^\pm_0(t)\right\|^2_{L^2(\Omega^\varepsilon)}, \\ w_2(t) &:= \left\|\nabla\left(\tilde{\Phi}_\varepsilon-\tilde{\Phi}^\varepsilon_1\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d} + \varepsilon\left\|\nabla\left(c^\pm_\varepsilon-c^{\pm,\varepsilon}_1\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}, \\ w_0 &:= \left\|c^{\pm,0}_\varepsilon-c^{\pm,0}_0\right\|^2_{L^2(\Omega^\varepsilon)}, \end{aligned}$$

then after integrating (5.4.31) and (5.4.25) from 0 to t, we are led to the following Gronwall-like estimate:

$$w_1(t)+\int_0^t w_2(s)\,ds \le C\left(\varepsilon+(1+\varepsilon)w_0+\int_0^t w_1(s)\,ds\right),$$

which provides that

$$w_1(t)+\int_0^t w_2(s)\,ds \le C\left(\varepsilon+(1+\varepsilon)w_0\right) \quad \text{for } t\in[0,T].$$

Assuming

$$\left\|c^{\pm,0}_\varepsilon-c^{\pm,0}_0\right\|^2_{L^2(\Omega^\varepsilon)} \le C\varepsilon^\mu \quad \text{for some } \mu\in\mathbb{R}_+, \tag{5.4.33}$$

we thus obtain

$$\begin{aligned} &\left\|\tilde{\Phi}_\varepsilon-\tilde{\Phi}_0\right\|^2_{L^2((0,T)\times\Omega^\varepsilon)} + \left\|c^\pm_\varepsilon-c^\pm_0\right\|^2_{L^2((0,T)\times\Omega^\varepsilon)} + \left\|\nabla\left(\tilde{\Phi}_\varepsilon-\tilde{\Phi}^\varepsilon_1\right)\right\|^2_{[L^2((0,T)\times\Omega^\varepsilon)]^d} \\ &\qquad + \varepsilon\left\|\nabla\left(c^\pm_\varepsilon-c^{\pm,\varepsilon}_1\right)\right\|^2_{[L^2((0,T)\times\Omega^\varepsilon)]^d} \le C\max\{\varepsilon,\varepsilon^\mu\}. \end{aligned} \tag{5.4.34}$$

Since the obtained estimate for $\left\|\nabla\left(\tilde{\Phi}_\varepsilon-\tilde{\Phi}^\varepsilon_1\right)\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d}$ is of the order of $\mathcal{O}(\max\{\varepsilon,\varepsilon^\mu\})$, we can also increase the rate of $\left\|\nabla\left(c^\pm_\varepsilon-c^{\pm,\varepsilon}_1\right)\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d}$. Indeed, let us consider the estimate (5.4.28) and (5.4.30) for $\left\|c^\pm_\varepsilon-c^\pm_0\right\|_{L^2((0,T)\times\Omega^\varepsilon)}$ and $\left\|\nabla\left(\tilde{\Phi}_\varepsilon-\tilde{\Phi}^\varepsilon_1\right)\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d}$, respectively. Then, we combine again (5.4.21), (5.4.26), (5.4.28), (5.4.29), (5.4.30) and (5.4.32) to get another Gronwall-like estimate:

$$\left\|\nabla\left(c^\pm_\varepsilon-c^{\pm,\varepsilon}_1\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d} \le C\left(\varepsilon^{\frac{1}{2}}+\max\{\varepsilon,\varepsilon^\mu\}+\varepsilon\int_0^t\left\|\nabla\left(c^\pm_\varepsilon-c^{\pm,\varepsilon}_1\right)(s)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}ds\right).$$

As a result, we have

$$\left\|\nabla\left(c^\pm_\varepsilon-c^{\pm,\varepsilon}_1\right)\right\|^2_{[L^2((0,T)\times\Omega^\varepsilon)]^d} \le C\max\left\{\varepsilon^{\frac{1}{2}},\varepsilon^\mu\right\}. \tag{5.4.35}$$

Note that with $\gamma>\alpha$, the drift term in the macroscopic Nernst-Planck system is not present. Thus, this term does not appear in (5.4.28) and (5.4.30). Due to the *a priori* estimate that $\left\|\tilde{\Phi}_\varepsilon\right\|_{L^2(0,T;H^1(\Omega^\varepsilon))}\le C$ (cf. Theorem 5.3.13) in combination with the boundedness of $c^\pm_\varepsilon$ (cf. Theorem 5.3.5), it is straightforward to get the same corrector estimate as (5.4.34). Moreover, if $\alpha<0$, the corrector becomes of the order $\mathcal{O}(\max\{\varepsilon,\varepsilon^{-\alpha},\varepsilon^\mu\})$. This explicitly illustrates the effect of the scaling parameter α on the rate of the convergence.

For the time being, it only remains to come up with the corrector estimates for the Stokes equation. At this point, we must pay a regularity price[1] concerning the smoothness of the

[1] Compare to the two-scale convergence method when deriving the structure of the macroscopic system in [99].

boundaries to make use of Lemma 5.3.19. With $\partial\Omega \in C^4$, we adapt the ideas of [80] to define the following velocity corrector:

$$\begin{aligned}\mathscr{V}^{\varepsilon,\delta}(t,x) := &-\sum_{j=1}^{d} w_j\left(\frac{x}{\varepsilon}\right)\left[\left(c_0^+ - c_0^-\right)\partial_{x_j}\tilde{\Phi}_0(t,x) + \partial_{x_j}p_0(t,x) + \left(\mathbb{K}^{-1}\eta^\delta\right)_j\right] \\ &-\varepsilon\sum_{i,j=1}^{d} r_{ij}\left(\frac{x}{\varepsilon}\right)(1-m^\varepsilon)\,\partial_{x_i}\left(\left(c_0^+ - c_0^-\right)\partial_{x_j}\tilde{\Phi}_0(t,x) + \partial_{x_j}p_0(t,x) + \left(\mathbb{K}^{-1}\eta^\delta\right)_j\right),\end{aligned} \tag{5.4.36}$$

and the pressure corrector:

$$\mathscr{P}^{\varepsilon,\delta}(t,x) := p_0(t,x) - \varepsilon\sum_{j=1}^{d}\pi_j\left(\frac{x}{\varepsilon}\right)\left[\left(c_0^+ - c_0^-\right)\partial_{x_j}\tilde{\Phi}_0(t,x) + \partial_{x_j}p_0(t,x) + \left(\mathbb{K}^{-1}\eta^\delta\right)_j\right], \tag{5.4.37}$$

where w_j, π_j and r_{ij} are solutions of the problems (5.3.1) and (5.3.8), respectively, for $1 \le i,j \le d$; and η^δ is a function defined in Lemma 5.3.19.
From (5.4.36), one can structure the divergence of the corrector $\mathscr{V}^{\varepsilon,\delta}$. In fact, by definition of the function η^δ and the structure of the macroscopic system for the velocity in Theorem 5.3.8, the divergence of the first term of vanishes (5.4.36) itself. Therefore, one computes that

$$\begin{aligned}\nabla\cdot\mathscr{V}^{\varepsilon,\delta} = &-\sum_{i,j=1}^{d}\left(w_j^i\left(\frac{x}{\varepsilon}\right) - |Y_l|^{-1}K_{ij}\right)(1-m^\varepsilon)\,\partial_{x_i}\left[\left(c_0^+ - c_0^-\right)\partial_{x_j}\tilde{\Phi}_0 + \partial_{x_j}p_0 + \left(\mathbb{K}^{-1}\eta^\delta\right)_j\right] \\ &-\varepsilon\sum_{i,j=1}^{d} r_{ij}\left(\frac{x}{\varepsilon}\right)(1-m^\varepsilon)\,\nabla\cdot\left[\partial_{x_i}\left(\left(c_0^+ - c_0^-\right)\partial_{x_j}\tilde{\Phi}_0 + \partial_{x_j}p_0 + \left(\mathbb{K}^{-1}\eta^\delta\right)_j\right)\right] \\ &+\varepsilon\sum_{i,j=1}^{d} r_{ij}\left(\frac{x}{\varepsilon}\right)\nabla m^\varepsilon\,\partial_{x_i}\left[\left(c_0^+ - c_0^-\right)\partial_{x_j}\tilde{\Phi}_0 + \partial_{x_j}p_0 + \left(\mathbb{K}^{-1}\eta^\delta\right)_j\right],\end{aligned}$$

where we also use the structure of the cell problem (5.3.8).
Taking into account that

$$\begin{aligned}&-\sum_{i,j=1}^{d} K_{ij}\partial_{x_i}\left(\left(c_0^\pm - c_0^-\right)\partial_{x_j}\tilde{\Phi}_0 + \partial_{x_j}p_0\right) = 0, \\ &\sum_{i,j=1}^{d} K_{ij}\partial_{x_i}\left(\mathbb{K}^{-1}\eta^\delta\right)_j = 0,\end{aligned}$$

hold (see again the macroscopic system for the velocity in Theorem 5.3.8 as well as the properties of η^δ in Lemma 5.3.19), the estimate for the divergence of $\mathscr{V}^{\varepsilon,\delta}$ in L^2-norm

$$\left\|\nabla\cdot\mathscr{V}^{\varepsilon,\delta}\right\|_{L^2(\Omega^\varepsilon)} \le C\left(\varepsilon^{\frac{1}{2}}\delta^{-1} + \varepsilon\delta^{-\frac{3}{2}} + \varepsilon^{\frac{1}{q}}\delta^{-\frac{1}{2}-\frac{1}{q}}\right) \quad \text{for } q \in [2,\infty],$$

is directly obtained from Lemma 5.3.19 and the inequalities in (5.3.12).
At this stage, if we choose $q = 2$ and $\delta \gg \varepsilon$, we get

$$\left\|\nabla\cdot\mathscr{V}^{\varepsilon,\delta}\right\|_{L^2(\Omega^\varepsilon)} \le C\left(\varepsilon\delta^{-\frac{3}{2}} + \varepsilon^{\frac{1}{2}}\delta^{-1}\right), \tag{5.4.38}$$

and hence,

$$\left\|\nabla\cdot\mathscr{V}^{\varepsilon,\delta}\right\|_{L^2((0,T)\times\Omega^\varepsilon)} \le C\left(\varepsilon\delta^{-\frac{3}{2}} + \varepsilon^{\frac{1}{2}}\delta^{-1}\right).$$

Next, we introduce the following function:

$$\Psi^{\varepsilon}(t,x) := \Delta \mathscr{V}^{\varepsilon,\delta}(t,x) - \varepsilon^{-2}\nabla \mathscr{P}^{\varepsilon,\delta} - \left(c_0^+(t,x) - c_0^-(t,x)\right)\nabla \tilde{\Phi}_0(t,x).$$

Thus, for any $\varphi_1 \in \left[H_0^1(\Omega^{\varepsilon})\right]^d$ we have, after direct computations, that

$$\begin{aligned}
&\langle \Psi^{\varepsilon}, \varphi_1 \rangle_{\left([H^1]^d\right)', [H^1]^d} \\
&= -\sum_{j=1}^{d} \int_{\Omega^{\varepsilon}} \left(\Delta w_j\left(\frac{x}{\varepsilon}\right) - \varepsilon^{-1}\nabla \pi_j\left(\frac{x}{\varepsilon}\right)\right)\left[\left(c_0^+ - c_0^-\right)\partial_{x_j}\tilde{\Phi}_0 + \partial_{x_j} p_0 + \left(\mathbb{K}^{-1}\eta^{\delta}\right)_j\right]\varphi_1 dx \\
&- \varepsilon^{-2}\int_{\Omega^{\varepsilon}} \left(\nabla p_0 + \left(c_0^+ - c_0^-\right)\nabla \tilde{\Phi}_0\right)\varphi_1 dx \\
&- \sum_{j=1}^{d} \int_{\Omega^{\varepsilon}} \left(2\nabla w_j\left(\frac{x}{\varepsilon}\right) - \varepsilon^{-1}\pi\left(\frac{x}{\varepsilon}\right)\mathbb{I}\right)\nabla\left[\left(c_0^+ - c_0^-\right)\partial_{x_j}\tilde{\Phi}_0 + \partial_{x_j} p_0 + \left(\mathbb{K}^{-1}\eta^{\delta}\right)_j\right]\varphi_1 dx \\
&- \sum_{j=1}^{d} \int_{\Omega^{\varepsilon}} w_j\left(\frac{x}{\varepsilon}\right)\Delta\left[\left(c_0^+ - c_0^-\right)\partial_{x_j}\tilde{\Phi}_0 + \partial_{x_j} p_0 + \left(\mathbb{K}^{-1}\eta^{\delta}\right)_j\right]\varphi_1 dx \\
&- \varepsilon\sum_{j=1}^{d} \int_{\Omega^{\varepsilon}} \nabla\left[r_{ij}\left(\frac{x}{\varepsilon}\right)(1-m^{\varepsilon})\partial_{x_j}\left(\left(c_0^+ - c_0^-\right)\partial_{x_j}\tilde{\Phi}_0 + \partial_{x_j} p_0 + \left(\mathbb{K}^{-1}\eta^{\delta}\right)_j\right)\right]\cdot \nabla\varphi_1 dx \\
&:= \mathscr{I}_1 + \mathscr{I}_2 + \mathscr{I}_3 + \mathscr{I}_4 + \mathscr{I}_5.
\end{aligned} \tag{5.4.39}$$

Note that $\mathbb{I}$ here stands for the identity matrix. From now on, to get the estimate for Ψ^{ε} in $\left(H^1\right)'$-norm, we need bounds of $\mathscr{I}_i$ for $1 \le i \le 5$. Indeed, with the help of Lemma 5.3.20 applied to the test function φ_1, and the estimates of the involved functions, one immediately obtains from Hölder's inequality that

$$|\mathscr{I}_3| + \left|\mathscr{I}_4\right| \le C\left(\delta^{-\frac{1}{2}} + \varepsilon\delta^{-\frac{3}{2}}\right)\|\nabla\varphi_1\|_{[L^2(\Omega^{\varepsilon})]^d}, \tag{5.4.40}$$

where we also apply again the estimate of η^{δ} in Lemma 5.3.19.
To estimate $\mathscr{I}_5$, we notice

$$|\mathscr{I}_5| \le C\left(\delta^{-\frac{1}{2}} + \varepsilon\delta^{-\frac{3}{2}}\right)\|\nabla\varphi_1\|_{[L^2(\Omega^{\varepsilon})]^d}, \tag{5.4.41}$$

where we also employ the estimates for m^{ε} in (5.3.12).
In addition, we have

$$\begin{aligned}
&|\mathscr{I}_1 + \mathscr{I}_2| \\
&\le \left|\int_{\Omega^{\varepsilon}} \varepsilon^{-2}\left[-\sum_{j=1}^{d}\left(\left(c_0^+ - c_0^-\right)\partial_{x_j}\tilde{\Phi}_0 + \partial_{x_j} p_0 + \left(\mathbb{K}^{-1}\eta^{\delta}\right)_j\right) + \nabla p_0 + \left(c_0^+ - c_0^-\right)\nabla\tilde{\Phi}_0\right]\varphi_1 dx\right| \\
&\le C\varepsilon^{-1}\delta^{\frac{1}{2}}\|\nabla\varphi_1\|_{[L^2(\Omega^{\varepsilon})]^d}.
\end{aligned} \tag{5.4.42}$$

Consequently, collecting (5.4.39)-(5.4.42) and according to the definition of the $\left(H^1\right)'$-norm, we arrive at

$$\begin{aligned}
\|\Psi^{\varepsilon}\|_{\left([H^1(\Omega^{\varepsilon})]^d\right)'} &= \sup_{\varphi_1 \in [H^1(\Omega^{\varepsilon})]^d, \|\varphi_1\|_{[H^1(\Omega^{\varepsilon})]^d} \le 1} \langle \Psi^{\varepsilon}, \varphi_1 \rangle_{\left([H^1]^d\right)', [H^1]^d} \\
&\le C\left(\varepsilon^{-1}\delta^{\frac{1}{2}} + \delta^{-\frac{1}{2}} + \varepsilon\delta^{-\frac{3}{2}}\right)\|\nabla\varphi_1\|_{[L^2(\Omega^{\varepsilon})]^d}.
\end{aligned} \tag{5.4.43}$$

Now, we have available a couple of estimates related to the correctors $\mathscr{V}^{\varepsilon,\delta}$ and $\mathscr{P}^{\varepsilon,\delta}$. To go on, we consider the differences

$$\mathscr{D}_1^\varepsilon := v_\varepsilon - |Y_l|^{-1}\,\mathbb{D}\mathscr{V}^{\varepsilon,\delta}, \quad \mathscr{D}_2^\varepsilon := p_\varepsilon - |Y_l|^{-1}\,\mathbb{D}\mathscr{P}^{\varepsilon,\delta},$$

and observe that the equation

$$-\varepsilon^2\Delta\mathscr{D}_1^\varepsilon + \nabla\mathscr{D}_2^\varepsilon = \varepsilon^2\left[|Y_l|^{-1}\,\mathbb{D}\Psi^\varepsilon - \varepsilon^{-2}\left(\left(c_\varepsilon^+ - c_\varepsilon^-\right)\nabla\tilde{\Phi}_\varepsilon - \left(c_0^+ - c_0^-\right)|Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0\right)\right] \quad (5.4.44)$$

holds a.e. in Ω^ε.
It now remains to estimate the second term on the right-hand side of the equation (5.4.47) in $\left(H^1\right)'$-norm. This estimate fully relies on the corrector estimate for the electrostatic potentials in (5.4.34), the boundedness of concentration fields in Theorem 5.3.5 with the assumption that $c_0^\pm \in W^{1,\infty}(\Omega^\varepsilon)\cap H^2(\Omega^\varepsilon)$. In fact, the estimate resembles very much the one in (5.4.30), viz.

$$\begin{aligned}
&\left\langle\left(c_\varepsilon^+ - c_\varepsilon^-\right)\nabla\tilde{\Phi}_\varepsilon - \left(c_0^+ - c_0^-\right)|Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0, \varphi_1\right\rangle_{\left([H^1]^d\right)',[H^1]^d}\\
&\le C\left\|\nabla\tilde{\Phi}_\varepsilon - |Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0\right\|_{[L^2(\Omega^\varepsilon)]^d}\|\varphi_1\|_{L^2(\Omega^\varepsilon)}\\
&\le C\max\left\{\varepsilon^{\frac{3}{2}}, \varepsilon^{\frac{\mu}{2}+1}\right\}\|\nabla\varphi_1\|_{[L^2(\Omega^\varepsilon)]^d},
\end{aligned} \quad (5.4.45)$$

for all $\varphi_1 \in \left[H_0^1(\Omega^\varepsilon)\right]^d$ and where we also use Lemma 5.3.20.
For ease of presentation, we put

$$\mathscr{L}^\varepsilon = \varepsilon^{-2}\left(\left(c_\varepsilon^+ - c_\varepsilon^-\right)\nabla\tilde{\Phi}_\varepsilon - \left(c_0^+ - c_0^-\right)|Y_l|^{-1}\,\mathbb{D}\nabla\tilde{\Phi}_0\right).$$

The corrector for the pressure can be obtained by the use of the following results which are deduced from [111] and [80]:

- there exists an extension $E\left(\mathscr{D}_2^\varepsilon\right) \in L^2(\Omega)/\mathbb{R}$ of $\mathscr{D}_2^\varepsilon$ such that

$$\left\|E\left(\mathscr{D}_2^\varepsilon\right)\right\|_{L^2(\Omega)/\mathbb{R}} \le C\varepsilon\left(\|\Psi^\varepsilon - \mathscr{L}^\varepsilon\|_{\left([H^1(\Omega^\varepsilon)]^d\right)'} + \left\|\nabla\mathscr{D}_1^\varepsilon\right\|_{[L^2(\Omega^\varepsilon)]^{d^2}}\right), \quad (5.4.46)$$

- the following estimates hold:

$$\left\|\nabla\mathscr{D}_1^\varepsilon\right\|_{[L^2(\Omega^\varepsilon)]^{d^2}} \le C\left(\|\Psi^\varepsilon - \mathscr{L}^\varepsilon\|_{\left([H^1(\Omega^\varepsilon)]^d\right)'} + \varepsilon^{-1}\left\|\nabla\cdot\mathscr{V}^{\varepsilon,\delta}\right\|_{L^2(\Omega^\varepsilon)}\right), \quad (5.4.47)$$

$$\left\|\mathscr{D}_1^\varepsilon\right\|_{[L^2(\Omega^\varepsilon)]^d} \le C\left(\varepsilon\|\Psi^\varepsilon - \mathscr{L}^\varepsilon\|_{\left([H^1(\Omega^\varepsilon)]^d\right)'} + \left\|\nabla\cdot\mathscr{V}^{\varepsilon,\delta}\right\|_{L^2(\Omega^\varepsilon)}\right). \quad (5.4.48)$$

Collecting (5.4.43) and (5.4.45), we get

$$\|\Psi^\varepsilon - \mathscr{L}^\varepsilon\|_{\left([H^1(\Omega^\varepsilon)]^d\right)'} \le C\left(\varepsilon^{-1}\delta^{\frac{1}{2}} + \delta^{-\frac{1}{2}} + \varepsilon\delta^{-\frac{3}{2}} + \max\left\{\varepsilon^{-\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}-1}\right\}\right)\|\nabla\varphi_1\|_{[L^2(\Omega^\varepsilon)]^d}. \quad (5.4.49)$$

We thus observe from (5.4.48), (5.4.38) and (5.4.49) that

$$\left\|\mathscr{D}_1^\varepsilon\right\|_{[L^2(\Omega^\varepsilon)]^d} \le C\left(\delta^{\frac{1}{2}} + \varepsilon\delta^{-\frac{1}{2}} + \varepsilon^2\delta^{-\frac{3}{2}} + \max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\} + \varepsilon\delta^{-\frac{3}{2}} + \varepsilon^{\frac{1}{2}}\delta^{-1}\right).$$

Since $\delta \gg \varepsilon$, we can take $\delta = \varepsilon^\lambda$ for $\lambda \in (0,1)$ to obtain

$$\begin{aligned}
\left\|\mathscr{D}_1^\varepsilon\right\|_{[L^2(\Omega^\varepsilon)]^d} &\le C\left(\varepsilon^{\frac{\lambda}{2}} + \varepsilon^{1-\frac{\lambda}{2}} + \varepsilon^{2-\frac{3\lambda}{2}} + \varepsilon^{1-\frac{3\lambda}{2}} + \varepsilon^{\frac{1}{2}-\lambda} + \max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\}\right)\\
&\le C\left(\max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\} + \varepsilon^{\frac{\lambda}{2}} + \varepsilon^{1-\frac{3\lambda}{2}} + \varepsilon^{\frac{1}{2}-\lambda}\right).
\end{aligned}$$

On the other hand, the optimal value for λ is $1/3$ which leads to the following estimate:

$$\left\|\mathscr{D}_1^\varepsilon\right\|_{[L^2(\Omega^\varepsilon)]^d} \leq C \max\left\{\varepsilon^{\frac{1}{6}}, \varepsilon^{\frac{\mu}{2}}\right\}. \tag{5.4.50}$$

Hereafter, it follows from (5.4.50), (5.4.46), (5.4.47) and (5.4.49) that

$$\begin{aligned}\left\|E\left(\mathscr{D}_2^\varepsilon\right)\right\|_{L^2(\Omega)/\mathbb{R}} &\leq C\left(\varepsilon\left\|\Psi^\varepsilon - \mathscr{L}^\varepsilon\right\|_{\left([H^1(\Omega^\varepsilon)]^d\right)'} + \left\|\nabla\cdot\mathscr{V}^{\varepsilon,\delta}\right\|_{[L^2(\Omega^\varepsilon)]^{d^2}}\right)\\ &\leq C\left(\max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\} + \varepsilon^{\frac{\lambda}{2}} + \varepsilon^{1-\frac{3\lambda}{2}} + \varepsilon^{\frac{1}{2}-\lambda}\right).\end{aligned}$$

This indicates the following estimate:

$$\|p_\varepsilon - p_0\|_{L^2(\Omega)/\mathbb{R}} \leq C\left(\max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\} + \varepsilon^{\frac{\lambda}{2}} + \varepsilon^{1-\frac{3\lambda}{2}} + \varepsilon^{\frac{1}{2}-\lambda}\right). \tag{5.4.51}$$

Finally, we gather (5.4.11), (5.4.34), (5.4.35), (5.4.50) and (5.4.51) to conclude the proof of Theorem 5.4.2.

5.4.3 Proof of Theorem 5.4.3

We turn the attention to the Dirichlet boundary condition for the electrostatic potential on the micro-surface. Based on Theorem 5.3.15, we observe that the structure of the macroscopic systems for the Stokes and Nernst-Planck equations are the same as the corresponding systems in the Neumann case (see Theorem 5.3.8). Therefore, the corrector estimates for these systems remain unchanged in Theorem 5.4.2. Also, some regularity properties are not needed in this case. We derive first the corrector estimates for the velocity and pressure and then the corrector estimates of the concentration fields. Thereby, the corrector for the electrostatic potential can also be obtained. Here, the macroscopic reconstructions are defined as follows:

$$v_0^\varepsilon(t,x) := v_0\left(t,x,\frac{x}{\varepsilon}\right), \tag{5.4.52}$$

$$v_1^\varepsilon(t,x) := v_1\left(t,x,\frac{x}{\varepsilon}\right), \tag{5.4.53}$$

$$c_0^{\pm,\varepsilon}(t,x) := c_0^\pm(t,x), \tag{5.4.54}$$

$$c_1^{\pm,\varepsilon}(t,x) := c_0^{\pm,\varepsilon}(t,x) + \varepsilon\sum_{j=1}^d \varphi_j\left(\frac{x}{\varepsilon}\right)\partial_{x_j} c_0^{\pm,\varepsilon}(t,x). \tag{5.4.55}$$

Recall $\tilde{\Phi}_\varepsilon := \varepsilon^{\alpha-2}\Phi_\varepsilon^{\text{hom}}$. By Theorem 5.3.14, $\tilde{\Phi}_\varepsilon$ obeys the weak formulation

$$\int_{\Omega^\varepsilon} \varepsilon^2\nabla\tilde{\Phi}_\varepsilon\cdot\nabla\varphi_2 dx = \int_{\Omega^\varepsilon}\left(c_\varepsilon^+ - c_\varepsilon^-\right)\varphi_2 dx \quad \text{for all } \varphi_2 \in H_0^1(\Omega^\varepsilon).$$

Therefore, we define the following macroscopic reconstructions:

$$\tilde{\Phi}_0^\varepsilon(t,x) := \tilde{\Phi}_0\left(t,x,\frac{x}{\varepsilon}\right), \tag{5.4.56}$$

$$\overline{\tilde{\Phi}}_0^\varepsilon(t,x) := |Y_l|^{-1}\,\overline{\tilde{\Phi}}_0(t,x), \tag{5.4.57}$$

and recall that the strong formulation for $\tilde{\Phi}_0$ (see [99, Theorem 4.12]) is given by

$$\begin{aligned}&-\Delta_y\tilde{\Phi}_0(t,x,y) = c_0^\pm(t,x) - c_0^-(t,x) \text{ in } (0,T)\times\Omega\times Y_l,\\ &\tilde{\Phi}_0 = 0 \text{ in } (0,T)\times\Omega\times\Gamma.\end{aligned}$$

Consequently, the difference equation for the Poisson equation can be written as

$$-\varepsilon^2\Delta\tilde{\Phi}_\varepsilon+\left(\Delta_y\tilde{\Phi}_0\right)^\varepsilon=\left(c_\varepsilon^+-c_0^+\right)+\left(c_0^--c_\varepsilon^-\right).$$

Choosing the test function $\varphi_2=\tilde{\Phi}_\varepsilon-\tilde{\Phi}_0^\varepsilon$, let us now estimate the following integral:

$$\mathscr{T}=\int_{\Omega^\varepsilon}\left(\Delta_y\tilde{\Phi}_0\right)^\varepsilon\varphi_2dx.$$

Using the simple relation $\nabla_y=\varepsilon\left(\nabla-\nabla_x\right)$ and the decomposition

$$\left(\Delta_y\tilde{\Phi}_0\right)^\varepsilon=(1-m^\varepsilon)\left(\Delta_y\tilde{\Phi}_0\right)^\varepsilon+\varepsilon m^\varepsilon\nabla\cdot\left(\nabla_y\left(\tilde{\Phi}_0\right)^\varepsilon\right)-\varepsilon m^\varepsilon\left(\nabla_x\cdot\left(\nabla_y\tilde{\Phi}_0\right)\right)^\varepsilon,$$

and we obtain, after integrating by parts of the term $\nabla\cdot\left(\nabla_y\left(\tilde{\Phi}_0\right)^\varepsilon\right)$, that

$$\begin{aligned}\int_{\Omega^\varepsilon}\left(\Delta_y\tilde{\Phi}_0\right)^\varepsilon\varphi_2dx=&\int_{\Omega^\varepsilon}\Big[(1-m^\varepsilon)\left(\Delta_y\tilde{\Phi}_0\right)^\varepsilon\\&-\varepsilon m^\varepsilon\left(\nabla_x\cdot\left(\nabla_y\tilde{\Phi}_0\right)\right)^\varepsilon-\varepsilon\nabla m^\varepsilon\cdot\nabla_y\left(\tilde{\Phi}_0\right)^\varepsilon\Big]\varphi_2dx\\&+\varepsilon\int_{\Omega^\varepsilon}(1-m^\varepsilon)\nabla_y\left(\tilde{\Phi}_0\right)^\varepsilon\cdot\nabla\varphi_2dx-\varepsilon\int_{\Omega^\varepsilon}\nabla_y\left(\tilde{\Phi}_0\right)^\varepsilon\cdot\nabla\varphi_2dx\\&:=\mathscr{F}_1+\mathscr{F}_2+\mathscr{F}_3.\end{aligned}\tag{5.4.58}$$

The first and second integrals on the right-hand side of (5.4.58) can be estimated by

$$\begin{aligned}|\mathscr{F}_1|+|\mathscr{F}_2|\le&\,C\left\|1-m^\varepsilon\right\|_{L^2(\Omega^\varepsilon)}\left\|\Delta_y\tilde{\Phi}_0\right\|_{L^\infty(\Omega^\varepsilon;C(Y_l))}\left\|\varphi_2\right\|_{L^2(\Omega^\varepsilon)}\\&+C\varepsilon\left\|\nabla_x\cdot\left(\nabla_y\tilde{\Phi}_0\right)\right\|_{L^2(\Omega^\varepsilon;C(Y_l))}\left\|\varphi_2\right\|_{L^2(\Omega^\varepsilon)}\\&+C\varepsilon\left\|\nabla m^\varepsilon\right\|_{L^2(\Omega^\varepsilon)}\left\|\nabla_y\tilde{\Phi}_0\right\|_{L^\infty(\Omega^\varepsilon;C(Y_l))}\left\|\varphi_2\right\|_{L^2(\Omega^\varepsilon)}\\&+C\varepsilon\left\|1-m^\varepsilon\right\|_{L^2(\Omega^\varepsilon)}\left\|\nabla_y\tilde{\Phi}_0\right\|_{L^\infty(\Omega^\varepsilon;C(Y_l))}\left\|\nabla\varphi_2\right\|_{L^2(\Omega^\varepsilon)},\end{aligned}$$

where we assume here that $\tilde{\Phi}_0\in L^\infty\left(\Omega^\varepsilon;W^{2+s,2}\left(Y_l\right)\right)\cap H^1\left(\Omega^\varepsilon;W^{1+s,2}\left(Y_l\right)\right)$ and make use of the compact embeddings $W^{2+s,2}\left(Y_l\right)\subset C^2\left(Y_l\right)$, $W^{1+s,2}\left(Y_l\right)\subset C^1\left(Y_l\right)$ for $s>d/2$. Applying the inequalities (5.3.12), we thus have

$$|\mathscr{F}_1|+|\mathscr{F}_2|\le C\left(\varepsilon+\varepsilon^{\frac{1}{2}}\right)\left\|\varphi_2\right\|_{L^2(\Omega^\varepsilon)}+C\varepsilon^{\frac{3}{2}}\left\|\nabla\varphi_2\right\|_{L^2(\Omega^\varepsilon)}.\tag{5.4.59}$$

It now remains to estimate the following integral:

$$\int_{\Omega^\varepsilon}\varepsilon^2\nabla\tilde{\Phi}_\varepsilon\cdot\nabla\varphi_2dx=\int_{\Omega^\varepsilon}\varepsilon\nabla\tilde{\Phi}_\varepsilon\cdot\varepsilon\nabla\left(\tilde{\Phi}_\varepsilon-\tilde{\Phi}_0^\varepsilon\right)dx.$$

Its right-hand side can be estimated by

$$\int_{\Omega^\varepsilon}\varepsilon\nabla\tilde{\Phi}_\varepsilon\cdot\varepsilon\nabla\left(\tilde{\Phi}_\varepsilon-\tilde{\Phi}_0^\varepsilon\right)dx\le C\varepsilon\left\|\nabla\left(\tilde{\Phi}_\varepsilon-\tilde{\Phi}_0^\varepsilon\right)\right\|_{[L^2(\Omega^\varepsilon)]^d},\tag{5.4.60}$$

where we use the fact that $\varepsilon\left\|\nabla\tilde{\Phi}_\varepsilon\right\|_{L^2(\Omega^\varepsilon)}\le C$ in Theorem 5.3.13.
Based on the corrector estimates for the concentration fields $c_\varepsilon^\pm$, we see that

$$\int_{\Omega^\varepsilon}\left[\left(c_\varepsilon^+-c_0^+\right)+\left(c_0^--c_\varepsilon^-\right)\right]\varphi_2dx\le C\left\|c_\varepsilon^\pm-c_0^\pm\right\|_{L^2(\Omega^\varepsilon)}\left\|\tilde{\Phi}_\varepsilon-\tilde{\Phi}_0^\varepsilon\right\|_{L^2(\Omega^\varepsilon)}.\tag{5.4.61}$$

Setting

$$
\begin{aligned}
w_1(t) &= \left\|\tilde{\Phi}_\varepsilon(t) - \tilde{\Phi}_0^\varepsilon(t)\right\|^2_{L^2(\Omega^\varepsilon)} + \left\|c_\varepsilon^\pm(t) - c_0^\pm(t)\right\|^2_{L^2(\Omega^\varepsilon)}, \\
w_2(t) &= \left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0^\varepsilon\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d} + \left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)(t)\right\|^2_{[L^2(\Omega^\varepsilon)]^d}, \\
w_0 &= \left\|c_\varepsilon^{\pm,0} - c_0^{\pm,0}\right\|^2_{L^2(\Omega^\varepsilon)},
\end{aligned}
$$

the combination of the estimates (5.4.59)-(5.4.61) with the respective estimates for the concentration fields (which are similar to the Neumann case) and the application of suitable Hölder's inequalities give

$$
w_1(t) + \int_0^t w_2(s)\,ds \le C\left(\varepsilon + (1+\varepsilon)\,w_0 + \int_0^t w_1(s)\,ds\right).
$$

Using Gronwall's inequality yields

$$
w_1(t) + \int_0^t w_2(s)\,ds \le C\left(\varepsilon + (1+\varepsilon)\,w_0\right).
$$

As a consequence, we obtain

$$
\begin{aligned}
&\left\|\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0^\varepsilon\right\|_{L^2((0,T)\times\Omega^\varepsilon)} + \left\|\nabla\left(\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0^\varepsilon\right)\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d} + \left\|c_\varepsilon^\pm - c_0^{\pm,\varepsilon}\right\|_{L^2((0,T)\times\Omega^\varepsilon)} \\
&+ \left\|\nabla\left(c_\varepsilon^\pm - c_1^{\pm,\varepsilon}\right)\right\|_{[L^2((0,T)\times\Omega^\varepsilon)]^d} \le C\max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\} \text{ for } \mu \in \mathbb{R}_+,
\end{aligned}
$$

where we have used (5.4.33).
Finally, we apply Lemma 5.3.18 to get

$$
\begin{aligned}
\left\|\tilde{\Phi}_\varepsilon - \overline{\tilde{\Phi}}_0^\varepsilon\right\|_{L^2((0,T)\times\Omega^\varepsilon)} &\le \left\|\tilde{\Phi}_\varepsilon - \tilde{\Phi}_0^\varepsilon\right\|_{L^2((0,T)\times\Omega^\varepsilon)} + \left\|\tilde{\Phi}_0^\varepsilon - \overline{\tilde{\Phi}}_0^\varepsilon\right\|_{L^2((0,T)\times\Omega^\varepsilon)} \\
&\le C\max\left\{\varepsilon^{\frac{1}{2}}, \varepsilon^{\frac{\mu}{2}}\right\}.
\end{aligned}
$$

This completes the proof of Theorem 5.4.3.

5.5 Concluding remarks

In [99], the two-scale convergence method has discovered possible macroscopic structures of a non-stationary SNPP model coupled with various scaling factors and different boundary conditions. In this chapter, we have justified such homogenization limits by deriving several corrector estimates (cf. Theorem 5.4.2 and Theorem 5.4.3). The techniques we have presented here are mainly based on the construction of suitable macroscopic reconstructions and on a number of energy-like estimates. The employed methodology is applicable to more complex scenarios, where coupled systems of partial differential equations posed in perforated media are involved.

CHAPTER 6

Concluding remarks. Outlook

This is the moment to review briefly what we have done in this thesis and point out to what remains to be done. This chapter has two parts. The first part is devoted to summarizing the main results of this thesis, while the second part provides some ideas to be explored in the near future.

6.1 Summary

The main results of this work are reported in Chapter 2, Chapter 3, Chapter 4 and Chapter 5 where our investigations concentrate on derivation of convergence rates for the homogenization limit applied to certain systems of partial differential equations with coupled fluxes.

In Chapter 2, Chapter 3 and Chapter 4, we focused on Smoluchowski-Soret-Dufour models posed in a perforated domain. This type of model describes the interplay between heat and diffusion in transporting and interacting hot colloidal particles. Recent studies by [74, 75] have derived the structure of the macroscopic model as well as the weak solvability of these systems. Also, [75] has validated the upscaled equations for realistic soils.

As first step, we studied in Chapter 2 and in Chapter 3 as a simplified model of Smoluchowski-Soret-Dufour-type, a stationary semi-linear reaction-diffusion system. We ensured the L^∞-bounds for the active concentrations and then proved the existence and uniqueness of positive and bounded weak solutions to the microscopic system. In the proofs, we applied an energy minimization method as in [22] and further extended in [55]. The contributions in these two chapters rely on the explicit use of the high-order two-scale asymptotic expansions. To do so, we collected the high-order auxiliary and cell problems, from which the macroscopic system as well as the corrector estimates can be ultimately derived. It turns out that there exist cases where the cell problems are semi-linear elliptic problems due to the structure of the production term. An iterations-based technique was used to treat this nonlinear scenario. Essentially, our proofs in this part are based on the accumulation of the energy estimates for each species.

In Chapter 4, we tackled the original Smoluchowski-Soret-Dufour model expressed as a coupled thermo-diffusion system. This system consists of a set of nonlinear reaction-diffusion equations for hot colloidal concentrations coupled with a family of linear ordinary differential equations for the immobile species. Due to the coupled-flux structure of the system, it is difficult to apply the formal asymptotic expansion to gain the corrector estimates. Instead, we employed the concept of macroscopic reconstruction (of [40]) which allowed us to construct a bridge between the microscopic and macroscopic systems. Energy estimates for the

reconstructed system were used to derive the structure of the correctors.
Most of our results yield that the difference in L^2-norm between the microscopic and macroscopic solutions is of the order $\mathcal{O}\left(\varepsilon^{\frac{1}{2}}\right)$, agreeing with the classical corrector estimates in e.g. the monograph [31]. This is due to the influence of the elliptic part of the oscillating systems. For reaction-drift-convection problems or for some general problems with coupled fluxes, the situation is more complicated (see Chapter 5) and derivations for the standard estimates appear.
In Chapter 5, we turn our attention to a non-stationary Stokes-Nernst-Planck-Poisson model with various scaling choices. The challenging part in deriving the correctors for this model lies in handling the Stokes equation. In fact, the energy-type estimates for correctors of the Stokes equation could not be obtained as in the previous chapters. Fortunately, the *a priori* estimates (derived in [99]) enable us to choose a suitable structure of the correctors, partly inspired from the so-called boundary layer asymptotics. When doing so, the corrector estimates we gained highlighted a corrector of the pressure of order $\mathcal{O}\left(\varepsilon^{\frac{1}{6}}\right)$. Note also that to obtain such order of convergence we needed the internal micro-surfaces to be C^2 and the exterior boundary to be C^4 (compared to the Lipschitz boundary regularity as requested in Chapter 4).

6.2 Outlook

Once corrector estimates are available for systems of partial differential equations, with coupled fluxes, three potential research directions open:

1. For the systems (2.1.1), (4.2.2)-(4.2.12) and (5.1.1)-(5.1.8), we can now design convergent MsFEM schemes with explicit convergence rates;

2. We can now start handling multiscale inverse problems where ε plays a double role – a regularization parameter in an inverse question as well as a small geometry parameter characteristic to a vanishing microstructure length scale;

3. We were able to justify the homogenization asymptotics only for the case of two interplaying separated scales. It would be interesting to handle situations where scales are not separated (or are weakly separated like in the case of the very weak homogenization asymptotics [48]).

It is worth mentioning that inverse problems are omnipresent in both physics (e.g. [115]) and biology (e.g. [113]). As a starting point, one can think of the inverse heat transfer problem with multiple space scales. This problem would fit the very first perspectives including the heat source identification problem e.g. [67] and the backward problem e.g. [114]. In this direction, it would be interesting to design also a certain regularization coupled with the homogenization method, for particular microscopic problems. Working on problems with coupled fluxes can perhaps be made, but one flux must be identified. Observe, on the other hand, that the two-scale convergence can be helpful in establishing a multiscale theory of filter regularization operators following up [36].

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APPENDIX A

Miscellaneous results

We collect in this appendix the definition and main properties of the two-scale convergence as well as related compactness results. We refer the reader to the original works by [5] and [89].
The notation used here is introduced in Chapter 2.

Definition A.0.1. Two-scale convergence
Let $(u^\varepsilon)_{\varepsilon>0}$ be a sequence of functions in $L^2\left(0,T;L^2(\Omega)\right)$, then it two-scale converges to a unique function $u^0 \in L^2((0,T)\times\Omega\times Y)$ if for any $\varphi \in C_0^\infty\left((0,T)\times\Omega; C_\#^\infty(Y)\right)$ we have

$$\lim_{\varepsilon\to 0}\int_0^T\int_\Omega u^\varepsilon(t,x)\,\varphi\left(t,x,\frac{x}{\varepsilon}\right)dxdt = \frac{1}{|Y|}\int_0^T\int_\Omega\int_Y u^0(t,x,y)\,\varphi(t,x,y)\,dydxdt.$$

We denoted this convergence by $u^\varepsilon \overset{2}{\rightharpoonup} u^0$ as $\varepsilon\to 0$. If in addition $(u^\varepsilon)_{\varepsilon>0}$ satisfies

$$\lim_{\varepsilon\to 0}\|u^\varepsilon\|_{L^2((0,T)\times\Omega)} = \left\|u^0\right\|_{L^2((0,T)\times\Omega\times Y)},$$

then the sequence is said to be strongly two-scale convergent to u^0 in $L^2((0,T)\times\Omega\times Y)$ and we write $u^\varepsilon \overset{2}{\to} u^0$.

Theorem A.0.2. Two-scale compactness

- Let $(u^\varepsilon)_{\varepsilon>0}$ be a bounded sequence in $L^2((0,T)\times\Omega)$. Then there exists a function $u^0 \in L^2((0,T)\times\Omega\times Y)$ such that, up to a subsequence, u^ε two-scale converges to u^0.
- Let $(u^\varepsilon)_{\varepsilon>0}$ be a bounded sequence in $L^2\left(0,T;H^1(\Omega)\right)$, then up to a subsequence, we have the two-scale convergence $\nabla u^\varepsilon \overset{2}{\rightharpoonup} \nabla_x u^0 + \nabla_y u^1$, where $u^0 \in L^2\left(0,T;H^1(\Omega)\right)$ and $u^1 \in L^2\left((0,T)\times\Omega; H^1_\#(Y)/\mathbb{R}\right)$.

Next, we recall the concepts of two-scale convergence and compactness for ε-periodic hypersurfaces. They were originally introduced in [87, 6] and have been used in many applications; see, for instance, [45, 74].

Definition A.0.3. Two-scale convergence on hypersurfaces
Let $(u^\varepsilon)_{\varepsilon>0}$ be a sequence of functions in $L^2(0,T;L^2(\Gamma^\varepsilon))\left(\equiv L^2((0,T)\times\Gamma^\varepsilon)\right)$. We say u^ε two-scale converges to a limit u^0 in $L^2((0,T)\times\Omega\times\Gamma)$ if for any $\varphi \in C_0^\infty((0,T)\times\Omega; C_\#^\infty(\Gamma))$ we have

$$\lim_{\varepsilon\to 0}\int_0^T\int_{\Gamma^\varepsilon}\varepsilon u^\varepsilon(t,x)\,\varphi\left(t,x,\frac{x}{\varepsilon}\right)dxdt = \frac{1}{|Y|}\int_0^T\int_\Omega\int_\Gamma u^0(t,x,y)\,\varphi(t,x,y)\,d\sigma(y)dxdt.$$

Theorem A.0.4. Two-scale compactness on surfaces
For each bounded sequence (u^ε) in $L^2\left(0,T;L^2(\Gamma^\varepsilon)\right)$, one can extract a subsequence which two-scale converges to $u^0 \in L^2((0,T)\times\Omega\times\Gamma)$. Furthermore, if (u^ε) is bounded in $L^\infty(0,T;L^\infty(\Gamma^\varepsilon))$, it then two-scale converges to a limit function $u^0 \in L^\infty((0,T)\times\Omega\times\Gamma)$.

The relation between the (weak) two-scale convergence and the ordinary weak convergence is collected in the following result (cf. e.g. [78, Theorems 9, 10, 17]).

Proposition A.0.5. *Let $(u^\varepsilon)_{\varepsilon>0}$ be a sequence in $L^2((0,T)\times\Omega)$ and given a function $u^0 \in L^2((0,T)\times\Omega\times Y)$. Then, one has*

1. *If $u^\varepsilon \xrightarrow{2} u^0$ in $L^2((0,T)\times\Omega\times Y)$, then it implies $u^\varepsilon \overset{2}{\rightharpoonup} u^0$ in $L^2((0,T)\times\Omega\times Y)$;*

   If $u^\varepsilon \overset{2}{\rightharpoonup} u^0$ in $L^2((0,T)\times\Omega\times Y)$, then it holds that
   $$u^\varepsilon \rightharpoonup \frac{1}{|Y|}\int_Y u^0(\cdot,y)\,dy \quad \text{in } L^2((0,T)\times\Omega).$$
   In particular, sequences that weakly two-scale converge in $L^2((0,T)\times\Omega\times Y)$ are bounded in $L^2((0,T)\times\Omega)$.

2. *If u^0 is independent of the third argument y, i.e. $u^0 \in L^2(\Omega)$, then the strong convergence in $L^2((0,T)\times\Omega)$ is equivalent to the strongly two-scale convergence in $L^2((0,T)\times\Omega\times Y)$.*

Theorem A.0.6. *(cf. [5, Theorem 1.8]) If $(u^\varepsilon)_{\varepsilon>0}$ and $(v^\varepsilon)_{\varepsilon>0}$ are sequences in $L^2((0,T)\times\Omega)$ such that*
$$u^\varepsilon \overset{2}{\rightharpoonup} u^0 \text{ in } L^2((0,T)\times\Omega\times Y),$$
$$v^\varepsilon \xrightarrow{2} v^0 \text{ in } L^2((0,T)\times\Omega\times Y),$$
then for every $\varphi \in C_c^\infty(\Omega)$ one has
$$\lim_{\varepsilon\to 0}\int_0^T\int_\Omega u^\varepsilon(x)v^\varepsilon(x)\varphi(x)\,dxdt = \frac{1}{|Y|}\int_0^T\int_\Omega\left(\int_Y u^0(x,y)v^0(x,y)\,dy\right)\varphi(x)\,dxdt.$$

Lemma A.0.7. *(A Young-type inequality) Let $\delta > 0$ and $a,b \geq 0$ be arbitrarily real numbers and take $q,q' > 1$ real constants that are the Hölder conjugates of each other. Then the following inequality holds*
$$ab \leq \frac{1}{q}\delta^q a^q + \frac{1}{q'}\delta^{-q'}b^{q'}. \tag{A.0.1}$$

Lemma A.0.8. *(Trace inequality for ε-dependent hypersurfaces Γ^ε) Let Γ^ε be as defined in Subsection 4.2.1. For $u^\varepsilon \in H^1(\Omega^\varepsilon)$, there exists a constant $C > 0$ (independent of ε) such that*
$$\varepsilon\,\|u^\varepsilon\|^2_{L^2(\Gamma^\varepsilon)} \leq C\left(\|u^\varepsilon\|^2_{L^2(\Omega^\varepsilon)} + \varepsilon^2\,\|\nabla u^\varepsilon\|^2_{[L^2(\Omega^\varepsilon)]^d}\right). \tag{A.0.2}$$

The proof of (A.0.2) can be found in [65, Lemma 3]. In the case of the homogeneous (bounded) domain Ω with smooth boundary, one has the usual trace inequality (cf. [64]):
$$\|u\|^2_{L^2(\Gamma)} \leq C\left(\|u\|^2_{L^2(\Omega)} + \|\nabla u\|^2_{L^2(\Omega)}\right) \quad \text{for all } u \in H^1(\Omega).$$

Lemma A.0.9. *(Poincaré's inequality) For $u^\varepsilon \in H^1(\Omega^\varepsilon)$, there exists a constant $C > 0$ independent of ε such that*
$$\|u^\varepsilon\|_{L^2(\Omega^\varepsilon)} \leq C\,\|\nabla u^\varepsilon\|_{[L^2(\Omega^\varepsilon)]^d}.$$

The proof is straightforward in [31, Lemma 2.1] and based on the Poincaré inequality for the homogeneous case, the result is similar up to the homogeneous domain Ω.

Lemma A.0.10. *(Hölder's inequality) Let $q, q\prime > 1$ be real constants that are Hölder conjugates of each other. Then, for $u^\varepsilon \in L^q(\Omega^\varepsilon)$ and $v^\varepsilon \in L^{q\prime}(\Omega^\varepsilon)$, the following inequality holds*

$$\|u^\varepsilon v^\varepsilon\|_{L^1(\Omega^\varepsilon)} \leq \|u^\varepsilon\|_{L^q(\Omega^\varepsilon)} \|v^\varepsilon\|_{L^{q\prime}(\Omega^\varepsilon)}.$$

Furthermore, this inequality also holds in the hypersurfaces Γ^ε.

The proof of the Hölder inequality is trivial by virtue of the Young inequality as presented in Lemma A.0.7.

Lemma A.0.11. *(Minkowski's inequality) Let $1 \leq p \leq \infty$ and let $u^\varepsilon, v^\varepsilon \in L^p(\Omega^\varepsilon)$. Then $u^\varepsilon + v^\varepsilon \in L^p(\Omega^\varepsilon)$ and the following inequality holds*

$$\|u^\varepsilon + v^\varepsilon\|_{L^p(\Omega^\varepsilon)} \leq \|u^\varepsilon\|_{L^p(\Omega^\varepsilon)} + \|v^\varepsilon\|_{L^p(\Omega^\varepsilon)}.$$

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