Scaling effects and homogenization of reaction-diffusion problems with nonlinear drift

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Faculty of Health, Science and Technology

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Abstract

We study the periodic homogenization of reaction-diffusion problems with nonlinear drift describing the transport of interacting particles in composite materials. The microscopic model is derived as the hydrodynamic limit of a totally asymmetric simple exclusion process for a population of interacting particles crossing a domain with obstacles. We are particularly interested in exploring how the scalings of the drift affect the structure of the upscaled model.

We first look into a situation when the interacting particles cross a thin layer that has a periodic microstructure. To understand the effective transmission condition, we perform homogenization together with the dimension reduction of the aforementioned reaction-diffusion-drift problem with variable scalings.

One particular physically interesting scaling that we look at separately is when the drift is very large compared to both the diffusion and reaction rate. In this case, we consider the overall process taking place in an unbounded porous media. Since we have the presence of a large nonlinear drift in the microscopic problem, we first upscale the model using the formal asymptotic expansions with drift. Then, with the help of two-scale convergence with drift, we rigorously derive the homogenization limit for a similar microscopic problem with a nonlinear Robin-type boundary condition. Additionally, we show the strong convergence of the corrector function.

In the large drift case, the resulting upscaled equation is a nonlinear reaction-dispersion equation that is strongly coupled with a system of nonlinear elliptic cell problems. We study the solvability of a similar strongly coupled two-scale system with nonlinear dispersion by constructing an iterative scheme. Finally, we illustrate the behavior of the solution using the iterative scheme.

Keywords: Homogenization; asymptotic expansion with drift; two-scale convergence with drift; effective transmission condition; dimension reduction; two-scale system; nonlinear dispersion.

MSC (2020): 35B27; 35Q92; 35A01; 35M30; 47J25.

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Karlstad, March 2024 Vishnu Raveendran

Contents

Overview of the thesis

1 Introduction

1.1 Background and main questions

In this thesis, we perform the periodic homogenization asymptotics for a particular class of reaction-diffusion-drift problems. In this way, we aim to get a sound theoretical understanding of how the Mean-Field representation (population) of a family of interacting particles can evolve driven by a nonlinear drift into composite materials.

We assume the composite material has a periodic microstructure in which the characteristic length scale of the microstructure is very small compared to the size of the macroscopic domain. For the macroscopic geometry of the material, we consider multiple possibilities such as thin layers with periodic microstructure in one direction and unbounded perforated domain.

To introduce the mathematical model, we take the composite materials as the domain for our problem. In this domain, we consider the microscopic equation that has a structure of reaction-diffusion with a nonlinear drift. The microscopic model describes the transport of interacting particles in the composite material driven by a drift. The derivation of the aforementioned model is based on the hydrodynamic limit of asymmetric simple exclusion process defined in a 2-dimensional lattice (see [14] and Section 1.2).

One way to investigate the problem is via direct numerical approximation of the solution to the microscopic equations. However, if the microscopic structure of the domain is very small compared to the macroscopic domain, the computational cost will be extremely high. Even for high-performing computers, it may take a long time and high energy to approximate the solution. To overcome this difficulty, we perform periodic homogenization for the microscopic problems and propose upscaled models that are computationally cheap and contain rich information from the microscopic data.

In this thesis, we mainly want to address the following questions:

- Q1: What is the macroscopic model and effective transmission condition for reaction-diffusion problem with nonlinear drift defined in a thin layer with periodic microstructure?
- Q2: How does the large scaling in the nonlinear drift affect the upscaled model in an unbounded porous media?
- Q3: Construct a two-scale iterative scheme to approximate numerically the solution of the upscaled model derived from the large nonlinear drift problem (strongly coupled two-scale system with nonlinear dispersion).

Homogenization of reaction-diffusion-drift problems has potential application in a number of directions like reactive transport in porous media [20], filtration combustion [21], material modeling for controlled heat transfer [28]. The main tools that we used to find homogenization limits are variations of the formal asymptotic expansion [19, 13] and variations of the two-scale convergence [32, 1, 24]. We choose the specific variation depending on the macroscopic geometry and the microscopic scaling.

To perform the homogenization in the thin periodic domains, we use concept of two-scale convergence for the thin layers introduced in [26] and later developed in [31, 9, 16, 17]. Some other thin layer homogenization methods are discussed in [10, 25, 8]. To upscale the model equation that involves a large nonlinear drift, we used two different averaging methods. Firstly, we relied on a formal homogenization technique called two-scale asymptotic expansion with drift [2], and then we made use of a rigorous homogenization tool – the two-scale convergence with drift. This new type of convergence was introduced in [27] and later developed in [6, 4, 5].

1.2 Motivation for the nonlinear drift structure

The major part of the thesis is to analyze the upscaling of the reaction-diffusion equation with nonlinear drift in the form

$$\partial_t u + \operatorname{div}(-D\nabla u + BP(u)) = f, \tag{1}$$

where $P(u) = u(1-u)$, the unknown u represents the concentration profile of a population of interacting particles, D is the diffusion coefficient, B denotes the drift coefficient and f represents the reaction rate. We study the problem (1) with multiple scalings and with different macroscopic geometry. The structure of the model equation (1) is derived in [14] via the Mean Field approximation and a rigorous derivation was provided in dimension one in the paper (for more recent techniques and generalizations we refer [23, 15]). Now, we give a small outline of the derivation of the structure of (1).

Let $\mathbb{Z}^2$ be a two-dimensional lattice and $(z_1, z_2) \in \mathbb{Z}\times\mathbb{Z}$ represents the points in the lattice. Consider interacting particles are moving on these lattice points. We say a site (z_1, z_2) is occupied if there is a particle present; otherwise, we say the site is unoccupied. We assume that one site can be occupied by at most one particle at a time. If a particle is present at time t, we indicate the occupation number at site (z_1, z_2) as 1; if not, we state that the occupation number is 0. Define the value $u(t, z_1, z_2)$ as the expectation of the occupation number on (z_1, z_2) at time t. Now, from this discrete model defined on the lattice, we derive a continuum equation for the expectation of occupation number based on a random walk rule of the particles. The random walk rule is defined as the particle from (z_1, z_2) moves to (z_1+1, z_2), (z_1-1, z_2), (z_1, z_2+1) or (z_1, z_2-1) with the following rates

$$u(t, z_1, z_2)(1 - u(t, z_1+1, z_2))p((1,0)),$$

$$
\begin{aligned}
u(t, z_1, z_2)(1 - u(t, z_1 - 1, z_2)p((-1, 0)),\\
u(t, z_1, z_2)(1 - u(t, z_1, z_2 + 1))p((0, 1)),\\
u(t, z_1, z_2)(1 - u(t, z_1, z_2 - 1))p((0, -1))
\end{aligned}
$$

respectively. Where, $p(\cdot)$ is the probability distribution with

$$
\begin{aligned}
p((1, 0)) &= \frac{1}{2}(1 - h)(1 + \delta),\\
p((0, 1)) &= \frac{1}{2}h,\\
p((-1, 0)) &= \frac{1}{2}(1 - h)(1 - \delta),\\
p((0, -1)) &= \frac{1}{2}h
\end{aligned}
$$

for some displacement probability $h \in [0, 1]$ and drift $\delta \in [0, 1]$. Now, by using the balance equation

$$
\begin{aligned}
u(t + \Delta t, z_1, z_2) - u(t, z_1, z) =& p((-1, 0))u(t, z_1 - 1, z_2)(1 - u(t, z_1, z_2))\\
&+ p((0, -1))u(t, z_1, z_2 - 1)(1 - u(t, z_1, z_2))\\
&+ p((1, 0))u(t, z_1 + 1, z_2)(1 - u(t, z_1, z_2))\\
&+ p((0, 1))u(t, z_1, z_2 + 1)(1 - u(t, z_1, z_2))\\
&- p((-1, 0))u(t, z_1, z_2)(1 - u(t, z_1 - 1, z_2))\\
&- p((0, -1))u(t, z_1, z_2)(1 - u(t, z_1, z_2 - 1))\\
&- p((1, 0))u(t, z_1, z_2)(1 - u(t, z_1 + 1, z_2))\\
&- p((0, 1))u(t, z_1, z_2)(1 - u(t, z_1, z_2 + 1)),
\end{aligned}
$$

and choosing the variables

$$
x_1 = \varepsilon z_1 \qquad x_2 = \varepsilon z_2 \qquad \Delta t = \varepsilon^2 \qquad \delta = \varepsilon\bar{\delta},
$$

by rearranging balance equation and passing $\varepsilon \to 0$, we get the Mean Field limit equation in the form (1), where D depends on h while B depends on $\bar{\delta}$ and h. For the details of the calculation, we direct the readers to [14].

1.3 Synopsis

The content of the thesis consists of four papers. Next, we briefly summarize the chapters.

- **Paper I**: [*Scaling effects on the periodic homogenization of a reaction-diffusion-convection problem posed in homogeneous domains connected by a thin composite layer*] We consider reaction-diffusion equation with nonlinear drift defined in two homogenous domain connected by a thin layer. The thin layer has periodic microstructure in one direction with microscopic length scale ε. For the nonlinear drift, we have a bounded polynomial type nonlinearity. Our main aim is to study how different scalings in diffusion, drift or reaction rate affect the macroscopic model as $\varepsilon \to 0$. The well-posedness of the microscopic problem is studied by the Galerkin approximation method. We prove the needed energy estimates and then, using the concept of thin layer two-scale convergence, we derive different macroscopic models and effective transmission conditions along the thin layer depending on the scaling parameter.

- **Paper II**: [*Upscaling of a reaction-diffusion-convection problem with exploding non-linear drift*] One physically relevant and interesting scaling we were not able to handle in Paper I is when the nonlinear drift is scaled by $\frac{1}{\varepsilon}$. In other words, the drift becomes large as $\varepsilon \to 0$. Such types of scaling are of potential interest when designing composite materials expected to withstand high-velocity particle impacts. Within this chapter, we consider a reaction-diffusion equation with polynomial drift in an unbounded porous media. Classical homogenization techniques like asymptotic expansion, two-scale convergence, and periodic unfolding are not enough to handle this situation. We use a modified asymptotic expansion with drift where the asymptotic expansion is performed in a fast-moving coordinate to overcome the exploding drift effect. Now, passing $\varepsilon \to 0$, we obtain the upscaled equation as a reaction-dispersion equation in the unbounded domain that is strongly coupled with elliptic cell problems in the bounded domain. We also study the existence result of the system by the Schauder fixed point argument.

- **Paper III**: [*Homogenization of a reaction-diffusion problem with large nonlinear drift and Robin boundary data*] In this chapter, we perform rigorously the homogenization of a reaction-diffusion equation with large second-order polynomial drift in an unbounded porous media. On the surface of pores, we consider a nonlinear Robin-type boundary condition. To prove the existence of the microscopic problem defined in the unbounded domain, we first study the well-posedness of a similar problem in the bounded domain and show that a particular extension of solutions of the bounded domain problem converges to the solution of our unbounded problem as the radius of domain goes to infinity. To perform the homogenization, we choose the technique of two-scale convergence with drift where the classical two-scale convergence is modified in such a way that the test function is defined in a fast-moving coordinate. Since our microscopic problem exhibits a nonlinear drift, the method of two-scale convergence with drift is not enough to pass $\varepsilon \to 0$. So, firstly, we prove the strong convergence of the solution in a fast-moving coordinate. Then we derive the homogenized equation which is a reaction-dispersion equation in the unbounded domain coupled with elliptic cell problems defined in a bounded domain. Finally, we show the strong convergence of the corrector function.

- **Paper IV**: [*Strongly Coupled Two-scale System with Nonlinear Dispersion: Weak Solvability and Numerical Simulation*] In Chapter 2 and Chapter 3, we see that the upscaled equation is a reaction-dispersion equation that is strongly coupled with a system of elliptic cell problems. The dispersion coefficient arising into the structure of the reaction-dispersion equation depends on the weak derivative of the solution of the elliptic cell problems, and the drift term in the elliptic cell problem depends on the solution of the reaction-dispersion equation. To investigate the solvability of such a problem, we propose a two-scale iterative scheme. By, showing the uniform ellipticity property for the dispersion tensor and using an auxiliary problem, we show that the solution to the iterative scheme converges to the solution of the two-scale coupled system. Finally, by using the iterative scheme combined with the finite element method, we illustrate how the dispersion tensor and the solution interact with nonlinear drift.

2 Main results

In this section, we collect the main results from Paper I ([38]), Paper II ([37]), Paper III ([36]), and Paper IV ([39]).

2.1 Paper I

The goal of this paper is to study the scaling effects of homogenization and dimension reduction of a reaction-diffusion equation with nonlinear drift. We study the problem defined in two bulk domains connected by a thin layer that has a periodic microstructure (see Figure 1 and Figure 2). Now, we introduce our microscopic equation:

$$\begin{aligned}
\frac{\partial u_l^\varepsilon}{\partial t} + \operatorname{div}(-D_L \nabla u_l^\varepsilon + B_L P_\delta(u_l^\varepsilon)) &= f_l \quad \text{in } \Omega_{\mathcal{L}}^\varepsilon \times (0,T),\\
\frac{\partial u_r^\varepsilon}{\partial t} + \operatorname{div}(-D_R \nabla u_r^\varepsilon + B_R P_\delta(u_r^\varepsilon)) &= f_r \quad \text{in } \Omega_{\mathcal{R}}^\varepsilon \times (0,T),\\
\varepsilon^\alpha \frac{\partial u_m^\varepsilon}{\partial t} + \operatorname{div}(-\varepsilon^\beta D_M^\varepsilon \nabla u_m^\varepsilon + \varepsilon^\gamma B_M^\varepsilon P_\delta(u_m^\varepsilon)) &= \varepsilon^\alpha f_m^\varepsilon \quad \text{in } \Omega_{\mathcal{M}}^\varepsilon \times (0,T),
\end{aligned}$$

where $P_\delta(\cdot)$ is a bounded polynomial type nonlinear function that is defined in paper I (see detailed description of data parameters and domain in Section 2 of Paper I). The problem mentioned above is endowed with

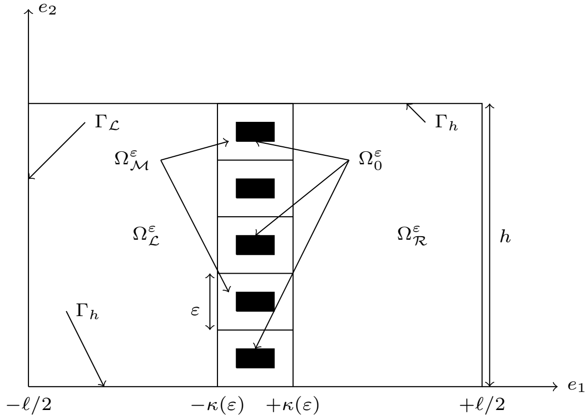

Figure 1: Schematic representation of the microscopic model.

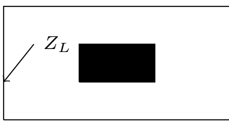

Figure 2: The standard cell Z exhibiting a rectangular obstacle placed in the center.

the following boundary and initial conditions:

$$u_l^\varepsilon = U_L \text{ on } \Gamma_{\mathcal{L}} \times (0,T),$$
$$u_r^\varepsilon = U_R \text{ on } \Gamma_{\mathcal{R}} \times (0,T),$$

$$(-\varepsilon^\beta D_M^\varepsilon \nabla u_m^\varepsilon + \varepsilon^\gamma B_M^\varepsilon P_\delta(u_m^\varepsilon)) \cdot n_m^\varepsilon = \varepsilon^\xi g_0^\varepsilon \text{ on } \Gamma_0^\varepsilon \times (0,T),$$
$$(-D_L \nabla u_l^\varepsilon + B_L P_\delta(u_l^\varepsilon)) \cdot n_l = g_l \text{ on } (\Gamma_h \cap \partial\Omega^\varepsilon_{\mathcal{L}}) \times (0,T),$$
$$(-D_R \nabla u_r^\varepsilon + B_R P_\delta(u_l^\varepsilon)) \cdot n_r = g_r \text{ on } (\Gamma_h \cap \partial\Omega^\varepsilon_{\mathcal{R}}) \times (0,T),$$

$$u_l^\varepsilon(0,x) = h_l^\varepsilon(x) \text{ for all } x \in \overline{\Omega}^\varepsilon_{\mathcal{L}},$$
$$u_r^\varepsilon(0,x) = h_r^\varepsilon(x) \text{ for all } x \in \overline{\Omega}^\varepsilon_{\mathcal{R}},$$
$$u_m^\varepsilon(0,x) = h_m^\varepsilon(x) \text{ for all } x \in \overline{\Omega}^\varepsilon_{\mathcal{M}},$$

and transmission conditions:

$$u_l^\varepsilon = u_M^\varepsilon \text{ on } \mathcal{B}^\varepsilon_{\mathcal{L}},$$
$$u_r^\varepsilon = u_M^\varepsilon \text{ on } \mathcal{B}^\varepsilon_{\mathcal{R}},$$
$$(-\varepsilon^\beta D_M^\varepsilon \nabla u_m^\varepsilon + \varepsilon^\gamma B_M^\varepsilon P_\delta(u_m^\varepsilon)) \cdot n_m^\varepsilon = (-D_L \nabla u_l^\varepsilon + B_L P_\delta(u_l^\varepsilon)) \cdot n_l \text{ on } \mathcal{B}^\varepsilon_{\mathcal{L}},$$
$$(-\varepsilon^\beta D_M^\varepsilon \nabla u_m^\varepsilon + \varepsilon^\gamma B_M^\varepsilon P_\delta(u_m^\varepsilon)) \cdot n_m^\varepsilon = (-D_R \nabla u_r^\varepsilon + B_R P_\delta(u_l^\varepsilon)) \cdot n_r \text{ on } \mathcal{B}^\varepsilon_{\mathcal{R}}.$$

We investigate the upscaled model and effective transmission condition for the microscopic problem with variable scalings along with two different thickness conditions. See Table 1 for the discussed scaling and thickness options.

Table 1: List of discussed scalings.

Scaling options for infinitely thin layer	
Choice S1	Choice S2
$\alpha = -1$	$\alpha = -1$
$\beta = 1$	$\beta \in (0,1)$
$\gamma \geq 1$	$\gamma \geq \beta$
$\xi \geq \frac{1}{2}$	$\xi \geq \min\{\beta - \frac{1}{2}, 0\}$

Scaling options for finitely thin layer	
Choice S3	Choice S4
$\alpha \in (-1, \infty)$	$\alpha \in (-1, \infty)$
$\beta - \alpha = 0$	$\beta - \alpha \in (0, \infty)$
$\gamma - \alpha \geq 0$	$\gamma - \alpha \geq 0$
$\xi - \alpha > 1$	$\xi - \alpha > 1$

For the infinitely thin layer case, we consider $\kappa(\varepsilon) = \varepsilon$ (see Figure 1). In this situation as $\varepsilon \to 0$, we attain the macroscopic domain as shown in Figure 3. For the layer with finite thickness, we consider $\kappa(\varepsilon)$ to be

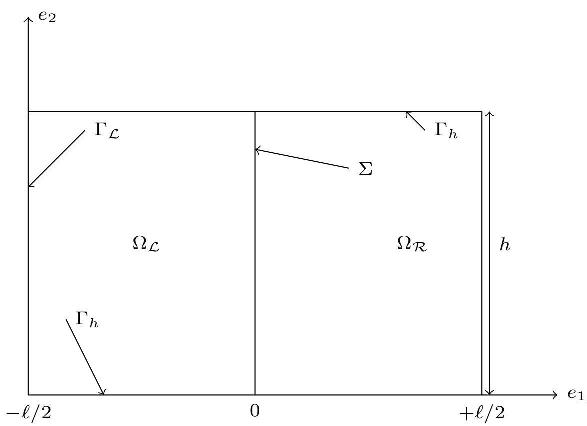

Figure 3: Schematic representation of the macroscopic model for the infinitely thin layer.

a constant independent of ε. In this situation, we get the macroscopic geometry as in Figure 4.

To work with the problem having a homogeneous Dirichlet boundary condition in the vertical boundary of the domain, we use the following transformation: $u_i^\varepsilon := v_i^\varepsilon - u_b$, where $u_b(t,x) := \frac{1}{2}(x_1 - \frac{\ell}{2})U_L - \frac{1}{2}(x_1 + \frac{\ell}{2})U_R$, with $x = (x_1, x_2)$. Under suitable assumptions on the data, by deriving the energy estimates (Theorem 4.1) and using two-scale convergence for thin layer, as $\varepsilon \to 0$, we obtain the upscaled models.

In every scaling option, we get the macroscopic equation in Ω_L and

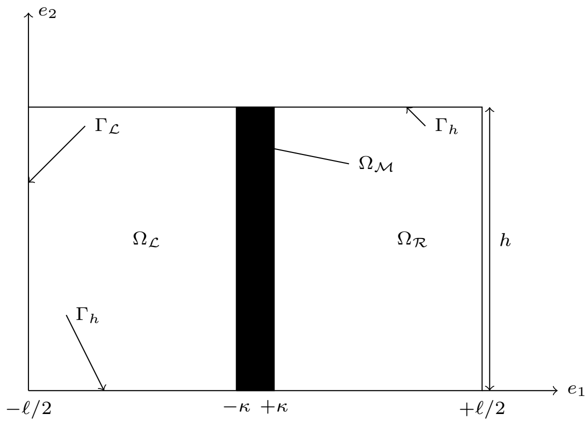

Figure 4: Schematic representation of the macroscopic model for finitely thin layer.

Ω_R as

$$\frac{\partial v_l^0}{\partial t} + \mathrm{div}(-D_L \nabla v_l^0 + B_L P_\delta(v_l^0 - u_b)) = f_{b_l} \quad \text{in } (0,T)\times\Omega_{\mathcal{L}},$$
$$\frac{\partial v_r^0}{\partial t} + \mathrm{div}(-D_R \nabla v_r^0 + B_R P_\delta(v_r^0 - u_b)) = f_{b_r} \quad \text{in } (0,T)\times\Omega_{\mathcal{R}}.$$

For the scaling choice $S1$, we obtain the effective transmission condition (see Theorem 5.3 for details) as

$$\begin{aligned}(-D_L\nabla v_l^0 + B_L P_\delta(v_l^0 - u_b) + D_R\nabla v_r^0 - B_R P_\delta(v_r^0 - u_b))\cdot n_l \\ = \int_{Z_L} D_M \nabla_y v_m^0 \cdot n_l + D_L \nabla_x u_b(t,\bar{x})\cdot n_l \\ - \int_{Z_R} D_M \nabla_y v_m^0 \cdot n_l + D_R \nabla_x u_b(t,\bar{x})\cdot n_l \\ \text{on } (0,T)\times\Sigma,\end{aligned}$$

where v_0^m solves the following cell problem

$$\frac{\partial v_m^0}{\partial t} + \mathrm{div_y}(-D_M\nabla_y v_m^0) = f_{a_0} \quad \text{on } (0,T)\times\Sigma\times Z,$$
$$(-D_M\nabla_y v_m^0)\cdot n = 0 \quad \text{on } (0,T)\times\Sigma\times(\partial Z\backslash(Z_L\cup Z_R))$$
$$v_l^0(t=0) = h_{b_l}^0 \quad \text{on } \Sigma\times\bar{Z}.$$

For the scaling choice $S2$, we have the following effective transmission condition (see Theorem 5.4)

$$(-D_L\nabla v_l^0 + B_L P_\delta(v_l^0 - u_b) + D_R\nabla v_r^0 - B_R P_\delta(v_r^0 - u_b))\cdot n_l$$
$$= -|Z|\frac{\partial v_m^0}{\partial t} + \int_Z f_{a_0} dy + D_L\nabla_x u_b(t,\bar{x})\cdot n_l - D_R\nabla_x u_b(t,\bar{x})\cdot n_l$$
$$\text{on } (0,T)\times\Sigma.$$

For scaling choice $S3$ (see details in Theorem 5.5), we obtain

$$(-D_M^*(\lambda_1\nabla_x v_m^0 - \lambda_2 B_M^* P_\delta(v_m^0 - u_b)))\cdot n_m$$
$$= (-D_L\nabla(v_l^\varepsilon - u_b) + B_L P_\delta(v_l^\varepsilon - u_b))\cdot n_l \text{ on } \mathcal{B}_{\mathcal{L}},$$
$$(-D_M^*(\lambda_1\nabla_x v_m^0 - \lambda_2 B_M^* P_\delta(v_m^0 - u_b)))\cdot n_m$$
$$= (-D_R\nabla(v_r - u_b) + B_R P_\delta(v_r - u_b))\cdot n_r \text{ on } \mathcal{B}_{\mathcal{R}},$$

where $\lambda_1 = 1$, and $\lambda_2 = 1$ if $\gamma - \alpha = 0$ and $\lambda_2 = 0$ if $\gamma - \alpha > 0$,

$$\frac{\partial v_m^0}{\partial t} + \mathrm{div}_x(-D_M^*(\lambda_1\nabla_x v_m^0 - \lambda_2 B_M^* P_\delta(v_m^0 - u_b))) = f_{a_m} \quad \text{in} \quad (0,T)\times\Omega_{\mathcal{M}},$$

$$D_M^* := \frac{1}{|Z|}\int_Z D(y)\left(I + \begin{bmatrix} 0 & 0 \\ \frac{\partial w_1}{\partial y_2} & \frac{\partial w_2}{\partial y_2}\end{bmatrix}\right) dy,$$
$$B_M^* := (D_M)^{-1} B_M$$

$\overline{B}_M$ chosen such a way that $D_M\overline{B}_M = B_M$, and w_i solves the cell problem

$$\begin{aligned} \mathrm{div}_y(D_M\nabla_y w_i) &= \mathrm{div}_y(D_M e_i) && \text{in} \quad Z \\ \nabla_y w_i\cdot n &= 0 && \text{on} \quad \partial Y_0 \\ w_i \text{ is } Z & \textit{ periodic} \end{aligned}$$

for $i \in \{1,2\}$.

2.2 Paper II

In this context, we are interested in deriving the upscaled equation for a reaction-diffusion problem with large polynomial drift in an unbounded perforated domain. The geometry of the perforated domain (denote as Ω_ε) can be seen as the standard cell Z (see Figure 5) scaled by ε and arranged periodically in whole $\mathbb{R}^2$.

In this perforated domain, we consider the following microscopic problem:

$$\frac{\partial u^\varepsilon}{\partial t} + \mathrm{div}(-D^\varepsilon\nabla u^\varepsilon + \frac{1}{\varepsilon}B^\varepsilon P(u^\varepsilon)) = f^\varepsilon \qquad \text{in} \qquad \Omega_\varepsilon\times(0,T),$$

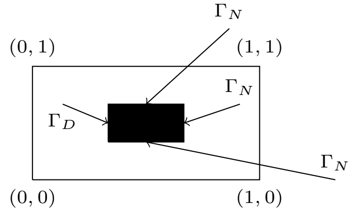

Figure 5: Standard cell Z exhibiting a obstacle Y_0 placed in the center.

$$
\begin{aligned}
(-D^\varepsilon \nabla u^\varepsilon + \frac{1}{\varepsilon} B^\varepsilon P(u^\varepsilon)) \cdot n_\varepsilon = \varepsilon g_N^\varepsilon \qquad & \text{on} \qquad \Gamma_N^\varepsilon \times (0,T),\\
u^\varepsilon = \varepsilon^\gamma g_D^\varepsilon \qquad & \text{on} \qquad \Gamma_D^\varepsilon \times (0,T),\\
u^\varepsilon(0) = g \qquad & \text{in} \qquad \overline{\Omega}_\varepsilon,
\end{aligned}
$$

where $P(\cdot)$ is a polynomial with variable coefficients and $\gamma > 1$. Concerning the boundary conditions along the obstacles, in some parts of the boundary, we assume the Dirichlet boundary condition, and in another part, we have the Neumann boundary condition. The main difficulty for upscaling the problem is the large nonlinear drift. In this situation, the classical techniques of homogenization such as formal asymptotic expansion, two-scale convergence, and periodic unfolding method cannot be used to obtain the upscaled model. Under suitable assumptions on data, by using asymptotic expansion with drift (in which the formal asymptotic expansion is defined in a moving coordinate), we obtain the following upscaled equation (see details in Section 4 in paper 2):

Find (u_0, W) satisfying the following system of equations:

$$
\begin{aligned}
\partial_t u_0 + \operatorname{div}(-D^*(u_0, W)\nabla_x u_0) = \frac{1}{|Z|}\int_Z f\,dy + \frac{-1}{|Z|}\int_{\Gamma_N} g_N\,d\sigma_y \\
\text{on } (0,T) \times \mathbb{R}^2, \\
u_0(0) = g \qquad \text{on} \qquad \mathbb{R}^2,
\end{aligned}
$$

$$
\begin{aligned}
&-\operatorname{div}_y(D(y)\nabla_y w_i) + P'(u_0)\operatorname{div}_y(B(y)w_i)\\
&= \operatorname{div}_y(D(y)e_i) + B^* \cdot e_i - P'(u_0)B(y)\cdot e_i \quad \text{on} \quad (0,T)\times Z,
\end{aligned}
$$

$$
\begin{aligned}
&(-D(y)\nabla_y w_i + BP'(u_0)w_i)\cdot n_y\\
&\qquad\qquad = (D(y)e_i)\cdot n_y \quad \text{on} \quad (0,T)\times \Gamma_N,
\end{aligned}
$$

$$
\begin{aligned}
&w_i = 0 && \text{on } (0,T)\times\Gamma_D,\\
&w_i \text{ is } Z\text{–periodic},
\end{aligned}
$$

where $i \in \{1,2\}$.

The effective dispersion tensor D^* is defined as

$$
\begin{aligned}
D^*(u_0, W) &= \frac{1}{|Z|}\int_Z D(y)\left(I + \begin{bmatrix} \frac{\partial w_1}{\partial y_1} & \frac{\partial w_2}{\partial y_1} \\ \frac{\partial w_1}{\partial y_2} & \frac{\partial w_2}{\partial y_2}\end{bmatrix}\right) dy\\
&\quad + \frac{1}{|Z|}B^*\int_Z W(y)^t\,dy - \frac{P'(u_0)}{|Z|}\int_Z B(y)W(y)^t\,dy.
\end{aligned}
$$

Finally, with additional assumptions, in Theorem 5.2, we show that there exists a weak solution for the upscaled model.

2.3 Paper III

The main aim of this paper is to derive rigorously the structure of the upscaled model corresponding to a reaction-diffusion equation with nonlinear drift and show the strong convergence of the corresponding corrector function. To set our problem, we consider unbounded perforated domain Ω_ε, in this domain, we investigate the following problem:

$$
\begin{aligned}
\frac{\partial u^\varepsilon}{\partial t} + \operatorname{div}(-D^\varepsilon \nabla u^\varepsilon + \frac{1}{\varepsilon}B^\varepsilon P(u^\varepsilon)) &= f^\varepsilon && \text{in} \quad \Omega^\varepsilon \times (0,T),\\
(-D^\varepsilon\nabla u^\varepsilon + \frac{1}{\varepsilon}B^\varepsilon P(u^\varepsilon))\cdot n_\varepsilon &= \varepsilon g_N(u^\varepsilon) && \text{in} \quad \Gamma_N^\varepsilon\times(0,T),\\
u^\varepsilon(0) &= g && \text{on} \quad \overline{\Omega}^\varepsilon,
\end{aligned}
$$

where $P(\cdot)$ is a second order polynomial in the form $P(r) = r(1-Cr)$ and $g_N(\cdot)$ is a Lipschitz continuous nonlinear function.

To perform the homogenization for our fast drift problem, we use the concept of two-scale convergence with drift (a generalized version of two-scale convergence in which the test function is defined in a fast-moving coordinate). Since both the drift and the boundary term are nonlinear, in addition to the two-scale convergence result, we need the strong convergence of our solution in moving coordinates. In Theorem 5.1 and Theorem 5.2 we establish that there exist a $u_0(t,x) \in L^2(0,T;H^1(\mathbb{R}^2))$, such that

$$\lim_{\varepsilon\to 0}\int_0^T\int_{\Omega^\varepsilon}\left|u^\varepsilon(t,x)-u_0\left(t,x-\frac{B^*t}{\varepsilon}\right)\right|^2 dxdt = 0,$$
$$\lim_{\varepsilon\to 0}\varepsilon\int_0^T\int_{\Gamma_N^\varepsilon}\left|u^\varepsilon(t,x)-u_0\left(t,x-\frac{B^*t}{\varepsilon}\right)\right|^2 d\sigma dt = 0.$$

In Theorem 5.5, we rigorously derive the upscaled model equations:

$$\partial_t u_0 + \operatorname{div}(-D^*(u_0,W)\nabla_x u_0) = \frac{1}{|Z|}\int_Z f\,dy - \frac{|\Gamma_N|}{|Z|}g_N(u_0) \quad \text{on} \quad (0,T)\times\mathbb{R}^2,$$
$$u_0(0) = g \quad \text{on} \quad \mathbb{R}^2,$$

$$-\operatorname{div}_y(D(y)\nabla_y w_i)+B(y)(1-2C(y)u_0)\cdot\nabla_y w_i = \operatorname{div}_y(D(y)e_i) + B^*\cdot e_i - B(y)(1-2C(y)u_0)\cdot e_i \quad \text{on} \quad (0,T)\times\mathbb{R}^2\times Z,$$

$$(-D(y)\nabla_y w_i + B(y)(1-2C(y)u_0)w_i)\cdot n_y = (D(y)e_i)\cdot n_y \quad \text{on} \quad (0,T)\times\mathbb{R}^2\times\Gamma_N,$$
$$w_i(t,x,\cdot) \text{ is } Z\text{–periodic},$$

where

$$B^*\cdot e_i := \frac{\int_Z B(y)\cdot e_i dy}{|Z|},$$

and

$$D^*(u_0,W) := \frac{1}{|Z|}\int_Z D(y)\left(I + \begin{bmatrix}\frac{\partial w_1}{\partial y_1} & \frac{\partial w_2}{\partial y_1}\\ \frac{\partial w_1}{\partial y_2} & \frac{\partial w_2}{\partial y_2}\end{bmatrix}\right)dy + \frac{1}{|Z|}B^*\int_Z W(y)^t\,dy - \frac{1}{|Z|}\int_Z B(y)(1-2C(y)u_0)W(y)^t\,dy$$

for all $t \in (0,T)$ and a.e. $x \in \mathbb{R}^2, y \in Z$, with

$$W := (w_1, w_2).$$

Finally, in Theorem 6.1, we show the following strong convergence of the corrector function

$$\lim_{\varepsilon\to 0} \left\| \nabla \left(u^\varepsilon(t, \frac{x}{\varepsilon}) - u_0(t, x - \frac{B^* t}{\varepsilon}) - \varepsilon u_1(t, x - \frac{B^* t}{\varepsilon}, \frac{x}{\varepsilon}) \right) \right\|_{L^2(0,T;L^2(\Omega^\varepsilon))} = 0.$$

2.4 Paper IV

Our goal is to investigate the solvability and numerical approximation of a two-scale system. The problem that we are interested in consists of a nonlinear reaction-dispersion equation which is strongly coupled with elliptic cell problems. The nonlinear two-scale structure is motivated by the upscaled model of large drift problem from Paper 2 and Paper 3. Let Ω and Y be two bounded spatial domains, in this domain we consider the following two-scale model:

$$\partial_t u + \operatorname{div}(-D^*(W)\nabla u) = f \quad \text{in } (0,T)\times\Omega, \tag{2}$$
$$u = 0 \quad \text{on } (0,T)\times\partial\Omega, \tag{3}$$
$$u(0) = g \quad \text{in } \overline{\Omega}, \tag{4}$$

$$\operatorname{div}_y\left(-D\nabla_y w_i + G_i(u)Bw_i\right) = \operatorname{div}_y(De_i) \quad \text{in } Y, \tag{5}$$
$$(-D\nabla_y w_i + BG_i(u)w_i)\cdot n_y = (De_i)\cdot n_y \quad \text{on } \Gamma_N, \tag{6}$$
$$w_i \text{ is } Y\text{–periodic}, \tag{7}$$

where $i \in \{1,2\}$, $G_i(\cdot)$ are nonlinear real-valued functions, and the dispersion tensor $D^*(W)$ defined as

$$D^*(W) := \frac{1}{|Y|}\int_Y D(y)\left(I + \begin{bmatrix} \frac{\partial w_1}{\partial y_1} & \frac{\partial w_2}{\partial y_1} \\ \frac{\partial w_1}{\partial y_2} & \frac{\partial w_2}{\partial y_2} \end{bmatrix}\right) \mathrm{d}y.$$

For details of other data parameters, see Section 2 from Paper 4.

To analyze the existence of solutions to the problem (2)–(7), we propose the following iterative scheme:

Set $u^0 = g$, for any $k \in \mathbb{N} \cup \{0\}$, u^{k+1}, w_1^k, and w_2^k satisfy:

$$\begin{aligned} \operatorname{div}_y \left(-D\nabla_y w_i^k + G_i(u^k)Bw_i^k\right) &= \operatorname{div}_y(De_i) && \text{in } Y, \\ \left(-D\nabla_y w_i^k + BG_i(u^k)w_i^k\right)\cdot n_y &= (De_i)\cdot n_y && \Gamma_N, \\ w_i^k \text{ is } Y\text{–periodic}, & && i \in \{1,2\} \end{aligned}$$

$$\begin{aligned} \partial_t u^{k+1} + \operatorname{div}(-D^*(W^k)\nabla u^{k+1}) &= f && \text{in } (0,T)\times\Omega, \\ u^{k+1}(0) &= g && \text{in } \overline{\Omega}, \\ u^{k+1} &= 0 && \text{on } (0,T)\times\partial\Omega, \end{aligned}$$

where the dispersion tensor $D^*(W^k)$ is given by

$$D^*(W^k) := \frac{1}{|Y|}\int_Y D(y)\left(I + \begin{bmatrix} \frac{\partial w_1^k}{\partial y_1} & \frac{\partial w_2^k}{\partial y_1} \\ \frac{\partial w_1^k}{\partial y_2} & \frac{\partial w_2^k}{\partial y_2} \end{bmatrix}\right) \mathrm{d}y.$$

In Theorem 3.1 and Lemma 3.4, we establish the well-posedness and k independent energy estimates of the solution to the iterative scheme. Using these results and suitable assumptions, in Theorem 3.2, we prove that there exists $(u, W) \in L^2((0,T); H_0^1(\Omega)) \times (H_\#^1(Y))^2$ such that

$$\begin{aligned} u^k &\to u && \text{strongly in} && L^2((0,T)\times\Omega), \\ \nabla u^k &\rightharpoonup \nabla u && \text{weakly in} && L^2((0,T)\times\Omega), \\ \partial_t u^k &\rightharpoonup \partial_t u && \text{weakly in} && L^2((0,T); H^{-1}(\Omega)), \\ D^*(W^k) &\to D^*(W) && \text{strongly in} && L^2((0,T)\times\Omega). \end{aligned}$$

and moreover, (u, W) is a weak solution to (2)–(7). Finally, using the finite element method together with the iterative scheme, we show several simulation studies for (2)–(7) (see Section 4 from Paper 4 for details).

3 Outlook

3.1 Conclusion

In this thesis, we derived upscaled equations for reaction-diffusion problems with nonlinear drift. The structure of the nonlinearity comes from a well-established mathematical model (see [14]) that describes the evolution of a population of interacting particles traveling through composite materials. We studied our microscopic problems posed in different geometries and with varying scaling. We looked particularly at bounded thin layers with periodically distributed microstructure and unbounded perforated domains.

In the thin layer case, we investigated the effect of the multiple scalings leading to slow and moderate drifts. For each scaling option, we derived the corresponding upscaled model and effective transmission condition. These results addressed the question (Q1) posed in Section 1.1.

In the unbounded perforated domain case, the microscopic problem has a large nonlinear drift. In this situation, we obtain the upscaled equation as a reaction-nonlinear dispersion structure that is coupled with elliptic cell problems. To study such strongly coupled two-scale system endowed with nonlinear dispersion, we proposed an iterative scheme. By this iterative scheme, we showed the existence of the solution to the original set of equations and used it to obtain numerical simulations. The aforementioned results address the questions (Q2) and (Q3), respectively.

3.2 Future work

The microscopic model that we focused on in this thesis comes from the hydrodynamic limit of a population of interacting particles driven by an asymmetric simple exclusion process. Now, it would be interesting to see how the mathematical model looks like when two (or more) different populations of interacting particles move in space by following the mentioned dynamics. We expect to see a nonlinear cross-diffusion system with coupled drift. The well-posedness and homogenization of such models need to be studied. We expect that a similar technique as used in [11] or [12] can help regarding the well-posedness part, while the two-scale convergent arguments discussed in [22] can be used to obtain the upscaled problem.

In the follow-up work [30], we proposed a precomputing strategy and a new time-discretization scheme to approximate the weak solution of the strongly coupled problem which is discussed in Paper 4. This new strategy allowed us to reduce a large amount of computational costs. However, the well-posedness and error analysis of this new scheme is yet to be done.

Another potentially relevant continuation of this research is to derive corrector estimates for all our upscaled models. This is a difficult task. We expect that for the thin layer case, we can adapt the technique used in [18]. Corrector estimates for the large drift problem (but in the linear case) are studied in [3, 33]. Thus, we anticipate that we might be able to extend such results to a nonlinear drift problem and then derive the corresponding corrector estimates for our large drift upscaled model.

The uniqueness of the weak solution of the upscaled large drift model (and the strongly coupled model that we studied in Paper 4) is yet to be proven. The main difficulty here is the presence of the nonlinear dispersion term. The standard technique of proving uniqueness by deriving the energy estimates for the difference between two weak solutions will not work in our case. However, we expect that the strong-weak uniqueness (in which case we assume one of the weak solutions to be the classical solution and then from that assumption conclude that all the weak solutions coincide (see [40])) can be achievable without much difficulty.

The homogenization technique that we used in this thesis is not suitable to handle the homogenization of large drift problems defined in a bounded domain. To the best of our knowledge, the only rigorous homogenization studies for large drift problems for bounded domains, without the assumption that the mean value of the drift coefficient is zero, are [7, 34]. Thus, extending the homogenization results from [7, 34] to our setting would be mathematically very interesting.

4 List of publications and author's contribution

The thesis is based on the following papers:

(I) V. Raveendran, E. N. M. Cirillo, I. de Bonis, and A. Muntean. "Scaling effects on the periodic homogenization of a reaction-diffusion-convection problem posed in homogeneous domains connected by a thin composite layer". In: *Quarterly of Applied Mathematics* 80 (2022), pp. 157–200

(II) V. Raveendran, E. N. M. Cirillo, and A. Muntean. "Upscaling of a reaction-diffusion-convection problem with exploding non-linear drift". In: *Quarterly of Applied Mathematics* 80 (2022), pp. 641–667

(III) V. Raveendran, I. de Bonis, E. N. M. Cirillo, and A. Muntean. "Homogenization of a reaction-diffusion problem with large nonlinear drift and Robin boundary data". In: *Quarterly of Applied Mathematics* (2024), pp. 1–39

(IV) V. Raveendran, S. Nepal, R. Lyons, M. Eden, and A. Muntean. "Strongly Coupled Two-scale System with Nonlinear Dispersion: Weak Solvability and Numerical Simulation". In: *arXiv:2311.12251* (2023)

Furthermore, work in related research has led to the following publications:

(V) V. Raveendran. *Homogenization of reaction-diffusion problems with nonlinear drift in thin structures*. Licentiate thesis, *Karlstads university*, 2022

(VI) S. Nepal, V. Raveendran, M. Eden, R. Lyons, and A. Muntean. "Numerical Study of a Strongly Coupled Two-scale System with Nonlinear Dispersion". In: *arXiv:2402.09607* (2024)

(VII) N. Avery, A. Contri, F. Heimann, A. Massing, S. Nepal, B. Rasheed, V. Raveendran, U. Schaarschmidt, H.G. Schaathun and K. Simmonds. *Modeling of soft tissue cutting for orthopedic surgery.* To appear in Proceedings of the European Study Group with Industry 156

Author's contributions

(I) I contributed to the major part of the theorems and proofs. A. Muntean, E. N. M. Cirillo, and I. de Bonis provided feedback, corrections, and valuable ideas for writing the manuscript. I drafted and submitted the manuscript.

(II) I derived the major part of the result presented in the manuscript. A. Muntean and E. N. M. Cirillo continuously provided discussions, feedback, and corrections in the manuscript. I was responsible for the drafting of the manuscript and correspondence with the journal editor.

(III) I was responsible for a significant part of the mathematical analysis and drafting of the manuscript. A. Muntean, E. N. M. Cirillo, and I. de Bonis continuously provided feedback, corrections, and valuable ideas in the text. I was responsible for the submission procedure of the manuscript and correspondence with the journal editor.

(IV) I was responsible for the analysis part of the manuscript. S. Nepal provided the simulation results. M. Eden, R. Lyons, and A. Muntean did the conceptualization, revision, and discussion. I was responsible for the drafting and submission procedure of the manuscript.

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Scaling effects and homogenization of reaction-diffusion problems with nonlinear drift

We study the homogenization of reaction-diffusion problems with nonlinear drift. The microscopic model is derived as the hydrodynamic limit of a totally asymmetric simple exclusion process of interacting particles. We first look into a situation when the interacting particles cross a thin composite layer. To understand the effective transmission condition, we perform the homogenization and dimension reduction of the model with variable scalings. One physically interesting scaling that we look at separately is when the drift is large. In this case, we consider the overall process taking place in an unbounded porous media. We first upscale the model using the asymptotic expansions with drift. Then, using two-scale convergence with drift, we rigorously derive the homogenization limit for a similar microscopic problem with a nonlinear boundary condition. Additionally, we show the strong convergence of the corrector function. In the large drift case, the resulting upscaled model is a nonlinear reaction-dispersion equation strongly coupled with a system of nonlinear elliptic cell problems. We study the solvability of a similar strongly coupled two-scale system with nonlinear dispersion by constructing an iterative scheme. Finally, we illustrate the behavior of the solution using the iterative scheme.

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