Upscaling the interplay between diffusion and polynomial drifts through a composite thin strip with periodic microstructure

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Abstract We study the upscaling of a system of many interacting particles through a heterogeneous thin elongated obstacle as modeled via a two-dimensional diffusion problem with a one-directional nonlinear convective drift. Assuming that the obstacle can be described well by a thin composite strip with periodically placed microstructures, we aim at deriving the upscaled model equations as well as the effective transport coefficients for suitable scalings in terms of both the inherent thickness at the strip and the typical length scales of the microscopic heterogeneities. Aiming at computable scenarios, we consider that the heterogeneity of the strip is made of an array of periodically arranged impenetrable solid rectangles and identify two scaling regimes what concerns the small asymptotics parameter for the upscaling

procedure: the characteristic size of the microstructure is either significantly smaller than the thickness of the thin obstacle or it is of the same order of magnitude. We scale up the diffusion–polynomial drift model and list computable formulas for the effective diffusion and drift tensorial coefficients for both scaling regimes. Our upscaling procedure combines ideas of two-scale asymptotics homogenization with dimension reduction arguments. Consequences of these results for the construction of more general transmission boundary conditions are discussed. We illustrate numerically the concentration profile of the chemical species passing through the upscaled strip in the finite thickness regime and point out that trapping of concentration inside the strip is likely to occur in at least two conceptually different transport situations: (i) full diffusion/dispersion matrix and nonlinear horizontal drift, and (ii) diagonal diffusion matrix and oblique nonlinear drift.

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1 Introduction

1.1 Background. Motivation

The study of the physics of interfaces has known a great impulse in the last decades; different point of views have been adopted and several related problem have been investigated, ranging from the dynamical evolution of a membrane to its static morphology and, also, to the possibility of metastable behaviors [26]. In this paper we investigate flat static (not fluctuating) strips separating two regions of space and crossed by a flow of particles. This is a typical setup one is interested in when studying membrane filtration. Traditionally, membrane filtration is one of the most common methods for purifying fluids. Furthermore, recent advances in conductive and mass transport through a composite medium have led to increased interest in the process of mixed-matrix membrane separation. In both such cases, small particles of a microporous material, identified as a filler, are dispersed in a dense nonporous polymer material, identified as a matrix, and then processed into a thin composite layer, identified as a membrane. The objective is that the filler, chosen for its high adsorption affinity or transport rate for a molecular species of interest, improves the efficacy of the matrix in membrane-mediated separation [29]. Depending on pore sizes and level of microscopic activity, one also encounters the so-called enhanced matrix diffusion [30]. Our main motivation is to develop multiscale mathematical modelling strategies of transport processes that can describe, over several space scales, how internal structural features of the filler and of the local defects affect the effective diffusivity of the material, perceived here as a thin long composite membrane. As concrete applications, we have in mind the transport of O_2 and/or CO_2 molecules through packaging materials [28] (layered composite membranes) as well as the dynamics of human crowds through barrier-like heterogeneous environments (active particles walking inside geometries with obstacles). In both cases, a relevant question concerns the possibility of concentration trapping. The motivation of doing this work was originally inspired by our research on lattice dynamics of reduced jamming in interacting particles by barriers.

We study the diffusion of particles through such a thin heterogeneous membrane under a one-directional nonlinear drift. We consider the mean-field equation

$$\frac{\partial u}{\partial t} - d_1 \frac{\partial^2 u}{\partial x_1^2} - d_2 \frac{\partial^2 u}{\partial x_2^2} = -b \frac{\partial}{\partial x_1} [u(1-u)] + f(x), \quad (1.1)$$

where t is time, x_1 and x_2 the space coordinates, u the typical occupation number (a number in $[0, 1]$ representing the probability to find a particle at the specified position), d_1 and d_2 are the possibly different diffusion coefficients in the two spatial directions, $b > 0$ is found in the hydrodynamic limit of the two-dimensional random walk with simple exclusion and drift along the x_1 -direction, and f is a particle source. Then, we scale up the system and derive computable effective transport coefficients accounting for the presence of the strip (complementing our simulation study [10] with new results).

Essentially the same problem is addressed in [9, 10] for an interacting-particle system setup—a lattice model, known as *simple exclusion model*, is considered on a two-dimensional strip of $\mathbb{Z}^2$, where particles move randomly with the constraint that at most one particle at a time can occupy the sites of the lattice. Particles move while choosing at random one of the four neighboring sites, and additionally, a *drift* is introduced in the dynamics so that one of the four direction is more probable. This model is a generalization of the celebrated TASEP (total asymmetric simple exclusion model) which is a one-dimensional simple exclusion model in which particles move to the right at random times [14].

It is important to have in view that the Eq. (1.1) is derived in the macroscopic diffusive limit, i.e. when the space and the drift are rescaled with a small parameter and, correspondingly, the time is rescaled with the square of the same parameter. In “Appendix A”, see also [9], we report a heuristic derivation of this equation which, in the one-dimensional case, was rigorously proven in [15] (see, also, [22] for an account of more recent techniques developed for hydrodynamic limits). In particular, our heuristic computation shows that the two diffusion coefficients can be different as a consequence of the fact that, at the lattice level, the probability of a particle to move horizontally or vertically can differ drastically. This is an important feature in our context, since the peculiar

anisotropic structure of the transport term is related to the probability of a particle performing a move, which the simple exclusion might in fact prevent. Consequently, the factor u comes from the probability to find a particle at a given site and the factor $1 - u$ accounts for the probability that the site where the particle tries to move to is indeed empty. In other words, the structure of the nonlinearity of the right hand side of Eq. (1.1) is connected to the hard-core repulsion of the molecules at the lattice level.

We emphasize that the model we have in mind is (1.1), while the techniques that are developed in this article apply directly to more general transport terms obtained by substituting $u(1 - u)$ with general polynomials in terms of u . Note that polynomials drifts are not uncommon—they appear also in the structure of Forchheimer flows. The heterogeneities we account for in this context are assumed to be arranged periodically, but the same working methodology can be adapted to the locally periodic case.

We scale up our problem for two scaling regimes. In the first case, we simply average the information over the strip, by keeping the strip width unchanged, while in the second case we look for the structure of the upscaled model in the limit in which both the width and the height of the cells tend to zero and their number is increased so that the total height of the cells equals that of the whole strip. In this second limiting procedure, the strip is reduced to a solid line.

Additionally, we investigate also the effect of diffusion correlations and cross-diffusion (diagonal vs. full diffusion tensors) on the structure of the upscaled equations. We observe that in the case of the infinitely thin upscaled membrane¹ the structure of the limit equations is unchanged, while in the case of the finite-length upscaled membrane the presence of the off-diagonal terms does not permit the use of closed form representations of oscillations in terms of cell functions. Furthermore, it is worth mentioning that even a local clogging of the strip cannot be achieved with our model, i.e. pores cannot be blocked and hence transport always takes place. This effect occurs in such

diffusion context only if the boundaries of the microstructures would be allowed to grow freely (cf. a suitable moving-boundary formulation), leading, as time elapses, to contacts in a number of positions in space between micro-interfaces at neighboring cells. In similar situations, the effective diffusion coefficient degenerates. We refer the reader to [25] for a setting that accounts for local clogging of the pores. Instead, we will see that localization/trapping of concentration is in principle possible, as our simulations indicate. However, we are not able yet to quantify *a priori* how much concentration can be stored within the membrane for a given time interval. An open issue in this context relates to unveiling the microscopic origin of quenching—we would like to understand whether infinitely-thin periodic membrane models, where diffusion is accompanied also by chemical reactions, can be used to shed light on the nonlinear structure of singular reaction terms. In such a context, production terms in coupled reaction–diffusion equations take the form kr/s^γ for a certain asymptotic regime, where $k > 0, 0 < \gamma \leq 1$ with $r, s \in [0, \infty]$ (cf. [11] or [12]).

As working techniques, we employ scaling arguments as well as two-scale homogenization asymptotic expansions to guess the structure of the model equations and the corresponding effective transport coefficients. The research presented in this article pursues a formal two-scale asymptotics route; it follows the thread of the original mathematical analysis work by Neuss-Radu and Jäger [27] by adding to the discussion the presence of nonlinear transport terms and is remotely related to our work on filtration combustion through heterogeneous thin layers; compare [19, 20] and also related recent work [3]. Strongly connected scenarios to the transport–through–membranes problem are the theoretical estimation of the effective interfacial resistance of regular rough surfaces (cf. [16], e.g.) and the upscaling of reaction, diffusion, and flow processes in porous media with thin fissures (cf. [4, 32], e.g.).

As alternative approach to the two-scale asymptotics homogenization, one could also attempt of using a matched asymptotics approach, a volume averaging approach for a suitably defined representative elementary volume (REV), or a renormalization strategy. Each method brings in both advantages and disadvantages, depending on what assumptions (closure relations) one relies on. We refer the reader to [7, 13, 23] for critical discussions around this topic. We choose to perform the

¹ For a particular scaling regime, we perform a simultaneous homogenization asymptotics and dimension reduction, allowing us not only to replace the heterogeneous membrane by an homogeneous obstacle line, but also to provide the effective transmission conditions needed to complete the upscaled model equations.

homogenization via the so-called formal two-scale asymptotics [21] simply because we trust that we can justify rigorously the asymptotic expansions using a combination of arguments based on the two-scale convergence and on the periodic unfolding operator. The other upscaling techniques seem applicable as well, but their rigorous justification is much harder to guarantee.

1.2 Main findings. Organization of the paper

In this context, the challenge is the handling of the combination of heterogeneous strip structure and the presence of the transport term on the right-hand side in the evolution equation (1.1). Our results extend to a more general model obtained by assuming the transport term to be the x_1 -derivative of a polynomial of the field u with a finite arbitrary large degree. The main findings of this work are:

- We deduced the structure of the formal asymptotic expansions which are behind the concept of two-scale boundary layer convergence from [27]; possibly using working ideas from [21], this structure can be further employed to construct corrector estimates to justify the upscaling and to provide convergence rates for the upscaling procedure.
- We derived the structure of the upscaled transmission conditions valid across the obstacle line with the corresponding jumps in both transport fluxes and concentrations. These jumps are expressed in terms of the local physics of the situation, i.e. they incorporate microstructural information.
- Using finite element approximations of our upscaled model equations implemented in FEniCS [2], we illustrate numerically profiles of concentration within the upscaled strip in the finite thickness scaling regime. We simulate a basic scenario using a reference set of parameters corresponding to the penetration of gaseous CO_2 through a thin periodically perforated strip. We gain confidence that our model equations and their implementation can be used for testing practical applications and, in principle, can be extended to deal with more realistic membranes (multiple layers, different kind of periodicities in the arrangement of microstructures, defects, curvature effects, etc.).

The article is organized as follows: In Sect. 2 we present the equations of our mean-field model as well as the strip geometry. After a suitable scaling, we point out two relevant asymptotic regimes in terms of a small parameter ε which incorporates the periodicity and selected size effects of the internal structure of the strip. Section 3 contains the derivation of the finite thickness upscaled strip model, while in Sect. 4 we consider the more delicate case of the upscaling of the infinitely-thin strip. Here the two-scale homogenization asymptotics is performed simultaneously with a dimension reduction procedure—a non-standard singular perturbation problem. We illustrate numerically in Sect. 5 the approximation of the solution to the upscaled strip in the finite thickness regime and point out the possibility of concentration localization. Finally, we present our conclusions in Sect. 6.

2 The microscopic model

Let $\ell, h > 0$ and consider the two-dimensional strip $[-\ell/2, \ell/2] \times [0, h]$, say that ℓ and h are, respectively, its horizontal and vertical side lengths. Partition the strip into the blocks $\omega_l = [-\ell/2, -w/2] \times [0, h]$, $\omega_m = [-w/2, w/2] \times [0, h]$, $\omega_r = [w/2, \ell/2] \times [0, h]$, and call ω_m the *membrane*. Let $0 < \eta \leq h$ and $\varepsilon = 2\eta/\ell$. We partition the membrane into rectangular *cells* $\omega_c^i = (-w/2, w/2) \times ((i-1)\eta, i\eta) \cap (0, h)$ with i running from one to the smallest integer larger than or equal to h/η . In each cell consider an impenetrable rectangular region, called *obstacle*, with its center in the center of the cell and diameter $O(\varepsilon)$ in the limit $\varepsilon \rightarrow 0$. Denote by ω_o the union of all the obstacles.

We denote by γ_v and γ_h , the vertical and horizontal boundaries of the strip, by γ_o the boundary of the obstacle region ω_o and by γ_i the boundary of the region ω_i for $i = l, m, r$. The boundaries γ 's are considered deprived of singular points. The external normal vector to a smooth arc of a closed curve is denoted here by $\mathbf{n}$.

We let $\omega = (\omega_l \cup \omega_r \cup \omega_m) \setminus \omega_o$ and $f : \omega \rightarrow \mathbb{R}$ be a real function. Fixing the parameters $d_1, d_2 > 0$, we consider the differential problem

Fig. 1 Schematic representation of the model geometry

$$\frac{\partial u}{\partial t} - d_1 \frac{\partial^2 u}{\partial x_1^2} - d_2 \frac{\partial^2 u}{\partial x_2^2} = -b \frac{\partial}{\partial x_1} u(1-u) + f(\mathbf{x}) \quad \text{in } \omega, \quad (2.1)$$

endowed with the homogeneous Neumann boundary conditions

$$\left(d_1 \frac{\partial u}{\partial x_1} - bu(1-u), d_2 \frac{\partial u}{\partial x_2} \right) \cdot \mathbf{n} = 0 \quad \text{on } \gamma_h \cup \gamma_o, \quad (2.2)$$

as well as with the Dirichlet boundary conditions

$$u(\mathbf{x}, t) = u_l \quad \text{on } \gamma_v \cap \gamma_l \quad \text{and} \quad u(\mathbf{x}, t) = u_r \quad \text{on } \gamma_v \cap \gamma_r \quad (2.3)$$

for any $t \geq 0$, where $u_l, u_r \in \mathbb{R}$. As initial condition we take

$$u(\mathbf{x}, 0) = v(\mathbf{x}) \quad \text{on } \omega. \quad (2.4)$$

2.1 The non-dimensional model

To perform the upscaling of the diffusion and drift processes through the heterogeneous strip depicted in Fig. 1, we need first to identify the small parameter as well as the corresponding scaling of the geometry that fits to the situation at hand. It is therefore useful to introduce the dimensionless variables

$$\mathbf{X} = (X_1, X_2) = \left(\frac{2x_1}{\ell}, \frac{2x_2}{\ell} \right) \quad \text{and} \quad T = \frac{t}{\tau}, \quad (2.5)$$

where τ is a fixed positive real representing a suitable characteristic time scale.²

Using (2.5), the original strip is mapped to $[-1, 1] \times [0, 2h/\ell]$, which is partitioned into $\Omega_l = [-1, -w/\ell] \times [0, 2h/\ell]$, $\Omega_m = [-w/\ell, w/\ell] \times [0, 2h/\ell]$, and $\Omega_r = [w/\ell, 1] \times [0, 2h/\ell]$. The cells are mapped to $\Omega_c^i = (-w/\ell, w/\ell) \times ((i-1)\varepsilon, i\varepsilon) \cap (0, 2h/\ell)$, where we recall that $\varepsilon = 2\eta/\ell$. In the new variables, we denote by Ω_o the region occupied by the obstacle and by $\Gamma_v, \Gamma_h, \Gamma_l, \Gamma_m, \Gamma_r$, and Γ_o the boundaries introduced above.

Take a reference concentration u_{ref} . It is convenient to set

$$U(\mathbf{X}, T) = \frac{1}{u_{\text{ref}}} u\left(\frac{\ell \mathbf{X}}{2}, \tau T\right), \quad V(\mathbf{X}) = \frac{1}{u_{\text{ref}}} v\left(\frac{\ell \mathbf{X}}{2}\right), \quad (2.6)$$

$$F(\mathbf{X}) = \frac{\tau}{u_{\text{ref}}} f\left(\frac{\ell \mathbf{X}}{2}\right)$$

and rewrite the model (2.1) as follows

$$\frac{\partial U}{\partial T} + \nabla \cdot \mathbf{J} = F \quad (2.7)$$

in $\Omega = (\Omega_l \cup \Omega_r \cup \Omega_m) \setminus \Omega_o$, where we introduced the flux

² In this paper, the letter T is used to denote both the dimensionless time variable and the transpose of a matrix A , i.e. A^T . The context will make clear what we mean.

$$\mathbf{J} = -\mathbb{D}(\nabla U + \mathbf{G}(U)), \quad (2.8)$$

with the derivatives in ∇ taken with respect to the dimensionless variables X_1, X_2 , and let

$$\mathbb{D} = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix}, \quad D_1 = \frac{4\tau d_1}{\ell^2}, \quad D_2 = \frac{4\tau d_2}{\ell^2}, \quad \text{and} \\ \mathbf{G}(U) = \begin{pmatrix} g(U) \\ 0 \end{pmatrix}, \quad (2.9)$$

with $g(U) = \ell b u_{\text{ref}} p(U)/(2d_1)$, where $p(U) = -U(1-U)$ —a choice that makes (2.8) to correspond precisely to the setting discussed in [10]. Furthermore, we introduce $U_{\text{r}} = u_{\text{r}}/u_{\text{ref}}$ and $U_{\text{l}} = u_{\text{l}}/u_{\text{ref}}$.

The derivations done in this paper cover the more general case:

$$\mathbb{D} = \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix} \quad \text{and} \quad p(U) = \sum_{n=1}^k a_n U^n \quad (2.10)$$

with arbitrary coefficients $a_n \in \mathbb{R}$ and arbitrary polynomial order $k \in \mathbb{N}$. The parameter k is simply the degree of the polynomial appearing in (2.10); in the physical example described in the introduction k is equal to 2. In other words, the diffusion matrix is not necessarily diagonal and $p(U)$ is an arbitrary polynomial. If not mentioned otherwise, in the rest of the paper $\mathbb{D}$ is a full matrix as indicated in (2.10).

For any $T \geq 0$, problem (2.7) is endowed with the Dirichlet boundary conditions

$$\begin{aligned} U(\mathbf{X}, T) &= U_{\text{l}} \quad \text{on } \Gamma_{\text{v}} \cap \Gamma_{\text{l}} \quad \text{and} \\ U(\mathbf{X}, T) &= U_{\text{r}} \quad \text{on } \Gamma_{\text{v}} \cap \Gamma_{\text{r}}, \end{aligned} \quad (2.11)$$

the Neumann boundary conditions

$$\mathbf{J} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_{\text{h}} \cup \Gamma_{\text{o}}, \quad (2.12)$$

and the initial condition

$$U(\mathbf{X}, 0) = V(\mathbf{X}) \quad \text{for } \mathbf{X} \in \bar{\Omega}. \quad (2.13)$$

A few remarks are in order:

- (i) All diffusion coefficients mentioned in this section are given positive numbers. Typical values corresponding to the diffusion of CO_2 are indicated in Sect. 5. In the next sections, all diffusion coefficients acting within the strip become space-dependent functions depending

on the geometry of the periodic cell (of the strip).

- (ii) If a single species diffuses through an homogeneous medium, then the off-diagonal elements of $\mathbb{D}$ are zero. If two populations decide to diffuse together through an homogeneous medium, then cross-diffusion effects might come into play and the matrix $\mathbb{D}$ becomes full. If a single species diffuses through an heterogeneous medium, then the occurrence of non-zero off diagonal elements indicate deviations from geometric isotropy. In some textbooks on porous media, such diffusion matrix is referred to as dispersion tensor. The reason why we prefer to work with the full matrix is rather of technical nature—we wish to verify whether the upscaling results can be obtained for the case of a full matrix.

3 Derivation of the finite-thickness upscaled strip model

In this section, we use a two-scale homogenization approach to average the strip internal structure and then to derive the corresponding upscaled evolution equation for the mass transport as well as the effective transport coefficients. If the diffusion matrix is diagonal, then we point out explicitly the structure of the corresponding tortuosity tensor. Furthermore, it is worth noting that if the nonlinear drift term is neglected (hence, the model becomes linear), then the derivation of the finite-thickness upscaled membrane model can be made rigorous e.g. by following the strategy from Chapter 9 of Ref. [5]. We refer the reader also to the monograph [8].

3.1 Two-scale expansions

We look for upscaled model equations in the limit in which the height of the cells tends to zero and its number is increased so that the total height of the cell sequence is that of the whole strip. Due to the periodic micro-structure of the membrane Ω_{m} , with vertical spatial period $\varepsilon = 2\eta/\ell$, it is reasonable to attack the problem expanding the unknown function U in the strip region as

$$U(\mathbf{X}, T) = \sum_{n=0}^{\infty} \varepsilon^n U_n^{\text{m}}(\mathbf{X}, Y_2, T) \quad \text{in } \Omega_{\text{m}}, \quad (3.1)$$

where $Y_2 = X_2/\varepsilon$ and the functions U_n^m are Y_2 -periodic functions.

To keep the notation simple, we understand in (2.7)

$$\nabla = \nabla_{\mathbf{x}} + \frac{1}{\varepsilon} \nabla_{Y_2} \quad \text{with} \quad \nabla_{\mathbf{x}} = \begin{pmatrix} \frac{\partial}{\partial X_1} \\ \frac{\partial}{\partial X_2} \end{pmatrix} \quad \text{and} \quad \nabla_{Y_2} = \begin{pmatrix} 0 \\ \frac{\partial}{\partial Y_2} \end{pmatrix}.$$

We now compute the various terms appearing in (2.7) in the different regions of Ω . We have

$$\frac{\partial U}{\partial T} = \sum_{n=0}^{\infty} \varepsilon^n \frac{\partial U_n^m}{\partial T} \quad \text{and} \quad \frac{\partial U}{\partial X_1} = \sum_{n=0}^{\infty} \varepsilon^n \frac{\partial U_n^m}{\partial X_1} \quad \text{in } \Omega_m. \quad (3.2)$$

For handling the terms involving the gradient ∇ , we distinguish between the regions Ω_l , Ω_m , and Ω_r . In Ω_l and Ω_r , we simply have $\nabla U(\mathbf{X}, T) = \nabla U_0^l(\mathbf{X}, T)$ in Ω_l and $\nabla U(\mathbf{X}, T) = \nabla U_0^r(\mathbf{X}, T)$ in Ω_r . Instead of ∇U_0^l and ∇U_0^r , we use ∇U^l and ∇U^r , respectively.

In Ω_m , the computation of the gradient reads

$$\begin{aligned} \nabla U &= \nabla \sum_{n=0}^{\infty} \varepsilon^n U_n^m = \sum_{n=0}^{\infty} \varepsilon^n \nabla_{\mathbf{x}} U_n^m + \sum_{n=0}^{\infty} \varepsilon^n \frac{1}{\varepsilon} \nabla_{Y_2} U_n^m \\ &= \frac{1}{\varepsilon} \nabla_{Y_2} U_0^m + \sum_{n=0}^{\infty} \varepsilon^n (\nabla_{\mathbf{x}} U_n^m + \nabla_{Y_2} U_{n+1}^m). \end{aligned} \quad (3.3)$$

Hence, it yields

$$\begin{aligned} \nabla \cdot \mathbb{D} \nabla U &= \frac{1}{\varepsilon^2} \nabla_{Y_2} \cdot \mathbb{D} \nabla_{Y_2} U_0^m + \frac{1}{\varepsilon} \nabla_{\mathbf{x}} \cdot \mathbb{D} \nabla_{Y_2} U_0^m \\ &\quad + \sum_{n=0}^{\infty} \varepsilon^n \left[\nabla_{\mathbf{x}} \cdot \mathbb{D} \nabla_{\mathbf{x}} U_n^m + \nabla_{\mathbf{x}} \cdot \mathbb{D} \nabla_{Y_2} U_{n+1}^m \right. \\ &\quad \left. + \frac{1}{\varepsilon} \nabla_{Y_2} \cdot \mathbb{D} \nabla_{\mathbf{x}} U_n^m \right. \\ &\quad \left. + \frac{1}{\varepsilon} \nabla_{Y_2} \cdot \mathbb{D} \nabla_{Y_2} U_{n+1}^m \right] \\ &= \frac{1}{\varepsilon^2} \nabla_{Y_2} \cdot \mathbb{D} \nabla_{Y_2} U_0^m + \frac{1}{\varepsilon} [\nabla_{\mathbf{x}} \cdot \mathbb{D} \nabla_{Y_2} U_0^m \\ &\quad + \nabla_{Y_2} \cdot \mathbb{D} \nabla_{\mathbf{x}} U_0^m \\ &\quad + \nabla_{Y_2} \cdot \mathbb{D} \nabla_{Y_2} U_1^m] \\ &\quad + \sum_{n=0}^{\infty} \varepsilon^n [\nabla_{\mathbf{x}} \cdot \mathbb{D} \nabla_{\mathbf{x}} U_n^m + \nabla_{\mathbf{x}} \cdot \mathbb{D} \nabla_{Y_2} U_{n+1}^m \\ &\quad + \nabla_{Y_2} \cdot \mathbb{D} \nabla_{\mathbf{x}} U_{n+1}^m \\ &\quad + \nabla_{Y_2} \cdot \mathbb{D} \nabla_{Y_2} U_{n+2}^m]. \end{aligned} \quad (3.4)$$

Moreover, we have

$$\begin{aligned} \mathbb{D} \mathbf{G}(U) &= \mathbb{D} \mathbf{G}(U_0^m) \\ &\quad + \varepsilon \mathbb{D} \begin{pmatrix} U_1^m \sum_{n=1}^k n b_n (U_0^m)^{n-1} \\ 0 \end{pmatrix} + o(\varepsilon). \end{aligned} \quad (3.5)$$

It is worth noting already at this stage that if the matrix $\mathbb{D}$ is diagonal, then (3.5) implies

$$\nabla \cdot \mathbb{D} \mathbf{G}(U) = \nabla_{\mathbf{x}} \cdot \mathbb{D} \mathbf{G}(U_0^m) + o(1). \quad (3.6)$$

We consider now the equation inside the membrane region Ω_m at the lowest order ε^{-2} and we find

$$\nabla_{Y_2} \cdot \mathbb{D} \nabla_{Y_2} U_0^m = 0. \quad (3.7)$$

By expanding $\mathbf{J}$ and by collecting the terms with the lowest ε order, we get the Neumann boundary condition

$$(-\mathbb{D} \nabla_{Y_2} U_0^m) \cdot \mathbf{n} = 0 \quad \text{on } (\Gamma_o \cup \Gamma_h) \cap \Omega_m, \quad (3.8)$$

the transmission boundary conditions:

$$\begin{aligned} U_0^m(\mathbf{X}, T) &= U_0^l(\mathbf{X}, T) \quad \text{on } \Gamma_l \cap \Gamma_m \quad \text{and} \\ U_0^m(\mathbf{X}, T) &= U_0^r(\mathbf{X}, T) \quad \text{on } \Gamma_r \cap \Gamma_m, \end{aligned}$$

as well as

$$\begin{aligned} &-\mathbb{D}(\nabla U^l + \mathbf{G}(U^l)) \cdot \mathbf{n} \\ &= (-\mathbb{D}(\nabla U_0^m + \mathbf{G}(U_0^m))) \cdot \mathbf{n} \quad \text{at } \Gamma_l \cap \Gamma_m, \end{aligned} \quad (3.9)$$

$$\begin{aligned} &-\mathbb{D}(\nabla U^r + \mathbf{G}(U^r)) \cdot \mathbf{n} \\ &= (-\mathbb{D}(\nabla U_0^m + \mathbf{G}(U_0^m))) \cdot \mathbf{n} \quad \text{at } \Gamma_r \cap \Gamma_m, \end{aligned} \quad (3.10)$$

for any $T \geq 0$, where we used that $\mathbf{n}$ is horizontal.

We recall that U_0^m is Y_2 -periodic. Based on (3.7) and (3.8), we claim that U_0^m is independent of Y_2 , i.e. $U_0^m = U_0^m(\mathbf{X}, T)$.

At the order ε^{-1} , using that U_0^m does not depend on Y_2 , we get the equation

$$\nabla_{Y_2} \cdot \mathbb{D} \nabla_{Y_2} U_1^m = -\nabla_{Y_2} \cdot \mathbb{D} \nabla_{\mathbf{x}} U_0^m \quad (3.11)$$

with Neumann boundary condition (2.12) at order ε^0 in (3.3) and (3.5)

$$-\mathbb{D} \nabla_{Y_2} U_1^m \cdot \mathbf{n} = \mathbb{D} \nabla_{\mathbf{x}} U_0^m \cdot \mathbf{n} + \mathbb{D} \mathbf{G}(U_0^m) \cdot \mathbf{n} \quad \text{on } \Gamma_h \cup \Gamma_o. \quad (3.12)$$

Recall that U_1^m is Y_2 -periodic.

The structure of (3.11) allows us to assume that

$$U_1^m = \mathbf{W}(Y_2) \cdot [\nabla_{\mathbf{X}} U_0^m + \mathbf{G}(U_0^m)] + h, \quad (3.13)$$

where $\mathbf{W}(Y_2)$ is a vector with Y_2 -periodic components and $h = h(X)$ is some arbitrarily chosen function independent on Y_2 that will play no role in further calculations. We will refer to $\mathbf{W}(Y_2)$ as *cell function*. Substituting now the expression (3.13) in (3.11), we get

$$\begin{aligned} \nabla_{Y_2} \cdot \mathbb{D} \nabla_{Y_2} \mathbf{W}(Y_2) \cdot [\nabla_{\mathbf{X}} U_0^m + \mathbf{G}(U_0^m)] \\ = -\nabla_{Y_2} \cdot \mathbb{D} \cdot [\nabla_{\mathbf{X}} U_0^m + \mathbf{G}(U_0^m)], \end{aligned}$$

while substituting the same expression now in (3.12) leads to

$$\begin{aligned} -\mathbb{D} \nabla_{Y_2} \mathbf{W}(Y_2) \cdot [\nabla_{\mathbf{X}} U_0^m + \mathbf{G}(U_0^m)] \\ \cdot \mathbf{n} = \mathbb{D} [\nabla_{\mathbf{X}} U_0^m + \mathbf{G}(U_0^m)] \cdot \mathbf{n}. \end{aligned}$$

Now, we can introduce the following *cell problems*: find the Y_2 -periodic cell function $\mathbf{W} = (w_1, w_2)^T$ satisfying the following elliptic partial differential equations:

$$\nabla_{Y_2} \cdot (\mathbb{D} \nabla_{Y_2} w_j(Y_2)) = -\nabla_{Y_2} \cdot \mathbb{D} \mathbf{e}_j, \quad (3.14)$$

$$\nabla_{Y_2} w_j \cdot \mathbf{n} = 0 \text{ on } \Gamma_h \cup \Gamma_o, \quad (3.15)$$

for $j = 1, 2$. In (3.14), we use the coordinate vectors $\mathbf{e}_1 = (1 \ 0)^T$ and $\mathbf{e}_2 = (0 \ 1)^T$. When $\mathbb{D}$ is diagonal, we point out that (3.14) can be written explicitly as $\frac{\partial}{\partial Y_2} \left(D_{22} \frac{\partial w_1}{\partial Y_2} \right) = 0$ and $\frac{\partial}{\partial Y_2} \left[D_{22} \left(1 + \frac{\partial w_1}{\partial Y_2} \right) \right] = 0$, which in the absence of the internal heterogeneity can be solved analytically; see Proposition 3.3, p. 13 in [18].

For U_2^m , taking into account (3.2), (3.4), and (3.6), at the order ε^0 , we have the following equation

$$\begin{aligned} \frac{\partial U_0^m}{\partial T} - [\nabla_{\mathbf{X}} \cdot \mathbb{D} \nabla_{\mathbf{X}} U_0^m + \nabla_{\mathbf{X}} \cdot \mathbb{D} \nabla_{Y_2} U_1^m \\ + \nabla_{Y_2} \cdot \mathbb{D} \nabla_{\mathbf{X}} U_1^m + \nabla_{Y_2} \cdot \mathbb{D} \nabla_{Y_2} U_2^m \\ + \nabla_{\mathbf{X}} \cdot \mathbb{D} \mathbf{G}(U_0^m)] = F \end{aligned} \quad (3.16)$$

with boundary condition (2.12) across $(\Gamma_o \cup \Gamma_h) \cap \Omega_m$

$$\begin{aligned} -\mathbb{D} \left[\nabla_{\mathbf{X}} U_1^m + \nabla_{Y_2} U_2^m + \left(U_1^m \sum_{n=0}^k b_n n (U_0^m)^{n-1} \right) \right] \\ \cdot \mathbf{n} = 0, \end{aligned} \quad (3.17)$$

obtained by using the order ε of the expansions (3.3) and (3.5).

To derive the final form of the upscaled equations we use the Fredholm alternative argument as it applies to linear elliptic partial differential equations with periodic boundary conditions (see e.g. Lemma 1.3.21 in [1]). This boils down to integrating (3.16) with respect to Y_2 over a cell, say over the set $Z = [0, 2\eta/\ell]$. Using the divergence theorem with respect to the variable Y_2 and (3.13), we have

$$\begin{aligned} \int_Z \frac{\partial U_0^m}{\partial T} dY_2 - \nabla_{\mathbf{X}} \cdot \int_Z \mathbb{D} \nabla_{\mathbf{X}} U_0^m dY_2 \\ - \nabla_{\mathbf{X}} \cdot \int_Z \mathbb{D} \nabla_{Y_2} [\mathbf{W}(Y_2) \cdot (\nabla_{\mathbf{X}} U_0^m + \mathbf{G}(U_0^m))] dY_2 \\ - \nabla_{\mathbf{X}} \cdot \int_Z \mathbb{D} \mathbf{G}(U_0^m) dY_2 - \int_Z \nabla_{Y_2} \cdot \mathbb{D} \nabla_{\mathbf{X}} U_1^m dY_2 \\ = \int_Z F dY_2 + \int_{\partial Z} \mathbb{D} \nabla_{Y_2} U_2^m \cdot \mathbf{n} d\sigma. \end{aligned}$$

Notice that the last term in the above equation is nothing but the differences between the values of the function $\mathbb{D} \nabla_{Y_2} U_2^m \cdot \mathbf{n}$ evaluated at the extremes $2\eta/\ell$ and 0 of the integration interval. In that term $\mathbf{n}$ is the external normal to the horizontal parts of the boundary of the elementary cell, in particular it is a vertical unit vector. Hence, by using (3.17), we obtain

$$\begin{aligned} \int_Z \frac{\partial U_0^m}{\partial T} dY_2 - \nabla_{\mathbf{X}} \cdot \int_Z \mathbb{D} \nabla_{\mathbf{X}} U_0^m dY_2 \\ - \nabla_{\mathbf{X}} \cdot \int_Z \mathbb{D} \nabla_{Y_2} [\mathbf{W}(Y_2) \cdot (\nabla_{\mathbf{X}} U_0^m + \mathbf{G}(U_0^m))] dY_2 \\ - \nabla_{\mathbf{X}} \cdot \int_Z \mathbb{D} \mathbf{G}(U_0^m) dY_2 - \int_Z \nabla_{Y_2} \cdot \mathbb{D} \nabla_{\mathbf{X}} U_1^m dY_2 \\ = \int_Z F dY_2 \\ - \int_{\partial Z} \mathbb{D} \nabla_{\mathbf{X}} U_1^m \cdot \mathbf{n} d\sigma. \end{aligned}$$

By the divergence theorem, the last term of the left-hand side cancels the last term of the right-hand side. Thus, we get

$$\begin{aligned} & \int_Z \frac{\partial U_0^m}{\partial T} dY_2 - \nabla_{\mathbf{x}} \cdot \int_Z \mathbb{D}[\nabla_{\mathbf{x}} U_0^m + \mathbf{G}(U_0^m)] dY_2 \\ & - \nabla_{\mathbf{x}} \cdot \int_Z \mathbb{D} \nabla_{Y_2} [\mathbf{W}(Y_2) \cdot (\nabla_{\mathbf{x}} U_0^m + \mathbf{G}(U_0^m))] dY_2 \\ & = \int_Z F dY_2. \end{aligned}$$

Recalling that U_0^m does not depend on Y_2 , we finally get

$$\begin{aligned} & \frac{\partial U_0^m}{\partial T} - \nabla_{\mathbf{x}} \cdot \left[\frac{1}{|Z|} \int_Z \mathbb{D} \left(\mathbb{I} + \begin{pmatrix} 0 & 0 \\ \frac{\partial w_1}{\partial Y_2} & \frac{\partial w_2}{\partial Y_2} \end{pmatrix} \right) dY_2 \right] \\ & (\nabla_{\mathbf{x}} U_0^m + \mathbf{G}(U_0^m)) = \frac{1}{|Z|} \int_Z F dY_2. \end{aligned} \quad (3.18)$$

We refer to the coefficient

$$\mathbb{D}^\star := \frac{1}{|Z|} \int_Z \mathbb{D} \left(\mathbb{I} + \begin{pmatrix} 0 & 0 \\ \frac{\partial w_1}{\partial Y_2} & \frac{\partial w_2}{\partial Y_2} \end{pmatrix} \right) dY_2 \quad (3.19)$$

as effective transport coefficient.

The upscaled equation (3.18) for the zero term of the expansion has the same structure as the original Eq. (2.7). The source term F on the right-hand side is replaced by its average over the cell on the Y_2 . The diffusion matrix is replaced by its average over the cell on the Y_2 variable weighted by the function

$$\mathbb{I} + \begin{pmatrix} 0 & 0 \\ \frac{\partial w_1}{\partial Y_2} & \frac{\partial w_2}{\partial Y_2} \end{pmatrix},$$

which is referred to as tortuosity tensor in the porous media literature; we refer the reader to the review paper [19] for a discussion done in terms of this tortuosity tensor of the role played by microscopic anisotropies in understanding macroscopically a smoldering combustion scenario.

Summarizing, the upscaled model equation reads: Find $U_0^m(\mathbf{X}, Y_1, T)$ satisfying

$$\begin{aligned} & \frac{\partial U_0^m}{\partial T} - \nabla_{\mathbf{x}} \cdot \left[\frac{1}{|Z|} \int_Z \mathbb{D} \left(\mathbb{I} + \begin{pmatrix} 0 & 0 \\ \frac{\partial w_1}{\partial Y_2} & \frac{\partial w_2}{\partial Y_2} \end{pmatrix} \right) dY_2 \right] \\ & (\nabla_{\mathbf{x}} U_0^m + \mathbf{G}(U_0^m)) = \frac{1}{|Z|} \int_Z F dY_2. \end{aligned} \quad (3.20)$$

$$\begin{aligned} U_0^m &= U^l, -\mathbb{D}(\nabla U^l + \mathbf{G}(U^l)) \cdot \mathbf{n} = -\mathbb{D}(\nabla_{\mathbf{x}} U_0^m \\ & + \mathbf{G}(U_0^m)) \cdot \mathbf{n} \text{ at } \Gamma_l \cap \Gamma_m, \end{aligned} \quad (3.21)$$

$$\begin{aligned} U_0^m &= U^r, -\mathbb{D}(\nabla U^r + \mathbf{G}(U^r)) \cdot \mathbf{n} = -\mathbb{D}(\nabla_{\mathbf{x}} U_0^m \\ & + \mathbf{G}(U_0^m)) \cdot \mathbf{n} \text{ at } \Gamma_r \cap \Gamma_m, \end{aligned} \quad (3.22)$$

together with the initial condition

$$U_0^m(T=0) = v^m(\mathbf{X}, Y_1). \quad (3.23)$$

Using the transmission conditions at Γ_l and Γ_r , the information in Ω_m is now linked (in a well-posed way) with equation (2.7) posed in Ω_l and Ω_r , respectively.

4 Derivation of the infinitely-thin upscaled strip model

We look for the upscaled model in the limit in which both the width and the height of the cells tends to zero and the number of cells is increased so that the total height of the cells equals that of the whole strip. To handle such a situation, the equation inside the strip must be replaced by a matching condition between the solutions of the problems in the left and the right regions Ω_l and Ω_r . In this case, the upscaling procedure needs to be combined with a singular perturbation ansatz; see [17] for a remotely related case. We stress that within this new framework the scaling in terms of the small parameter ε is quite different than what was achieved in Sect. 3. A quick comparison between (4.3) and (2.7) indicates differences in size of order of $\mathcal{O}(1/\varepsilon)$ in the characteristic time scale of the process and in the forcing (production) term inside the membrane as well as differently scaled fluxes; compare (4.4) and (2.8).

4.1 Two-scale layer expansions

We consider the geometry introduced in Sect. 2.1 and assume $w = 2\eta$, so that the strip is the region $[-2\eta/\ell, 2\eta/\ell] \times [0, 2h/\ell]$ (see Fig. 2). Recalling the relation $\varepsilon = 2\eta/\ell$, in the homogenization limit $\varepsilon \rightarrow 0$ the strip shrinks to a sharp separating surface. The equations in Ω_l and Ω_r are as in Sect. 2.1, see Eqs. (2.7)–(2.9). More precisely, we have

$$\frac{\partial U^i}{\partial T} + \nabla \cdot \mathbf{J}^i = F^i \text{ in } \Omega_i \text{ with } \mathbf{J}^i = -\mathbb{D}^i(\nabla U^i + \mathbf{G}(U^i)) \text{ for } i = l, r, \quad (4.1)$$

where $F^l : [-1, -\varepsilon] \rightarrow \mathbb{R}$, $F^r : [\varepsilon, +1] \rightarrow \mathbb{R}$, $\mathbb{D}^i$ a general real 2×2 matrix, and

$$\mathbf{G}(U) = \begin{pmatrix} g(U) \\ 0 \end{pmatrix} \quad (4.2)$$

with $g(U) = \sum_{n=1}^k b_n U^n$ where b_n are real coefficients. In the strip $\Omega_m \setminus \Omega_o$, we consider the equation

$$\frac{1}{\varepsilon} \frac{\partial U^m}{\partial T} + \nabla \cdot \mathbf{J}^m = \frac{1}{\varepsilon} F^m\left(\frac{X_1}{\varepsilon}, X_2\right) \quad (4.3)$$

with $F^m : [-1, +1] \times [0, 2h/\ell] \rightarrow \mathbb{R}$ and the flux $\mathbf{J}^m$ defined as

$$\mathbf{J}^m = -\mathbb{D}^m\left(\frac{X_1}{\varepsilon}, X_2\right)(\varepsilon \nabla U^m + \mathbf{G}(U^m)), \quad (4.4)$$

where $\mathbb{D}^m$ is a 2×2 square matrix

$$\mathbb{D}^m = \begin{pmatrix} \mathbb{D}_{11}^m & \mathbb{D}_{12}^m \\ \mathbb{D}_{21}^m & \mathbb{D}_{22}^m \end{pmatrix}.$$

These equations are endowed with the Dirichlet boundary conditions

$$\begin{aligned} U^l(\mathbf{X}, T) &= U_l \text{ on } \Gamma_v \cap \Gamma_l \text{ and} \\ U^r(\mathbf{X}, T) &= U_r \text{ on } \Gamma_v \cap \Gamma_r \end{aligned} \quad (4.5)$$

for any $T \geq 0$, the initial condition

$$\begin{aligned} U^i(\mathbf{X}, 0) &= V^i(\mathbf{X}) \text{ in } \Omega_i \text{ for } i = l, r \text{ and} \\ U^m(\mathbf{X}, 0) &= V^m(\mathbf{X}) \text{ in } \Omega_m \setminus \Omega_o, \end{aligned} \quad (4.6)$$

the Neumann boundary conditions

$$\begin{aligned} \mathbf{J}^i(\mathbf{X}, T) \cdot \mathbf{n} &= 0 \text{ on } \Gamma_h \cap \Omega_i \text{ for } i = l, r \text{ and} \\ \mathbf{J}^m(\mathbf{X}, T) \cdot \mathbf{n} &= 0 \text{ on } (\Gamma_h \cap \Omega_m) \cup \Gamma_o \end{aligned} \quad (4.7)$$

for any $T \geq 0$, the continuity (linear transmission) conditions

$$\begin{aligned} U^i(\mathbf{X}, T) &= U^m(\mathbf{X}, T) \text{ and } \mathbf{J}^i(\mathbf{X}, T) \cdot \mathbf{n} \\ &= \mathbf{J}^m(\mathbf{X}, T) \cdot \mathbf{n} \text{ on } \Gamma_i \cap \Gamma_m \text{ for } i = l, r \end{aligned} \quad (4.8)$$

for any $T \geq 0$, where in the last equation $\mathbf{n}$ is the horizontal unit vector pointing to the left on Γ_l and to the right on Γ_r .

Inside the membrane we use the same two-scale expansion as the one introduced in the Sect. 3, namely we take

$$U^m(\mathbf{X}, T) = \sum_{n=0}^{\infty} \varepsilon^n U_n^m(\mathbf{X}, y_2, T) \text{ in } \Omega_m, \quad (4.9)$$

where $y_2 = X_2/\varepsilon$ and the functions U_n^i , with $i = l, m, r$, are y_2 -periodic functions. Since the domain where the two-scale expansion is defined vanishes as $\varepsilon \rightarrow 0$, we refer to (4.9) as two-scale layer expansion. We claim that this expansion formally discovers the limit point of the two-scale convergence for thin homogeneous layers (as presented cf. Definition 4.1 in [27]).

Fig. 2 Schematic representation of the dimensionless model geometry

We define the new variables

$$z_1 = \frac{X_1}{\varepsilon} \quad \text{and} \quad z_2 = X_2, \quad (4.10)$$

and we set

$$v^m(\mathbf{z}, T) = U^m(\varepsilon z_1, z_2, T) \quad (4.11)$$

for the original functions and

$$v_n^m(\mathbf{z}, y_2, T) = U_n^m(\varepsilon z_1, z_2, y_2, T) \quad (4.12)$$

for the perturbative terms $n \geq 0$.

It is immediate to deduce the following differentiation rules with respect to the new variables. We let

$$\begin{aligned} \nabla_{z_1} &= \begin{pmatrix} \frac{\partial}{\partial z_1} \\ 0 \end{pmatrix}, \quad \nabla_{z_2} = \begin{pmatrix} 0 \\ \frac{\partial}{\partial z_2} \end{pmatrix}, \quad \text{and} \\ \nabla_{y_2} &= \begin{pmatrix} 0 \\ \frac{\partial}{\partial y_2} \end{pmatrix} \end{aligned} \quad (4.13)$$

and prove

$$\nabla U_n^m = \frac{1}{\varepsilon} \nabla_{z_1} v_n^m + \nabla_{z_2} v_n^m + \frac{1}{\varepsilon} \nabla_{y_2} v_n^m \quad \text{for } n \geq 0. \quad (4.14)$$

Firstly, we note that the first term ε^0 in the expansion of $\mathbf{J}^m$ is

$$\mathbf{J}^m = -\mathbb{D}^m \nabla_{z_1} v_0^m - \mathbb{D}^m \nabla_{y_2} v_0^m - \begin{pmatrix} D_{11}^m g(v_0^m) \\ D_{21}^m g(v_0^m) \end{pmatrix} + o(1). \quad (4.15)$$

Hence, expanding the equation (4.3) in the region $\Omega_m \setminus \Omega_0$ and taking into account the order ε^{-1} we get the following equation

$$\begin{aligned} \frac{\partial v_0^m}{\partial T} - [\nabla_{z_1} \cdot \mathbb{D}^m \nabla_{z_1} v_0^m + \nabla_{y_2} \cdot \mathbb{D}^m \nabla_{y_2} v_0^m \\ + \nabla_{z_1} \cdot \mathbb{D}^m \nabla_{y_2} v_0^m + \nabla_{y_2} \cdot \mathbb{D}^m \nabla_{z_1} v_0^m] \\ - \frac{\partial}{\partial z_1} (\mathbb{D}_{11}^m g(v_0^m)) - \frac{\partial}{\partial y_2} (\mathbb{D}_{21}^m g(v_0^m)) = F^m. \end{aligned} \quad (4.16)$$

Integrating (4.16) with respect to the variable z_1 (or invoking once more the Fredholm alternative argument), it turns out that the limit function v_0^m will have to solve the equation

$$\frac{\partial v_0^m}{\partial T} - \nabla_{y_2} \cdot \mathbb{D}^m [\nabla_{y_2} v_0^m + \mathbf{G}(v_0^m)] = F^m \quad (4.17)$$

for any X_2 . The limit function v_0^m is periodic in y_2 and has to satisfy the conditions

$$\begin{aligned} v_0^m(z_2, y_2, T) &= U^i(0, z_2, T) \quad \text{for } i = l, r \quad \text{and} \\ v_0^m(z_2, y_2, 0) &= V^m. \end{aligned} \quad (4.18)$$

In the limit $\varepsilon \rightarrow 0$ the functions U^i , with $i = l, r$ will solve the equations (4.1) with the conditions (4.5), (4.6) (first equation), and (4.7) (first equation). Moreover, the matching conditions (4.8) will provide as with a jump condition on the flux associated to the limit solutions U^i . Indeed, we first note that at order ε^0 , using (4.15), the matching condition (4.8) (second equation) can be written as

$$\begin{aligned} -\mathbb{D}^l (\nabla U^l + \mathbf{G}(U^l)) \cdot \mathbf{n} \\ = \left(D_{11}^m \frac{\partial v_0^m}{\partial z_1} + D_{12}^m \frac{\partial v_0^m}{\partial y_2} + D_{11}^m g(v_0^m) \right) \cdot \mathbf{n} \end{aligned} \quad (4.19)$$

and

$$\begin{aligned} -\mathbb{D}^r (\nabla U^r + \mathbf{G}(U^r)) \cdot \mathbf{n} \\ = - \left(D_{11}^m \frac{\partial v_0^m}{\partial z_1} - D_{12}^m \frac{\partial v_0^m}{\partial y_2} - D_{11}^m g(v_0^m) \right) \cdot \mathbf{n}. \end{aligned} \quad (4.20)$$

The last two interface conditions act on the flat solid line, say Γ , where the strip Ω reduces as $\varepsilon \rightarrow 0$. It is worth noting that equations (4.19) and (4.20) complete the system of upscaled equations; compare e.g. how Corollary 7.1 in [27] proves a similar statement. These conditions emphasize that the macroscopic flux is obtained by averaging the corresponding microscopic flux.

4.2 Summary of the upscaled equations

The resulting upscaled problem corresponding to this asymptotic regime is: Find the triplet (U^l, v_0^m, U^r) satisfying the following set of equations:

$$\frac{\partial U^i}{\partial T} + \nabla \cdot [-\mathbb{D}^i(\nabla U^i + \mathbf{G}(U^i))] = F^i \quad \text{in } \Omega_i, i = l, r, \quad (4.21)$$

$$\frac{\partial v_0^m}{\partial T} - \nabla_{y_2} \cdot \mathbb{D}^m[\nabla_{y_2} v_0^m + \mathbf{G}(v_0^m)] = F^m \quad \text{in } \Gamma \times (0, 2h/\ell) \quad (4.22)$$

$$v_0^m \text{ is periodic in } y_2 \quad (4.23)$$

$$v_0^m(z_2, y_2, T) = U^i(0, z_2, T) \text{ for } i = l, r \text{ and } v_0^m(z_2, y_2, 0) = v^m, \quad (4.24)$$

$$\begin{aligned} & -\mathbb{D}^l(\nabla U^l + \mathbf{G}(U^l)) \cdot \mathbf{n} \\ &= \left(D_{11}^m \frac{\partial v_0^m}{\partial z_1} + D_{12}^m \frac{\partial v_0^m}{\partial y_2} + D_{11}^m g(v_0^m) \right) \cdot \mathbf{n} \text{ at } \Gamma, \end{aligned} \quad (4.25)$$

$$\begin{aligned} & -\mathbb{D}^r(\nabla U^r + \mathbf{G}(U^r)) \cdot \mathbf{n} \\ &= \left(-D_{11}^m \frac{\partial v_0^m}{\partial z_1} - D_{12}^m \frac{\partial v_0^m}{\partial y_2} - D_{11}^m g(v_0^m) \right) \cdot \mathbf{n} \text{ at } \Gamma, \end{aligned} \quad (4.26)$$

$$\begin{aligned} U^l(\mathbf{X}, T) &= U_l \quad \text{on } \Gamma_v \cap \Gamma_l \quad \text{and} \quad U^r(\mathbf{X}, T) \\ &= U_r \quad \text{on } \Gamma_v \cap \Gamma_r, \end{aligned} \quad (4.27)$$

$$\mathbf{J}^i(\mathbf{X}, T) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_h \cap \Omega_i \quad \text{for } i = l, r, \quad (4.28)$$

$$U^i(\mathbf{X}, 0) = V^i \quad \text{in } \Omega_i \quad \text{for } i = l, r. \quad (4.29)$$

4.3 Further remarks

In what follows, we deduce alternative transmission relations across the membrane, recovering expected structures as if one would have applied two-scale layer convergence arguments as indicated in [27]. Integrating the equation (4.16) with respect to z_1 we get

$$\begin{aligned} & \int_{-1}^1 \frac{\partial v_0^m}{\partial T} dz_1 - \left[D_{11}^m \frac{\partial v_0^m}{\partial z_1} \right]_{z_1=-1}^{z_1=+1} \\ & - \nabla_{y_2} \cdot \int_{-1}^1 \mathbb{D}^m \nabla_{y_2} v_0^m dz_1 - \left[D_{12}^m \frac{\partial v_0^m}{\partial y_2} \right]_{z_1=-1}^{z_1=+1} \\ & - \nabla_{y_2} \cdot \int_{-1}^1 \mathbb{D}^m \nabla_{z_1} v_0^m dz_1 - \left[D_{11}^m g(v_0^m) \right]_{z_1=-1}^{z_1=+1} \\ & - \int_{-1}^1 \frac{\partial}{\partial y_2} (D_{21}^m g(v_0^m)) dz_1 = \int_{-1}^1 F^m dz_1. \end{aligned}$$

By (4.19) and (4.20) we get

$$\begin{aligned} & \int_{-1}^1 \frac{\partial v_0^m}{\partial T} dz_1 - \nabla_{y_2} \cdot \int_{-1}^1 \mathbb{D}^m \nabla_{y_2} v_0^m dz_1 \\ & - \nabla_{y_2} \cdot \int_{-1}^1 \mathbb{D}^m \nabla_{z_1} v_0^m dz_1 \\ & - \int_{-1}^1 \frac{\partial}{\partial y_2} (D_{21}^m g(v_0^m)) dz_1 - \mathbb{D}^r \nabla U^r \cdot \mathbf{n}|_{z_1=+1} \\ & - \mathbb{D}^l \nabla U^l \cdot \mathbf{n}|_{z_1=-1} = \int_{-1}^1 F^m dz_1. \end{aligned}$$

Now we integrate with respect to y_2 and we obtain

$$\begin{aligned} & \int_0^1 \int_{-1}^1 \frac{\partial v_0^m}{\partial T} dy_2 dz_1 - \int_{-1}^1 \left[D_{22}^m \frac{\partial v_0^m}{\partial y_2} \right]_{y_2=0}^{y_2=1} dz_1 \\ & - \int_{-1}^1 \left[D_{21}^m \frac{\partial v_0^m}{\partial z_1} \right]_{y_2=0}^{y_2=1} dz_1 \\ & - \int_{-1}^1 [D_{21}^m g(v_0^m)]_{y_2=0}^{y_2=1} dz_1 \\ & - \int_0^1 \int_{-1}^1 \frac{\partial}{\partial y_2} (D_{21}^m g(v_0^m)) dy_2 dz_1 \\ & - \int_0^1 \left[\mathbb{D}^r \nabla U^r \cdot \mathbf{n}|_{z_1=+1} + \mathbb{D}^l \nabla U^l \cdot \mathbf{n}|_{z_1=-1} \right] dy_2 \\ & = \int_0^1 \int_{-1}^1 F^m dy_2 dz_1. \end{aligned}$$

Now, we note that the second equation in (4.7) yields

$$D_{21}^m \frac{\partial v_0^m}{\partial z_1} + D_{22}^m \frac{\partial v_0^m}{\partial y_2} + D_{21}^m g(v_0^m) = 0$$

on $\Gamma_h \cap \Omega_m$. Recalling that $\mathbb{D}^m$ and v_0^m are y_2 -periodic functions, we find the aforementioned jump condition

$$\begin{aligned} & \int_0^1 \left[\mathbb{D}^r \nabla U^r \cdot \mathbf{n} \Big|_{z_1=+1} + \mathbb{D}^l \nabla U^l \cdot \mathbf{n} \Big|_{z_1=-1} \right] dy_2 \\ &= \int_0^1 \int_{-1}^1 \left[\frac{\partial v_0^m}{\partial T} - \frac{\partial}{\partial y_2} (D_{21}^m g(v_0^m)) - F^m \right] dy_2 dz_1. \end{aligned}$$

The relations (4.19) and (4.20) provide direct access to the jump in the flux of matter when crossing the membrane. Interestingly from a modeling point of view, we can also obtain a quantitative description of the jump in concentrations across the reduced strip, say Γ ; the situation is somehow similar to the case described by Theorem 2.4 in [27];

5 Numerical illustration of the finite-thickness upscaled strip

We illustrate numerically the behavior of the finite-thickness upscaled strip derived in Sect. 3. To fix a simulation scenario, we imagine the diffusion and drift of a gaseous species (e.g. CO₂ or O₂) supposed to cross a heterogeneous strip with finite thickness. Experimental values of the diffusion coefficient of gaseous CO₂ in cells have been estimated to be around $d = 3.5 \text{ cm}^2 \text{ s}^{-1}$ (cf. [24]). We choose values for the diffusion coefficients within this range, viz. take $d_1 = 10 \text{ cm}^2 \text{ s}^{-1}$ and $d_2 = 1 \text{ cm}^2 \text{ s}^{-1}$, letting the horizontal diffusion dominate the process. Initially, we assume that there is no mass present in the system, i.e. $u(t=0) = 0$. We fix the inflow of the left boundary by choosing $u_r = 5.8 \times 10^{-5} \text{ g cm}^{-3}$ according to [24], $u_l = 0 \text{ g cm}^{-3}$, $u_{\text{ref}} = 1 \text{ g cm}^{-3}$. Concerning the strip geometry, we set: $l = 1 \text{ cm}$, $h = 0.4 \text{ cm}$, $w = 0.25 \text{ cm}$.

Case (i): Full diffusion/dispersion matrix and nonlinear horizontal drift. We choose the non-linear transport term from (1.1) with $b = 2 \text{ g cm}^2 \text{ s}^{-1}$. As D_{22} is an essentially bounded function on the set $\Omega_m \setminus \Omega_o$, i.e. it lies in $L^\infty(\Omega_m \setminus \Omega_o)$, solving the parameter-dependent ODEs

$$\frac{\partial}{\partial Y_2} \left(D_{22}(Y_1, Y_2) \frac{\partial w_1}{\partial Y_2} \right) = 0 \quad (5.1)$$

and

$$\frac{\partial}{\partial Y_2} \left[D_{22}(Y_1, Y_2) \left(1 + \frac{\partial w_2}{\partial Y_2} \right) \right] = 0, \quad (5.2)$$

is rather delicate since it involves distributions localized along $\partial\Omega_o$. To handle this issue, one needs a convenient regularization of the “contrast jump”. It is worth also noting that, based on (5.1)–(5.2), the coefficient D_{11} plays no role in the construction of the cell functions. Instead of smoothing the contrast, we suggest the following regularization: Take $\delta = \mathcal{O}(\eta)$. Find (w_1, w_2) such that

$$\begin{aligned} & \delta \frac{\partial}{\partial Y_1} \left(D_{11}(Y_1, Y_2) \frac{\partial}{\partial Y_1} w_1 \right) + \frac{\partial}{\partial Y_2} \left(D_{22}(Y_1, Y_2) \frac{\partial}{\partial Y_2} w_1 \right) \\ &= -\sqrt{\delta} \frac{\partial}{\partial Y_1} D_{11}(Y_1, Y_2), \end{aligned} \quad (5.3)$$

$$\begin{aligned} & \delta \frac{\partial}{\partial Y_1} \left(D_{11}(Y_1, Y_2) \frac{\partial}{\partial Y_1} w_2 \right) + \frac{\partial}{\partial Y_2} \left(D_{22}(Y_1, Y_2) \frac{\partial}{\partial Y_2} w_2 \right) \\ &= -\frac{\partial}{\partial Y_2} D_{22}(Y_1, Y_2). \end{aligned} \quad (5.4)$$

These formulations are obtained based on (3.14) by

interpreting ∇_{Y_2} as $\left(\sqrt{\delta} \frac{\partial}{\partial y_1}, \frac{\partial}{\partial y_2} \right)$ instead of

$\nabla_{Y_2} = \left(\frac{\partial}{\partial y_1}, \frac{\partial}{\partial y_2} \right)$. The boundary conditions needed to

complete the regularized problem are described in (3.15). Such a procedure appears to work well for symmetric obstacles. Note that both problems (5.3) and (5.4) are singular perturbations of linear elliptic PDEs. Under suitable assumptions, the convergence $\delta \rightarrow 0$ can be made rigorous in terms of weak solutions via a weak convergence procedure using symmetry restrictions and dimension reduction arguments.

To solve numerically the cell problems (5.3) and (5.4) (with corresponding boundary conditions), we use a FEM scheme implemented in FEniCS³. The cell problem and the macroscopic equations are solved on a triangular mesh with quadratic basis functions. We illustrate the behavior of the cell functions in Fig. 3.

³ This is an open source platform FEniCS [2]; see <https://fenicsproject.org>.

The explicit appearance of the variable Y_1 in (3.20)–(3.23) needs to be removed by integrating the system of equations with respect to the Y_1 variable. Using the transmission conditions at Γ_l and Γ_r , the information in Ω_m is now linked (in a well-posed way) with equation (2.7) posed in Ω_l and Ω_r , respectively. The numerical approximations of the cell functions can now be used to compute the effective diffusion tensor

$$\mathbb{D}^\star := \begin{pmatrix} D_{11}^\star & D_{12}^\star \\ D_{21}^\star & D_{22}^\star \end{pmatrix} = \mathbb{D} \left(\mathbb{I} + \begin{pmatrix} 0 & 0 \\ \frac{\partial w_1}{\partial Y_2} & \frac{\partial w_2}{\partial Y_2} \end{pmatrix} \right), \quad (5.5)$$

and hence, FEM approximations of the upscaled diffusion–drift equation can be reached. Note that $\mathbb{D}^{-1}\mathbb{D}^\star$ is the so-called tortuosity⁴ tensor for the strip. Typical macroscopic concentration profiles are shown in Fig. 4. For the chosen parameter regime, one can see that the strip is usually permeable. Interestingly, the efficiency of the transport through the strip reduces when increasing the strength of the drift b . Figure 4 (right) is obtained via turning the diagonal matrix $\mathbb{D}^\star$ into a full matrix by adding diffusion correlations. The off-diagonal entries are small $D_{12}^\star = -0.05 \text{ cm}^2 \text{ s}^{-1}$ and $D_{21}^\star = +0.05 \text{ cm}^2 \text{ s}^{-1}$. Combined with a polynomial drift (of type $bu(1-u)$ with $b = 54 \text{ g cm}^2 \text{ s}^{-1}$) this causes some sort of concentration localization that we refer here as concentration trapping. In such case, the strip might play the role of a barrier, especially if the geometric setting would be extended to account for a multilayer structure as it is the case of materials like paperboard.

Although the finite-thickness strip scaling is rather standard (in the sense that the structure of the upscaled coefficients was foreseeable), Fig. 5(left) points out an outstanding opportunity: The numerical example shows that changing the aspect ratio of the rectangular

obstacle can be used as tool to optimize the strip performance (in the spirit of shape optimization). This leads to the following key question: Is such non-monotonic behavior specific to the choice of rectangles as microstructures, or is it actually generic?

To answer this question, intensive simulations involving a large variety of shapes of microstructures need to be performed. Particularly, the role played by the asymmetry of the microstructure is one target of investigation. We expect that if the chosen microstructure has asymmetries, then δ is not a parameter anymore, but rather an internal length scale that is linked to the asymmetry of the microstructure. More insight based on numerical simulations is needed to clarify the situation. Such simulations are typically quite involved as they are expected to capture simultaneously effects at two distinct spatial scales. Furthermore, the possibility of concentration trapping needs to be studied by, for instance, carefully considering the effect of the curvature of the microboundaries on the macroscopic outflux. We will address this issue somewhere else. At this moment, relying on the numerical stability with respect to changes in η shown in Fig. 5(right), we only speculate that the answer to the question is affirmative. If this were true, then one could start optimizing filtration processes by searching for best-suitable microstructure shapes. This would be a useful tool for a number of engineering applications. For what the finite strip scaling is concerned, the optimization problem is straightforward, since it can be linked exclusively to the structure of the cell problem. For the second scaling, i.e. for the infinitely-thin upscaled strip model, the optimization problem is not easily accessible. Here, any route towards optimizing filtration needs to take into account the structure of the limit two-scale model with nonlinear transmission condition [cf. (4.21)–(4.29)]. Hence, a significant computational power is needed for each optimization task.

Case (ii): Diagonal diffusion matrix and oblique nonlinear drift.

In this section, we consider our starting problem endowed now with a diagonal diffusion tensor as well as with an oblique drift exhibiting the same type of polynomial nonlinearity as before. The heuristics done in Appendix can be adapted to the case of a full oblique drift. To be specific, we set

⁴ When dealing with mass transfer in porous materials, the tortuosity refers to the ratio of the effective diffusivity in the porous medium to the diffusivity in the free space to (analogous to arc-chord ratio of path) and is usually a tensor, say $\mathbb{T}$; see e.g. [6] and [31] for a discussion of the concept of tortuosity in 3D and 2D, respectively. To be specific, it holds $\mathbb{D}^\star = \mathbb{D}\phi\mathbb{T}$, where ϕ denotes here the volumetric porosity of the porous material. Note that the structure of the tortuosity tensor is usually unknown, excepting for the some of the cases when upscaling procedures are applicable.

Fig. 3 Cell functions profiles: w_1 (left) and w_2 (right) for $\delta = 10^{-1}$

Fig. 4 Typical macroscopic diffusion profiles. Left: A moderate diffusion regime; Right: Increased barrier regime exhibiting a nearly empty membrane. Interestingly, the membrane starts to behave like a barrier only in the high drift regime (i.e. for large b)

Fig. 5 Non-monotonicity of D_{22}^* with respect to δ , as arising in (5.3)–(5.4). Stability of D_{22}^* with respect to the height of the periodic cell η

$$D_{12} = D_{21} = 0, \text{ namely, } \mathbb{D} = \begin{pmatrix} D_{11} & 0 \\ 0 & D_{22} \end{pmatrix} \text{ and}$$

$$\mathbf{G}(U) = \begin{pmatrix} g(U) \\ \alpha g(U) \end{pmatrix},$$

with $\alpha > 0$ a dimensionless parameter.

In this context, we are using the parameter α to emphasize in our simulations the presence of a strong anisotropic drift. As before, due to the presence of the microstructure (“perforation”), $\mathbb{D}$ and $g(U)$ genuinely depend on (Y_1, Y_2) . The two-scale asymptotics homogenization proceeds in a similar way as in Sect. 3. Essentially, we are lead to the cell problem: Find (w_1, w_2) such that

$$\begin{aligned} \frac{\partial}{\partial Y_1} \left(D_{11}(Y_1, Y_2) \frac{\partial}{\partial Y_1} w_1 \right) + \frac{\partial}{\partial Y_2} \left(D_{22}(Y_1, Y_2) \frac{\partial}{\partial Y_2} w_1 \right) \\ = - \frac{\partial}{\partial Y_1} D_{11}(Y_1, Y_2), \end{aligned} \quad (5.6)$$

$$\begin{aligned} \frac{\partial}{\partial Y_1} \left(D_{11}(Y_1, Y_2) \frac{\partial}{\partial Y_1} w_2 \right) + \frac{\partial}{\partial Y_2} \left(D_{22}(Y_1, Y_2) \frac{\partial}{\partial Y_2} w_2 \right) \\ = - \frac{\partial}{\partial Y_2} D_{22}(Y_1, Y_2), \end{aligned} \quad (5.7)$$

which for $\delta = 1$ coincides with the former regularized cell problem (5.3) and (5.4) (with corresponding boundary conditions) and to the same upscaled Eqs. (3.20)–(3.23) (with updated drift nonlinearity).

In Fig. 6 we show snapshots of simulation results obtained with this modified model. If one compares the concentration localization patterns in Figs. 4(-right) and 6, then one sees that they seem to have a different structure. In the first case, the localization tends to take place inside the strip, while in the second case along a part of a Neumann boundary. We believe that as soon as one replaces the Dirichlet conditions of the original system with the more natural Robin boundary conditions, then localization patterns will be more prominent, i.e. the concentration field has “more time” to localize due to the surface resistance effect incorporated in the structure of a Robin boundary condition (say, in the mass transfer Biot number).

6 Discussion

Starting off from a hydrodynamic limit of an asymmetric simple exclusion process (ASEP), we have investigated the problem of diffusion interplaying with a polynomial drift through a composite membrane in two specific scaling regimes. We have obtained upscaled model equations for the finite-length strip as well as for the infinitely-thin strip. We have explicitly seen how the strip’s internal microstructure affects the resulting upscaled equations. The entries of the tensorial effective transport coefficients and our simulations show that these effects are visible at the macroscopic level. From the perspective of materials design, what concerns the penetration of CO_2 through a thin flat composite membrane, there are parameter options that can be used to optimize the membrane performance. A careful exploration of both the parameter space and of possible microstructure shapes can improve effective transport fluxes (e.g. speed-up transport or slow-down transport via enhancing the localization of concentration fields).

To gain additional confidence in the upscaled model equations further investigations are needed. In this spirit, two directions are more prominent:

- (a) The upscaling needs to be made mathematically rigorous. We foresee that the two-scale convergence and the boundary layer techniques employed in [27] can be adapted to our scenario, provided one can handle the passage to the homogenization limit in the non-linear drift terms for both scalings. Additionally, the knowledge of the asymptotic expansions behind the singular perturbation (dimension reduction)–homogenization procedure can potentially be used to derive convergence rates for the involved limiting processes. This would deliver quantitative information on the expected size of fluctuations.
- (b) The stochastic particle simulations from [10] need to be extended from the one-barrier-case to the multiple-thin-barriers case. Then the stationary concentration profiles and the particles residence time can be compared with findings based on the finite element approximations of the upscaled model (both single and two-scale). We have chosen to include solid rectangles as

Fig. 6 Typical macroscopic diffusion profiles. Left: A moderate permeability regime; Right: Increased barrier regime exhibiting a harder-to-cross strip. In both cases, the diffusion

microstructures precisely so that the comparison between the lattice model and the upscaled evolution equations becomes possible. Such comparison would shed light not only on purely transport matters through thin porous layers (like the motion of gaseous O_2 or CO_2 through layered composite membranes mimicking a paper sheet), but would also bring understanding on the effect the environment knowledge has on the stochastic dynamics of active particles (agents). Here, the concentration localization becomes an unwanted pattern if one considers e.g. pedestrian evacuation scenarios.

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Compliance with ethical standards

Conflict of interests The authors declare that they have no conflict of interests.

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tensor is diagonal with an oblique full nonlinear drift just that in the picture exhibiting concentration localization (right) the drift is five times stronger

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Appendix

Simple exclusion random walk

As we mentioned in the Introduction, the Eq. (1.1) can be derived as the hydrodynamic limit for the two-dimensional random walk with simple exclusion and drift along the x_1 -direction. The formal derivation is explained in detail in [9]; for a rigorous result in the symmetric case we refer the interested reader to [22, Chapter 4] from where we borrow the notation. To explain the physical meaning of the different terms appearing in the equation, we summarize in this Appendix the main points of the derivation for the case of a the two-dimensional torus, namely, when periodic boundary conditions are considered.

Let $\mathbb{Z}$ be the set of integers and $\mathbb{Z}^2$ the two-dimensional lattice. Given the positive integer N , we also let $\mathbb{T}_N = \mathbb{Z}/N\mathbb{Z}$ be the N points torus and set $\mathbb{T}_N^2 = (\mathbb{T}_N)^2$. The elements $\mathbf{z} = (z_1, z_2)$ of $\mathbb{T}_N^2$ are called *sites*. The direction associated with the first

(resp. second) coordinate will be called *horizontal* (resp. *vertical*). A configuration is a map $\eta : \mathbb{T}_N^2 \rightarrow \{0, 1\}$ and we say that $\eta(\mathbf{z})$ is the number of particles at site $\mathbf{z}$ in the configuration η ; if $\eta(\mathbf{z}) = 0$ we say that the site $\mathbf{z}$ is *empty*, whereas if $\eta(\mathbf{z}) = 1$ we say that the site $\mathbf{z}$ is *occupied* by a particle. Since a site can be occupied by at most one particle, we say that the system is governed by an *exclusion* (or *hard core repulsion*) rule.

The evolution of the system is a continuous time $\tau \geq 0$ Markov process η_τ defined as follows: particles jump from site $\mathbf{z}$ to site $\mathbf{z} + \mathbf{e}$, with $\mathbf{e} = \pm \mathbf{e}_1, \pm \mathbf{e}_2$, where $\mathbf{e}_1 = (1, 0)$ and $\mathbf{e}_2 = (0, 1)$, with rate $\eta(\mathbf{z})[1 - \eta(\mathbf{z} + \mathbf{e})]p(\mathbf{e})$ where p is the probability distribution

$$\begin{aligned} p(\mathbf{e}_1) &= \frac{1}{2}(1-h)(1+\delta), \quad p(\mathbf{e}_2) = \frac{1}{2}h, \\ p(-\mathbf{e}_1) &= \frac{1}{2}(1-h)(1-\delta), \quad p(-\mathbf{e}_2) = \frac{1}{2}h, \end{aligned} \quad (1.74)$$

on $\{\mathbf{e}_1, -\mathbf{e}_1, \mathbf{e}_2, -\mathbf{e}_2\}$, where $h \in [0, 1]$ is called *vertical displacement* probability and $\delta \in [0, 1]$ is called *drift*. Note that if $h = 0$ particles move only horizontally, if $h = 1$ they move only vertically, if $\delta = 0$ the horizontal motion is left–right symmetric, and if $\delta = 1$ the horizontal motion is *totally* biased to the right. Note, also, that the jump from site $\mathbf{z}$ to site $\mathbf{z} + \mathbf{e}$ can be performed only if $\mathbf{z}$ is occupied, i.e., $\eta(\mathbf{z}) = 1$, and $\mathbf{z} + \mathbf{e}$ is empty, i.e., $\eta(\mathbf{z} + \mathbf{e}) = 0$, otherwise the rate is zero.

We remark that for the jumping probabilities we are adopting the same notation that some of the authors used in the papers [9, 10] although in those papers the biased direction was supposed to be vertical. Moreover, we note that there we adopted the discrete time formalism for Markov processes, since it was more convenient to perform and discuss the numerical simulations. Here, we prefer to use the continuous time language, since it allows a more intuitive derivation of the hydrodynamic equation.

Coming back to the definition of the model, more formally, we are considering the continuous time Markov process with infinitesimal generator

$$\begin{aligned} (L_N f) &= \sum_{\mathbf{z} \in \mathbb{T}_N^2} \sum_{\mathbf{e} = \pm \mathbf{e}_1, \pm \mathbf{e}_2} \eta(\mathbf{z})[1 - \eta(\mathbf{z} + \mathbf{e})]p(\mathbf{e}) \\ &\quad [f(\eta^{\mathbf{z}, \mathbf{z} + \mathbf{e}}) - f(\eta)] \end{aligned} \quad (1.75)$$

for any function $f : \{0, 1\}^{\mathbb{T}_N^2} \rightarrow \mathbb{R}$, where $\eta^{\mathbf{z}, \mathbf{z} + \mathbf{e}}$ is the configuration obtained from η by moving a particle from site $\mathbf{z}$ to site $\mathbf{z} + \mathbf{e}$.

For an arbitrary site $\mathbf{z}$ in the torus we write the balance equation for the average occupation number $v(\mathbf{z}, \tau)$ of the site $\mathbf{z}$ in the interval of time between τ and $\tau + \Delta\tau$:

$$\begin{aligned} v(\mathbf{z}, \tau + \Delta\tau) - v(\mathbf{z}, \tau) &= \left\{ \frac{1}{2} h v(\mathbf{z} + \mathbf{e}_2, \tau) [1 - v(\mathbf{z}, \tau)] \right. \\ &\quad + \frac{1}{2} (1-h)(1+\delta) v(\mathbf{z} - \mathbf{e}_1, \tau) [1 - v(\mathbf{z}, \tau)] \\ &\quad + \frac{1}{2} h v(\mathbf{z} - \mathbf{e}_2, \tau) [1 - v(\mathbf{z}, \tau)] \\ &\quad + \frac{1}{2} (1-h)(1-\delta) v(\mathbf{z} + \mathbf{e}_1, \tau) [1 - v(\mathbf{z}, \tau)] \\ &\quad - \frac{1}{2} h v(\mathbf{z}, \tau) [1 - v(\mathbf{z} + \mathbf{e}_2, \tau)] \\ &\quad - \frac{1}{2} (1-h)(1-\delta) v(\mathbf{z}, \tau) [1 - v(\mathbf{z} - \mathbf{e}_1, \tau)] \\ &\quad - \frac{1}{2} h v(\mathbf{z}, \tau) [1 - v(\mathbf{z} - \mathbf{e}_2, \tau)] \\ &\quad \left. - \frac{1}{2} (1-h)(1+\delta) v(\mathbf{z}, \tau) [1 - v(\mathbf{z} + \mathbf{e}_1, \tau)] \right\} \Delta\tau \end{aligned}$$

where the first four terms on the right-hand-side account for particles moving to $\mathbf{x}$ from neighboring sites, while the remaining terms account for particles moving from $\mathbf{x}$ to neighboring sites. Hence,

$$\begin{aligned} v(\mathbf{z}, \tau + \Delta\tau) - v(\mathbf{z}, \tau) &= \left\{ \frac{1}{2} h [v(\mathbf{z} + \mathbf{e}_2, \tau) - 2v(\mathbf{z}, \tau) + v(\mathbf{z} - \mathbf{e}_2, \tau)] \right. \\ &\quad + \frac{1}{2} (1-h) [v(\mathbf{z} + \mathbf{e}_1, \tau) - 2v(\mathbf{z}, \tau) + v(\mathbf{z} - \mathbf{e}_1, \tau)] \\ &\quad - \frac{1}{2} \delta (1-h) \{ [1 - v(\mathbf{z}, \tau)] [v(\mathbf{z} + \mathbf{e}_1, \tau) - v(\mathbf{z} - \mathbf{e}_1, \tau)] \\ &\quad \left. + v(\mathbf{z}, \tau) [(1 - v(\mathbf{z} + \mathbf{e}_1, \tau)) - (1 - v(\mathbf{z} - \mathbf{e}_1, \tau))] \} \right\} \Delta\tau. \end{aligned} \quad (1.76)$$

To derive the limit hydrodynamic equation, we let

$$\xi = \frac{1}{N}, \quad (1.77)$$

consider the macroscopic variables

$$\mathbf{x} = \xi \mathbf{z} \in [0, 1]^2 \quad \text{and} \quad t = \xi^2 \tau \quad (1.78)$$

and set

$$u(\mathbf{x}, t) = v\left(\frac{\mathbf{x}}{\xi}, \frac{t}{\xi^2}\right). \quad (1.79)$$

Finally, letting $\Delta t = \xi^2 \Delta \tau$, the balance Eq. (1.76) in the new variables becomes

$$\begin{aligned} & [u(\mathbf{x}, t + \Delta t) - u(\mathbf{x}, t)] / \Delta t \\ &= \left\{ \frac{1}{2} h [u(\mathbf{x} + \xi \mathbf{e}_2, t) - 2u(\mathbf{x}, t) + u(\mathbf{x} - \xi \mathbf{e}_2, t)] \right. \\ &+ \frac{1}{2} (1 - h) [u(\mathbf{x} + \xi \mathbf{e}_1, t) - 2u(\mathbf{x}, t) + u(\mathbf{x} - \xi \mathbf{e}_1, t)] \\ &- \frac{1}{2} \bar{\delta} (1 - h) \{ [1 - u(\mathbf{x}, t)] [u(\mathbf{x} + \xi \mathbf{e}_1, t) - u(\mathbf{x} - \xi \mathbf{e}_1, t)] \\ &+ u(\mathbf{x}, t) [(1 - u(\mathbf{x} + \xi \mathbf{e}_1, t)) - (1 - v(\mathbf{x} - \xi \mathbf{e}_1, t))] \} \} / \varepsilon^2. \end{aligned} \quad (1.80)$$

Finally, if we assume that in the limit $\xi \rightarrow 0$, namely, $N \rightarrow \infty$, the drift scales to zero as

$$\bar{\delta} = \xi \bar{\delta},$$

we find the limit hydrodynamic equation

$$\frac{\partial u}{\partial t} = \frac{1}{2} h \frac{\partial^2 u}{\partial x_2^2} + \frac{1}{2} (1 - h) \frac{\partial^2 u}{\partial x_1^2} - \bar{\delta} (1 - h) \frac{\partial}{\partial x_1} [u(1 - u)]. \quad (1.81)$$

The above equation, which provides a microscopic interpretation of the different terms appearing in (1.1), is a diffusion-like equation with a nonlinear anisotropic flux. The diffusion part of the equation is linear, while the effect of the drift is captured in the nonlinear transport term which vanishes when $\bar{\delta} = 0$, so that linearity is approximatively restored at very small $\bar{\delta}$.

It is worth noting that a derivation of the mean-field equations can be done in a similar way for the case of oblique nonlinear drifts.

References

- Allaire G (2002) Shape optimization by the homogenization method. Springer, New York
- Alnaes MS, Blechta J, Hake J, Johansson A, Kehlet B, Logg A, Richardson C, Ring J, Rognes ME, Wells GN (2015) The FEniCS project Version 1.5. Arch Numer Softw 3
- Allaire G, Briane M, Brizzi R, Capdeboscq Y (2009) Two asymptotic models for arrays of underground waste containers. Appl Anal 88(10–11):1145–1467
- Amaziane B, Pankratov L, Prytula V (2010) Homogenization of one phase flow in a highly heterogeneous porous medium including a thin layer. Asymptot Anal 70:51–86
- Bakhvalov N, Panasenko G (1989) Homogenisation: averaging processes in periodic media. Kluwer, New York
- Bear J (1972) Dynamics of fluids in porous media. Dover, Illinois
- Braga GA, Furtado F, Moreira JM, Rolla LT (2003) Renormalization group analysis of nonlinear diffusion equations with periodic coefficients. Multiscale Model Simul 1:630–644
- Ciorănescu D, Saint-Jean-Paulin J (1999) Homogenization of reticulated structures. Springer, New York
- Cirillo ENM, Krehel O, Muntean A, van Santen R, Sengar A (2016) Residence time estimates for asymmetric simple exclusion dynamics on strips. Phys A 442:436–457
- Cirillo ENM, Krehel O, Muntean A, van Santen R (2016) A lattice model of reduced jamming by barrier. Phys Rev E 94:042115
- de Bonis I, De Cave LM (2014) Degenerate parabolic equations with singular lower order terms. Differ Integral Equ 27(9–10):949–976
- de Bonis I, Muntean A (2017) Existence of weak solutions to a nonlinear reaction–diffusion system with singular sources. Electron J Differ Equ 202:1–16
- Davit Y, Bell CG, Byrne HM, Chapman LAC, Kimpton LS, Lang GE, Leonard KHL, Oliver JM, Pearson NC, Shipley RJ, Waters SL, Whiteley JP, Wood BD, Quintard M (2013) Homogenization via formal multiscale asymptotics and volume averaging: how do the two techniques compare? Adv Water Resour 62:178–206
- Derrida B, Janowsky SA, Lebowitz JL, Speer ER (1993) Exact solution of the totally asymmetric simple exclusion process: shock profiles. J Stat Phys 73:813–842
- De Masi A, Presutti E, Scacciatelli E (1989) The weakly asymmetric simple exclusion process. Ann l’I.H.P., Sect B 25:1–38
- Donato P, Piatnitski A (2010) On the effective interfacial resistance through rough surfaces. Commun Pure Appl Anal 9(5):1295–1310
- Ene H, Vernescu B (1985) Homogenization of a singular perturbation problem. Rev Roum Math Pures Appl 30:815–822
- Hornung U (1997) Homogenization and porous media, vol 6. Interdisciplinary and Applied Mathematics. Springer, New York
- Ijioma ER, Muntean A, Ogawa T (2015) Effect of material anisotropy on the fingering instability in reverse smoldering combustion. Int J Heat Mass Transf 58:924–938
- Ijioma ER, Ogawa T, Muntean A, Fatima T (2014) Homogenization and dimension reduction of filtration combustion in heterogeneous thin layers. Netw Heterog Media 9(4):709–737
- Khoa VA, Thieu TKT, Ijioma ER (2020) On a pore-scale stationary diffusion equation: scaling effects and correctors for the homogenization limit. To appear on Discrete and Continuous Dynamical Systems—B
- Kipnis C, Landim C (1999) Scaling limits of interacting particle systems. Springer, Berlin
- Leguillon D (2007) Comparison of matched asymptotics, multiple scalings and averages in homogenization of periodic structures. Math Models Methods Appl Sci 7(5):663–680

24. Muntean A, Böhm M, Kropp J (2011) Moving carbonation fronts in concrete: a moving-sharp-interface approach. *Chem Eng Sci* 66:538–547
25. Muntean A, Nikolopoulos CV (2020) Colloidal transport in locally periodic evolving porous media—An upscaling exercise. *SIAM J Appl Math* 80(1):448–475
26. Nelson DR, Piran T, Weinberg S (2004) *Statistical mechanics of membranes and surfaces*. World Scientific, Singapore
27. Neuss-Radu M, Jäger W (2007) Effective transmission conditions for reaction–diffusion processes in domains separated by an interface. *SIAM J Math Anal* 9(4):709–737
28. Nyflött A, Axrup L, Carlson G, Järnström L, Lestelius M, Moons E, Wahlström T (2015) Influence of kaolin addition on the dynamics of oxygen mass transport in polyvinyl alcohol dispersion coatings. *Coat Nord Pulp Pap Res J* 30:3
29. Pozrikidis C, Ford DM (2017) Conductive transport through a mixed–matrix membrane. *J Eng Math* 105:189–202
30. Sato K, Fujimoto K, Nakata M, Shikazono N (2013) Evidence for enhanced matrix diffusion in geological environment. *J Phys Soc Jpn* 82:014901
31. Watanabe Y, Nakashima Y (2001) Two-dimensional random walk program for the calculation of the tortuosity of porous media. *J Groundw Hydrol* 43:13–22
32. Zhao H, Yao Z (2012) Effective models of the Navier–Stokes flow in porous media with a thin fissure. *J Math Anal Appl* 387:542–555

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