Upscaling flow and transport in an evolving porous medium with general interaction potentials

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Abstract

Flow and transport in porous media are a classical multi-scale problem. In recent research, upscaling approaches have been undertaken for models integrating electrostatics or deformations of the porous matrix. The objective of this research is to investigate the upscaling of flow and transport models including both an evolving solid-liquid interface and a quite general interaction potential. Starting from a comprehensive pore-scale model, formal two-scale asymptotic expansion in a level set framework is applied. In doing so, the interplay between flow, transport, and evolving geometry is exposed. As a result of an averaging procedure, a fully coupled micro-macro in new principle variables is maintained. Moreover, time- and space-dependent coefficient functions are explicitly characterized by means of supplementary, fully coupled cell problems. Because of the general framework considered in this research, numerous application are expected, such as in biology or colloidal dynamics.

1 Introduction

Considering flow and transport through porous media is a classical multi-scale problem. The numerous applications range from geology and biology to technical applications. Recently, two related aspects have attracted an increased interest in upscaling flow and transport through porous media: the integration of electrostatics and an evolving porous matrix to the model. On the issue of electrostatic interaction, the research to date has tended to focus on a linearized model according to the work of [12], c.f. [1, 8]. Likewise, in [3, 5, 15, 20, 21] a fully nonlinear aspect has been investigated in a rigid porous medium. So far, however, little attention has been paid to more general interaction potentials such as in [17]. Additionally, upscaling methods have thus far been mainly applied in rigid porous

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media. To overcome this drawback, mechanical aspects have, on the one hand, been integrated to flow and transport models to account for small elastic deformations [10, 11]. On the other hand, an extension of homogenization techniques was introduced in [13] which is, however, restricted to smooth geometrical transformations of the porous matrix without topology change. In comparison to these approaches, an approach capable of more flexible variations within the geometry is introduced in [22]. Here, an extension of formal two-scale asymptotic expansion including a level set description for the evolving solid-liquid interface was introduced. This method has recently been applied to locally periodic media, biofilm growth, colloid dynamics, and drug delivery [16, 17, 23, 24].

In this research, we combine both of the aforementioned aspects in a comprehensive pore-scale model. More precisely, we integrate a general interaction potential as a transport mechanism (drift) to the model equations and account for the evolving microstructure. To this end, a general surface reaction rate that comprises immobilization and detachment processes completes the model and determines the changes in the underlying microstructure. In summary, transport and fluid flow is modeled by a fully coupled system of partial differential equations, namely convection-diffusion-drift-reaction equation combined with incompressible Stokes equations and a level set equation.

In this paper, we seek to address the following aspects: We carry out the upscaling of the underlying model equations while focusing on coupling the geometry to transport and fluid flow via surface reactions and the general interaction potential. In our investigations, we distinguish between two cases: first, a purely macroscopic interaction potential, and second, an interaction potential admitting for microscopic components. As a result of the averaging procedure by formal two-scale asymptotic expansion in a level set framework, we maintain a fully coupled two-scale model. In other words, we obtain a coupled system of partial differential equations consisting of Darcy’s law and an upscaled transport equation, perhaps defined in new principle variables (macro level). Moreover, time- and space-dependent coefficient functions are determined by supplementary, fully coupled cell problems (micro level). In conclusion, the upscaled problems have a micro-macro structure and, additionally, both levels are coupled to each other by the geometrical description.

Outline: In Section 2, a microscopic model at the pore scale is established. Thereafter, in Section 3, we state the main upscaling results. Moreover, we introduce the method of formal two-scale asymptotic expansion in a level set framework, which is applied to our model system in Section 4 and Section 5. Finally, in Section 6, we discuss the results obtained.

2 Mathematical model

In this section, a mathematical model describing transport and fluid dynamics in an evolving porous medium at the pore scale is presented, c.f. [17] and references cited therein. To this end, we start by describing the underlying geometric setting: We consider a bounded and connected domain Ω with exterior boundary ∂Ω and with an associated periodic microstructure. The microstructure is defined by unit cells \( Y = \left[ -\frac{1}{2}, \frac{1}{2} \right] ^n \) containing a solid
inclusion $Y_s$. Moreover, the liquid part $Y_l := Y \setminus Y_s$ and the solid part $Y_s$ define the solid-liquid interface $\Gamma = \bar{Y}_l \cap \bar{Y}_s$. We assume that at initial time $t = 0$, the solid part does not touch the boundary of the unit cell $Y$. As a consequence, the fluid part is connected.

We call $\varepsilon < 1$ the scale parameter and assume the macroscopic domain $\Omega$ is an ideal porous medium and is therefore given by the periodic composition of scaled unit cells $Y_\varepsilon = \varepsilon Y$ that are shifted in such a way that their midpoint $(i, j)$ coincides with a regular mesh of size $\varepsilon$. The scaled and shifted cells, which are denoted by $Y^{ij}_\varepsilon$, are divided into an analogously scaled fluid part $Y^{ij}_\varepsilon,l$ and solid part $Y^{ij}_\varepsilon,s$. The scaled and shifted solid-liquid interface is denoted by $\Gamma^{ij}_\varepsilon$ with the unit outer normal $\nu^i$. The fluid part/pore space, the solid part and the inner boundary of the porous medium are defined by

$$\Omega_\varepsilon := \bigcup_i Y^{ij}_\varepsilon,l, \quad \Omega^{\bar{i}}_\varepsilon := \bigcup_i Y^{ij}_\varepsilon,s, \quad \text{and} \quad \Gamma_\varepsilon := \bigcup_i \Gamma^{ij}_\varepsilon.$$ 

The distribution of the solid and liquid phase is characterized by a level set function

$$L_\varepsilon(t, x) = \begin{cases} > 0 & \text{liquid phase}, \\ = 0 & \text{interface}, \\ < 0 & \text{solid phase}, \end{cases}$$

Having these notations at hand, we are able to define the pore-scale model describing transport and fluid dynamics in an evolving porous medium including general surface reactions $f$ and interaction potential $\Phi$. In summary, we consider Stokes’ equations (1a) and (1b) for the fluid velocity $v_\varepsilon$ and pressure $p_\varepsilon$, the transport equation (2a) for the concentration $c_\varepsilon$, and the level set equation (3a). At the evolving interface $\Gamma_\varepsilon$, boundary conditions are derived from the conservation law [17, 22] and appropriate initial conditions are chosen. Accounting for the multi-scale framework, the different terms in (1), (2), and (3) are scaled with powers of the scale parameter $\varepsilon$. In the following, the parameter $\rho$ denotes the constant density of the solid and the parameter $\alpha, \beta$ refer to volume change [17, 22].

$$-\varepsilon^2 \Delta v_\varepsilon + \nabla p_\varepsilon = -c_\varepsilon \nabla \Phi_\varepsilon \quad x \in \Omega_\varepsilon(t), \ t \in (0, T), \quad (1a)$$

$$\nabla \cdot v_\varepsilon = 0 \quad x \in \Omega_\varepsilon(t), \ t \in (0, T), \quad (1b)$$

$$v_\varepsilon = -\varepsilon \beta \alpha f(c_\varepsilon, \rho) \nu^i \quad x \in \Gamma_\varepsilon(t), \ t \in (0, T), \quad (1c)$$

$$v_\varepsilon = 0 \quad x \in \partial \Omega, \ t \in (0, T). \quad (1d)$$

$$\partial_t c_\varepsilon - \nabla \cdot (-v_\varepsilon c_\varepsilon + \nabla c_\varepsilon + c_\varepsilon \nabla \Phi_\varepsilon) = 0 \quad x \in \Omega_\varepsilon(t), \ t \in (0, T), \quad (2a)$$

$$(-v_\varepsilon c_\varepsilon + \nabla c_\varepsilon + c_\varepsilon \nabla \Phi_\varepsilon) \cdot \nu_\varepsilon - \varepsilon \alpha f(c_\varepsilon, \rho)(c_\varepsilon - \rho) = 0 \quad x \in \Gamma_\varepsilon(t), \ t \in (0, T), \quad (2b)$$

$$(-v_\varepsilon c_\varepsilon + \nabla c_\varepsilon + c_\varepsilon \nabla \Phi_\varepsilon) \cdot \nu = 0 \quad x \in \partial \Omega, \ t \in (0, T), \quad (2c)$$

$$c_\varepsilon = c^0 \quad x \in \Omega_\varepsilon(0). \quad (2d)$$
\[
\begin{align*}
\partial_t L_\varepsilon - \varepsilon f(c_\varepsilon, \rho)|\nabla L_\varepsilon| &= 0 & x \in \Omega, \ t \in (0, T), & \quad (3a) \\
L_\varepsilon &= L^0 & x \in \Omega, \ t = 0. & \quad (3b)
\end{align*}
\]

Considering an electrostatic interaction potential, the above system is known to be the Stokes-Nernst-Planck-Poisson system [14, 25]. In that case, the system is complemented with Poisson’s equation for the electrostatic potential and the concentrations relating to the corresponding charge density. A thermodynamic consistent derivation of that model is found in [6]. In the literature, it is quite common to consider the associated linearized problem going back to the original work of O’Brian [12].

For the reaction rate \( f \) and the interaction potential \( \Phi_\varepsilon \), structural assumptions or constitutive laws must be assumed. In [17], several examples are also cited and illustrated with numerical simulations. However, we point out that a rather different scaling is used in Stokes’ equations (1). In contrast to [17], we aim to thoroughly investigate the coupling between fluid flow and transport including general interaction potentials. Further, we focus on the case that both processes are on par. Hand in hand with this assumption, the upscaling procedure requires rather elaborate investigations. Finally, much more sophisticated models arise that contain various ways of coupling. As a remark note that scaling the boundary terms is conducted in such a way that it compensates for the behavior of the interior boundary’s measure \(|\Gamma_\varepsilon|\) which is proportional to \(1/\varepsilon\).

3 Upscaling and main results

Our main goal is maintain a macroscopic model description starting from system (1), (2), and (3). To this end, we formally identify, in this case, the limit \( \varepsilon \to 0 \). A commonly used method is that of two-scale asymptotic expansion, c.f. [4, 7, 19]. A short mathematical introduction accounting for an extension to evolving microstructures as introduced in [22] is given in Section 3.2. For the readers’ convenience, the upscaling results are summarized in the following section. In Theorem 3.1 and Theorem 3.2 respectively, the cases of a purely macroscopic interaction potential and a potential including microscopic components are addressed.

3.1 Main results

The main result from upscaling for a macroscopic interaction potential, i.e. in the case of \( \Phi(t, x, y) = \Phi(t, x) \) is summarized in Theorem 3.1:

**Theorem 3.1**

The leading order terms \( \tau_0, p_0, c_0 \) fulfill the following limit equations:
Darcy’s law describes the averaged water movement

\[ \begin{align*}
\tau_0 &= -K(\nabla_x p_0 + c_0 \nabla_x \Phi_0) \\
\nabla_x \cdot \tau_0 &= \int_{\Gamma_0(t,x)} \beta f(c_0) \, dy 
\end{align*} \]

with permeability tensor $K$ defined as

\[ K_{ij} := \int_{Y_{l,0}(t,x)} w^i_j \, dy \]

and $w^i_j$ being the $i$-th component of the solutions $w_j$ of the supplementary family of cell problems of Stokes type in $(w_j, \pi_j)$ for $j = 1, 2$

\[ \begin{align*}
-\Delta_y w_j + \nabla_y \pi_j &= e_j & \text{in } Y_{l,0}(t,x), \\
\nabla_y \cdot w_j &= 0 & \text{in } Y_{l,0}(t,x), \\
w_j &= 0 & \text{on } \Gamma_0(t,x), \\
w_j, \pi_j & \text{ periodic in } y.
\end{align*} \]

The transport equation for averaged concentration is given by

\[ \begin{align*}
\partial_t (|Y_{l,0}| c_0) + \nabla_x \cdot (\nabla_x c_0) - \nabla_x \cdot (D(\nabla_x c_0 + c_0 \nabla_x \Phi_0)) &= -|\Gamma_0| f(c_0, \rho) & x \in \Omega
\end{align*} \]

with diffusion tensor $D$ defined as

\[ D_{ij} := \int_{Y_{l,0}(t,x)} \partial_y \zeta_j + \delta_{ij} \, dy \]

and $\zeta_j$ being the solutions in the supplementary family of cell problems for $j = 1, 2$

\[ \begin{align*}
-\nabla_y \cdot (\nabla_y \zeta_j) &= 0 & \text{in } Y_{l,0}(t,x), \\
\nabla_y \zeta_j \cdot \nu_0 &= -e_j \cdot \nu_0 & \text{on } \Gamma_0(t,x), \\
\zeta_j & \text{ periodic in } y,
\end{align*} \]

\[ \frac{1}{|Y|} \int_{Y_{l,0}} \zeta_j \, dy = 0. \]

Furthermore, the level set function fulfills

\[ \partial_t L_0 - \alpha f(c_0, \rho) |\nabla_y L_0| = 0 \text{ in } Y \times \Omega. \]

In Theorem 3.2, the main result for an interaction potential including microscopic and macroscopic components, i.e. the case of $\Phi(t, x, y) = \Phi(t, x, y)$, is summarized:
Theorem 3.2
The leading order terms \( \tau_0, \tilde{p}_0, u_0 \) (including new principle variables) fulfill the following limit equations:

Darcy’s law describes the averaged water movement

\[
\tau_0 = -K^1(t, x) \nabla_x \tilde{p}_0 - K^2(t, x) \nabla_x u_0 \quad x \in \Omega
\]

\[
\nabla_x \cdot \tau_0 = \int_{\Gamma_0(t, x)} \beta f(c_0) \, dy \quad x \in \Omega
\]

with permeability tensors \( K^1, K^2 \) defined as

\[
K^1_{ij} := \int_{Y_{i,0(t,x)}} (w^1)^i_j \, dy
\]

\[
K^2_{ij} := \int_{Y_{i,0(t,x)}} (w^2)^i_j \, dy
\]

and \( w_j \) being the solutions in the supplementary family of cell problems of Stokes type in \((w_j, \pi_j)\) for \( j = 1, 2 \)

\[
-\Delta_y w^1_j + \nabla_y \tilde{\pi}^1_j + e^{-\Phi_0} \nabla_y \zeta^1_j = -e_j \quad \text{in } Y_{i,0(t,x)},
\]

\[
\nabla_y \cdot w^1_j = 0 \quad \text{in } Y_{i,0(t,x)},
\]

\[
w^1_j = 0 \quad \text{on } \Gamma_0(t, x),
\]

\[
w^1_j, \tilde{\pi}^1_j \text{ periodic in } y.
\]

\[
-\Delta_y w^2_j + \nabla_y \tilde{\pi}^2_j + e^{-\Phi_0} \nabla_y \zeta^2_j = -e^{-\Phi_0} e_j \quad \text{in } Y_{i,0(t,x)},
\]

\[
\nabla_y \cdot w^2_j = 0 \quad \text{in } Y_{i,0(t,x)},
\]

\[
w^2_j = 0 \quad \text{on } \Gamma_0(t, x),
\]

\[
w^2_j, \tilde{\pi}^2_j \text{ periodic in } y.
\]

The averaged transport equation for the new concentration is given by

\[
\partial_t (A u_0) + \nabla_x \cdot (D^1 \nabla_x \tilde{p}_0 + D^2 \nabla_x u_0) = - \int_{\Gamma_0(t,x)} \alpha f(e^{-\Phi_0} u_0, \rho) \rho \, dy.
\]

with effective porosity \( A := \int_{Y_{i,0(t,x)}} e^{-\Phi_0} \, dy \) and diffusion tensors \( D^3, D^4 \) defined as

\[
D^1_{ij} := \int_{Y_{i,0(t,x)}} e^{-\Phi_0} \partial_y \zeta^1_i + e^{-\Phi_0} (w^1)^i_j u_0 \, dy
\]

\[
D^4_{ij} := \int_{Y_{i,0(t,x)}} e^{-\Phi_0} \partial_y \zeta^2_i + e^{-\Phi_0} (w^2)^i_j u_0 + e^{\Phi_0} \delta_{ij} \, dy
\]
i.e. as the integration over the fluxes of the corresponding cell problems in $\zeta_j^1, \zeta_j^2$ for $j = 1, 2$:

\[
\begin{align*}
-\nabla_y \cdot (e^{-\Phi_0} \nabla_y \zeta_j^1) &= \nabla_y \cdot (e^{-\Phi_0} w_j^1 u_0) \quad \text{in } Y_{1,0}(t, x), \\
(e^{-\Phi_0} \nabla_y \zeta_j^1) \cdot \nu_0 &= -e^{-\Phi_0} w_j^1 u_0 \cdot \nu_0 \quad \text{on } \Gamma_0(t, x), \\
\zeta_j^1 \text{ periodic in } y, \\
\frac{1}{|Y|} \int_{Y_{1,0}} \zeta_j^1 \, dy &= 0,
\end{align*}
\]

\[
\begin{align*}
-\nabla_y \cdot (e^{-\Phi_0} \nabla_y \zeta_j^2) &= \nabla_y \cdot (e^{-\Phi_0} w_j^2 u_0 + e^{-\Phi_0} e_j) \quad \text{in } Y_{1,0}(t, x), \\
(e^{-\Phi_0} \nabla_y \zeta_j^2) \cdot \nu_0 &= -(e^{-\Phi_0} w_j^2 u_0 + e^{-\Phi_0} e_j) \cdot \nu_0 \quad \text{on } \Gamma_0(t, x), \\
\zeta_j^2 \text{ periodic in } y, \\
\frac{1}{|Y|} \int_{Y_{1,0}} \zeta_j^2 \, dy &= 0.
\end{align*}
\]

Furthermore, the Level Set function fulfills

\[\partial_t L_0 - \alpha f(e^{-\Phi_0} u_0, \rho)|\nabla_y L_0| = 0 \text{ in } Y \times \Omega.\]

### 3.2 Method of two-scale asymptotic expansion

In this section, we give a short introduction to formal two-scale asymptotic expansion in evolving microstructures [22]. This method is then applied to (1), (2), and (3) for both of the following cases: first, for a purely macroscopic interaction potential, and then followed by investigations for an interaction potential including microscopic dependencies.

Concerning scale separation, in addition to the global variable $x$, a microscopic variable $y$ is introduced. Both are connected via the relation $y = x/\varepsilon$. As a consequence, the expansion of the spatial gradient reads

\[\nabla_\varepsilon = \nabla_x + \frac{1}{\varepsilon} \nabla_y.\]  

(4)

Higher order spatial derivatives may be calculated analogously by applying the chain rule. Furthermore it is assumed that all variable functions can be expanded as a series of the scale parameter $\varepsilon$, i.e.

\[\varphi_\varepsilon(t, x) = \varphi_0(t, x, y) + \varepsilon \varphi_1(t, x, y) + \varepsilon^2 \varphi_2(t, x, y) + \ldots, \quad y = x/\varepsilon, \quad \varphi_\varepsilon \in \{v_\varepsilon, p_\varepsilon, c_\varepsilon, \Phi_\varepsilon\}.\]  

(5)

By applying Taylor’s expansion, we obtain

\[
\begin{align*}
f(\varphi_\varepsilon, \psi_\varepsilon)(t, x) &= f(\varphi_0, \psi_0)(t, x, y) \\
+ \varepsilon \left( D_\varphi f(\varphi_\varepsilon, \psi_\varepsilon) |_{(\varphi_0, \psi_0)} \varphi_1 \right)(t, x, y) + \left( D_\psi f(\varphi_\varepsilon, \psi_\varepsilon) |_{(\varphi_0, \psi_0)} \psi_1 \right)(t, x, y) \\
+ \ldots.
\end{align*}
\]  

(6)
Beyond the standard expansions introduced above in the framework of a level set description, the level set function \( L_\varepsilon \) itself and the normal vector \( \nu_\varepsilon \) must also be expanded due to the evolving microstructure. For a two-dimensional setting, the expansion of the normal vector can be expressed in terms of the level set function to obtain the following expressions, c.f. e.g., [22]:

\[
L_\varepsilon(t, x) = L_0(t, x, y) + \varepsilon L_1(t, x, y) + \varepsilon^2 L_2(t, x, y) + \ldots, \quad y = x/\varepsilon, \tag{7}
\]

\[
\nu_\varepsilon = \nu_0 + \varepsilon \nu_1 + O(\varepsilon^2), \quad \nu_0 = \nabla_y L_0 / |\nabla_y L_0|, \quad \nu_1 = \tau_0 \cdot \nabla_x L_0 + \nabla_y L_1 / |\nabla_y L_0| \tag{8}
\]

with \( \tau_0 := \nu_0^\perp \). The zero order expansion of the level set function is also used to describe the zero order time evolving domain \( Y_{l,0}(t, x) := \{ y : L_0(t, x, y) < 0 \} \) and interface \( \Gamma_0(t, x) := \{ y : L_0(t, x, y) = 0 \} \), [22]. Applying these expansions to our problem and analyzing the different orders in \( \varepsilon^k \), \( k \in \mathbb{Z} \) we derive the desired macroscopic homogenized problem description. The necessary technical calculations for this derivation are performed in the following subsections.

4 Macroscopic interaction potential

In this section, we investigate the case that the interaction potential is a macroscopic quantity, i.e. \( \Phi_0(t, x, y) = \Phi_0(t, x) \). In comparison to the approach in [15], additional work must be conducted in the following to account for the evolving microstructure.

4.1 Lowest order problems

In this section, we investigate the lowest order terms of (1), (2), and (3) that arise after inserting expansion (4) - (8).

The transport equation of lowest order is of order \( \varepsilon^{-2} \) with a corresponding boundary condition of order \( \varepsilon^{-1} \) and reads

\[
-\nabla_y \cdot (\nabla_y c_0) = 0,
\]

\[
\nabla_y c_0 \cdot \nu_0 = 0.
\]

As a consequence, we conclude that

\[
c_0(t, x, y) = c_0(t, x) \tag{9}
\]

holds, in that the leading order concentration \( c_0 \) is a macroscopic variable.

Since we assume that the interaction potential is a macroscopic variable (\( \Phi_0(t, x, y) = \Phi_0(t, x) \)), the lowest order problem of Stokes’ equation, which is of order \( \varepsilon^{-1} \), reads:

\[
\nabla_y p_0 = 0.
\]

which in fact yields

\[
p_0(t, x, y) = p_0(t, x). \tag{10}
\]

Consequently, the leading order pressure \( p_0 \) is also a macroscopic variable.
Remark 1 The above results coincide perfectly with standard theory in upscaling flow and transport problems in periodic porous media, c.f. e.g. [7]. In particular, the interaction potential does not play a role in investigating the lowest order problems of (1), (2), and (3). This is a direct result of the assumption that the interaction potential is a macroscopic quantity, compare also Section 5.1 and Remark 4.

4.2 Next order problems

For the next step in upscaling, we consider the subsequent higher order terms in \( \varepsilon^k \), \( k \in \mathbb{Z} \) of (1) and (2).

For Stokes’ equation, we investigate the corresponding equation of order \( \varepsilon^0 \), supplemented by the incompressibility condition of order \( \varepsilon^{-1} \) and boundary condition of order \( \varepsilon^0 \):

\[
-\Delta_y v_0 + \nabla_y p_1 + \nabla_x p_0 = -c_0 \nabla_x \Phi_0 - c_0 \nabla_y \Phi_1,
\]

\[
\nabla_y \cdot v_0 = 0, \\
v_0 = 0.
\]

As already maintained in (9), the leading order concentration \( c_0 \) is a macroscopic quantity. Consequently, defining the correction \( \tilde{p}_1 \) of the first order pressure \( p_1 \) by

\[
\tilde{p}_1 := p_1 + c_0 \Phi_1
\]

leads to

\[
-\Delta_y v_0 + \nabla_y \tilde{p}_1 = -\nabla_x p_0 - c_0 \nabla_x \Phi_0, \\
\nabla_y \cdot v_0 = 0, \\
v_0 = 0.
\]

Since the leading order pressure \( p_0 \) is also a macroscopic quantity, c.f. (10), we are able to extract the following cell problems (12) of Stokes type for \( j = 1, 2 \) by linearity. This is again synonymous to the standard procedure in upscaling flow and transport in porous media [7].

\[
-\Delta_y w_j + \nabla_y \pi_j = e_j  \quad \text{in } Y_{i,0}(t,x), \\
\nabla_y \cdot w_j = 0  \quad \text{in } Y_{i,0}(t,x), \\
w_j = 0  \quad \text{on } \Gamma_0(t,x), \\
w_j, \pi_j \text{ periodic in } y.
\]

Due to the linearity of the problem, the leading order velocity \( v_0(x,y) \) is expressed in terms of the solutions \( w_j \) of the cell problems (12) via

\[
v_0(t,x,y) = -\sum_j w_j(t,x;y) \left( \partial_{x_j} p_0(t,x) + c_0(t,x) \partial_{x_j} \Phi_0(t,x) \right) .
\]
Integrating with respect to the fast variable $y$, we derive Darcy’s law for the averaged velocity $\overline{v}_0(x) := \int_{Y_{l,0}(t,x)} v_0(x,y)dy$:

$$\overline{v}_0 = -K(\nabla_x p_0 + c_0 \nabla_x \Phi_0), \quad (13)$$

with the permeability tensor

$$K_{ij} := \int_{Y_{l,0}(t,x)} w^j dy. \quad (14)$$

Here, we point out the first difference to the standard theory: in addition to the proportionality of the leading order velocity $v_0$ to the leading order pressure gradient, a forcing term related to the interaction potential’s gradient, or more precisely to the interaction force density, emerges.

This new Darcy’s law (13) is supplemented by the following compressibility condition

$$\nabla_x \overline{v}_0 = \int_{\Gamma_0(t,x)} \beta f(c_0) dy,$$

and by the no-slip boundary condition

$$\overline{v}_0 = 0$$

as has been shown in [22].

For the transport equation, we investigate the corresponding equation of (2) in order $\varepsilon^{-1}$ supplemented by the boundary condition of order $\varepsilon^0$:

$$-\nabla_y \cdot (\nabla_y c_1 + \nabla_x c_0 + c_0 \nabla_y \Phi_1 + c_0 \nabla_x \Phi_0) = 0,$$

$$\nabla_y \tilde{c}_1 \cdot \nu_0 = -e_j \cdot \nu_0 \quad \text{on } \Gamma_0(t,x), \quad (15b)$$

$$\tilde{c}_1 \text{ periodic in } y. \quad (15c)$$

Consequently, we are able to extract the following cell problems (15) in $\zeta_j$ for $j = 1, 2$ by linearity. As discussed above in deriving Darcy’s law, this procedure is synonymous to upscaling basic flow and transport in porous media [7].
Due to the linearity of the problem, the following representation of \( \tilde{c}_1 \) can be obtained:

\[
\tilde{c}_1(t, x, y) = \sum_j \zeta_j(t, x; y)(\partial_{x_j} c_0(t, x) + c_0(t, x)\partial_{x_j} \Phi_0(t, x)).
\]  

(16)

**Remark 2** In summary, we have proposed a macroscopic equation describing fluid flow: a new Darcy’s law (13) that, apart from the pressure gradient, directly involves the interaction force density in leading order. It is supplemented by cell problems (12) that enable us to calculate the permeability tensor \( \mathbb{K} \) (14), which is a time- and space-dependent macroscopic coefficient function. Moreover, we established a representation of the first order’s concentration correction \( \tilde{c}_1 \), c.f. (16).

### 4.3 Zero order problems

The last step in upscaling consists of investigating the zero order equations of (2) and (3). For the transport equation we obtain

\[
\partial_t c_0 - \nabla_x \cdot (-v_0 c_0 + \nabla_x c_0 + \nabla_y c_1 + c_0 \nabla_x \Phi_0 + c_0 \nabla_y \Phi_1)
\]

\[-\nabla_y \cdot (-v_0 c_0 - v_0 c_1 + \nabla_x c_1 + \nabla_y c_2 + c_0 \nabla_x \Phi_0 + c_1 \nabla_x \Phi_1 + c_0 \nabla_y \Phi_1 + c_0 \nabla_y \Phi_2) = 0.
\]

The corresponding boundary condition is of order \( \varepsilon^1 \). Here, it is crucial to bear the additional terms that come along with the evolving pore geometry in mind, c.f. [22]. In summary, we obtain

\[
(-v_1 c_0 - v_0 c_1 + \nabla_x c_1 + \nabla_y c_2) \cdot \nu_0 + (c_0 \nabla_x \Phi_1 + c_1 \nabla_x \Phi_0 + c_1 \nabla_y \Phi_1 + c_0 \nabla_y \Phi_2) \cdot \nu_0
\]

\[+ (-v_0 c_0 + \nabla_x c_0 + \nabla_y c_1 + c_0 \nabla_x \Phi_0 + c_0 \nabla_y \Phi_1) \cdot \nu_1
\]

\[+ y \cdot \nabla_x (-v_0 c_0 + \nabla_x c_0 + \nabla_y c_1 + c_0 \nabla_x \Phi_0 + c_0 \nabla_y \Phi_1) \cdot \nu_0
\]

\[+ \lambda \nu_0 \cdot \nabla_y (-v_0 c_0 + \nabla_x c_0 + \nabla_y c_1 + c_0 \nabla_x \Phi_0 + c_0 \nabla_y \Phi_1) \cdot \nu_0
\]

\[\partial_t c_0 - \alpha f(c_0, \rho)(c_0 - \rho) = 0.
\]

From these equations, we derive a macroscopic description of the transport processes via integration with respect to the fast variable \( y \), applying the boundary condition and the transport theorem in order to interchange integration and spatial derivation. With (8) and the Lemmata 3.1 and 3.2 in [22], which can be applied directly, several terms cancel and the cell problems (15) may be inserted as usual to derive

\[
\int_{Y_i(t, x)} \partial_t c_0 \, dy - \nabla_x \cdot \int_{Y_i(t, x)} (-v_0 c_0 + \nabla_x c_0 + \nabla_y \tilde{c}_1 + c_0 \nabla_x \Phi_0) \, dy
\]

\[= \int_{\Gamma_0(t, x)} \frac{1}{\rho} f(c_0, \rho)(c_0 - \rho) \, dy.
\]

Finally, interchanging integration and time derivative, we obtain

\[
\partial_t (|Y_i| c_0) + \nabla_x \cdot (\nabla_0 c_0) - \nabla_x \cdot (\mathbb{D}(\nabla_x c_0 + c_0 \nabla_x \Phi_0)) = -|\Gamma_0| f(c_0, \rho) \quad x \in \Omega
\]

(17)
with the diffusion tensor $D$ defined as
\[ D_{ij} := \int_{Y_{t_0}(t,x)} (\partial_i \zeta_j + \delta_{ij}) \, dy \] (18)

Finally, analyzing (3), the leading order level set $L_0$ fulfills
\[ \partial_t L_0 - \alpha f(c_0, \rho) |\nabla y L_0| = 0 \text{ in } Y \times \Omega. \] (19)

Remark 3 In summary, we have proposed a macroscopic equation describing transport of the leading order concentration $c_0$, c.f. (17). This description accounts for advection, diffusion, and drift as in (2a), but includes effective quantities. More precisely, cell problems (15) allow calculating the diffusion tensor $D$, c.f. (18), which is a time- and space-dependent macroscopic coefficient function. Moreover, the level set equation (19) changes to an equation comprising micro-macro structure.

5 Microscopic interaction potential

In this section, we consider the more general and sophisticated case of an interaction potential that has microscopic components, i.e. $\Phi_0(t, x, y) = \Phi_0(t, x, y)$. In comparison to the investigations in Section 4, here the upscaling procedure requires rather elaborate investigations including a change of principle variables. Moreover, accounting for the different scaling in Stokes’ equations (1) compared to [17], it is crucial to separate appropriate supplementary cell problems. Contrary to the cell problems arising in Section 4, c.f. (12) and (15), they exhibit a rather complex structure since they are fully coupled.

5.1 Lowest order problems

Starting our investigations, we analyze the lowest order terms of (1), (2), and (3) that arise after inserting expansion (4) - (8).

For the transport equation of lowest order ($\epsilon^{-2}$) with corresponding boundary condition of order $\epsilon^{-1}$, we obtain
\[ -\nabla_y \cdot (\nabla_y c_0 + c_0 \nabla_y \Phi_0) = 0, \]
\[ (\nabla_y c_0 + c_0 \nabla_y \Phi_0) \cdot \nu_0 = 0. \]

Applying the transformation
\[ c_\epsilon = e^{-\Phi_0} c_0 \] (20)

and inserting its zeroth order term according to the expansion (6), i.e. $c_0(t, x, y) = e^{-\Phi_0(t,x,y)} u_0(t, x, y)$, the above problem reduces to
\[ -\nabla_y \cdot (e^{-\Phi_0} \nabla_y u_0) = 0, \]
\[ e^{-\Phi_0} \nabla_y u_0 \cdot \nu_0 = 0. \]
This problem admits a uniquely defined solution (up to a constant with respect to $y$) and understandably every macroscopic solution $u_0(t,x)$ is a solution of this problem. As a consequence, we derive the following representation for the leading order concentration

$$c_0(t,x,y) = e^{-\Phi_0(t,x,y)}u_0(t,x).$$

(21)

Summarizing this result, the leading order concentration has microscopic components according to the influence of the general interaction potential, whereas the new principle variable $u_0(t,x)$ is a macroscopic quantity.

The lowest order problem of Stokes’ equation (1a) is of order $\varepsilon^{-1}$ and reads:

$$\nabla_y p_0 = -c_0 \nabla_y \Phi_0.$$

Inserting the transformation (20) and the properties being encoded in (21), we obtain

$$\nabla_y (p_0 - c_0) = 0,$$

which in fact yields the new principle variable

$$\tilde{p}_0 := p_0 - c_0$$

as a macroscopic quantity, i.e.

$$\tilde{p}_0(t,x,y) = \tilde{p}_0(t,x).$$

Remark 4 The transformation (20) is well known in the stationary theory of semiconductor devices [9, 18]. Moreover, it is strongly related to the linearization procedure of [12].

In summary, we have chosen two new principle variables, the transformed leading order concentration $u_0$ and the corrected pressure $\tilde{p}_0$ which are both macroscopic quantities.

5.2 Next order problems

We now consider the subsequent higher order terms of (1) and (2).

For Stokes’ equation (1a) we analyze the equation of order $\varepsilon^0$, supplemented by the incompressibility condition (1b) of order $\varepsilon^{-1}$ and boundary condition (1c) of order $\varepsilon^0$:

$$-\Delta_y v_0 + \nabla_y p_1 + \nabla_x p_0 = -c_0 \nabla_x \Phi_0 - c_1 \nabla_y \Phi_0 - c_0 \nabla_y \Phi_1,$$

$$\nabla_y \cdot v_0 = 0,$$

$$v_0 = 0.$$

We reformulate the problem taking into consideration the next order representation of (20) according to (6):

$$c_1(t,x,y) = e^{\Phi_0}u_1 - e^{-\Phi_0}u_0\Phi_1.$$

(23)
Bearing in mind the correction \( \tilde{p}_0 \) of the leading order pressure, c.f. (22), we define analogously the first order pressure correction \( \tilde{p}_1 := p_1 - e^{\Phi_0} u_1 + e^{-\Phi_0} u_0 \Phi_1 = p_1 - c_1 \). Finally, applying the chain rule leads to

\[
-\Delta_y v_0 + \nabla_y \tilde{p}_1 = -\nabla_x \tilde{p}_0 - e^{-\Phi_0} \nabla_x u_0 - e^{-\Phi_0} \nabla_y u_1, \\
\nabla_y \cdot v_0 = 0,
\]

\( v_0 = 0 \).

For the transport equation (2a), we consider the problem of order \( \varepsilon^{-1} \):

\[
- \nabla_y \cdot (v_0 c_0 + \nabla_y c_1 + \nabla_x c_0 + c_0 \nabla_y \Phi_1 + c_1 \nabla_y \Phi_0 + c_0 \nabla_x \Phi_0) - \nabla_x \cdot (\nabla_y c_0 + c_0 \nabla_y \Phi_0) - \nu_0 = 0.
\]

This equation is supplemented by the boundary condition (2b) of order \( \varepsilon^0 \):

\[
( -v_0 c_0 + \nabla_y c_1 + \nabla_x c_0 + c_0 \nabla_y \Phi_1 + c_1 \nabla_y \Phi_0 + c_0 \nabla_x \Phi_0 ) \cdot \nu_0 \\
+ (\nabla_y c_0 + c_0 \nabla_y \Phi_0) \cdot \nu_1 + y \cdot \nabla_x (\nabla_y c_0 + c_0 \nabla_y \Phi_0) \cdot \nu_0 \\
+ \lambda \nu_0 \cdot \nabla_y (\nabla_y c_0 + c_0 \nabla_y \Phi_0) \cdot \nu_0 = 0.
\]

Since the boundary conditions have to be applied to \( \Gamma_0(t, x) \), additional terms emerge due to the evolution of the pore space. The parameter \( \lambda \) occurring in the boundary condition is related to the expansion of the level set function \( L_\varepsilon \) in the following way [22]:

\[
\lambda = \frac{L_1}{|\nabla_y L_0|} - \frac{y \cdot \nabla_x L_0}{|\nabla_y L_0|} \quad y \in \Gamma_0(t, x).
\]

We now reformulate this problem by applying the chain rule in combination with (23).

\[
-\nabla_y \cdot (e^{-\Phi_0} \nabla_y u_1) = \nabla_y \cdot (-v_0 e^{-\Phi_0} u_0 + e^{-\Phi_0} \nabla_x u_0),
\]

\[
e^{-\Phi_0} \nabla_y u_1 \cdot \nu_0 = (v_0 e^{-\Phi_0} u_0 - e^{-\Phi_0} \nabla_x u_0) \cdot \nu_0.
\]

A crucial step at this point is to identify reasonable cell problems. First of all, we define the following, fully coupled cell problems of Stokes type in \((w_j, \pi_j)\) for \( j = 1, 2 \):

\[
-\Delta_y w_j^1 + \nabla_y \pi_j^1 + e^{-\Phi_0} \nabla_y \pi_j^1 = -e_j \quad \text{in } Y_{t,0}(t, x), \quad (24a)
\]

\[
\nabla_y \cdot w_j^1 = 0 \quad \text{in } Y_{t,0}(t, x), \quad (24b)
\]

\[
w_j^1 = 0 \quad \text{on } \Gamma_0(t, x), \quad (24c)
\]

\[
w_j^1, \pi_j^1 \text{ periodic in } y. \quad (24d)
\]

\[
-\Delta_y w_j^2 + \nabla_y \pi_j^2 + e^{-\Phi_0} \nabla_y \pi_j^2 = -e_j \quad \text{in } Y_{t,0}(t, x), \quad (25a)
\]

\[
\nabla_y \cdot w_j^2 = 0 \quad \text{in } Y_{t,0}(t, x), \quad (25b)
\]

\[
w_j^2 = 0 \quad \text{on } \Gamma_0(t, x), \quad (25c)
\]

\[
w_j^2, \pi_j^2 \text{ periodic in } y. \quad (25d)
\]
Due to the linearity of the problem, the leading order velocity term $v_0(x, y)$ and the higher order pressure correction $\tilde{p}_1$ are expressed in terms of the solutions $w_j$ and $\pi_j$ of the above cell problems (24) and (25), respectively. For the leading order velocity term $v_0(x, y)$ it holds that

$$v_0(x, y) = v_0^1(x, y) + v_0^2(x, y) = -\sum_j w_j^1(y) \partial_x \tilde{p}_0(x) + w_j^2(y) \partial_x u_0(x).$$

Hereby, the partial solutions $v_0^1$ and $v_0^2$ are defined as

$$v_0^1(x, y) = -\sum_j w_j^1(y) \partial_x \tilde{p}_0(x),$$

$$v_0^2(x, y) = -\sum_j w_j^2(y) \partial_x u_0(x).$$

Moreover, we obtain the following representation for the higher order pressure correction $\tilde{p}_1$

$$\tilde{p}_1(x, y) = \tilde{p}_1^1(x, y) + \tilde{p}_1^2(x, y) = -\sum_j \tilde{\pi}_j^1(y) \partial_x \tilde{p}_0(x) + \tilde{\pi}_j^2(y) \partial_x u_0(x)$$

and the partial solutions $\tilde{p}_1^1$ and $\tilde{p}_1^2$ are defined as

$$\tilde{p}_1^1(x, y) = -\sum_j \tilde{\pi}_j^1(y) \partial_x \tilde{p}_0(x),$$

$$\tilde{p}_1^2(x, y) = -\sum_j \tilde{\pi}_j^2(y) \partial_x u_0(x).$$

By integration with respect to the fast variable $y$, we derive Darcy’s law for the macroscopic velocity $\bar{v}_0(x)$.

$$\bar{v}_0 := \int_{Y_{t,0}(t,x)} v_0(x, y) dy = -\int_{Y_{t,0}(t,x)} \sum_j w_j^1(y) \partial_x \tilde{p}_0(x) + w_j^2(y) \partial_x u_0(x) dy$$

$$= -K_1 \nabla_x \tilde{p}_0 + K_2 \nabla_x u_0,$$

In this context, the permeability tensors

$$K^1_{ij} := \int_{Y_{t,0}(t,x)} (w^1)_i dy,$$

$$K^2_{ij} := \int_{Y_{t,0}(t,x)} (w^2)_i dy$$

are defined. Darcy’s law (26) is supplemented by the compressibility condition

$$\nabla_x \cdot \bar{v}_0 = \int_{\Gamma_{t,0}(t,x)} \beta f(c_0) do_y,$$
and by the boundary condition
\[ \mathbf{n}_0 = 0 \]
as was shown in [22].

By means of reformulating of Stokes’ equations and from the definition of the cell problems (24) and (25), we establish a representation of \( u_1 \)
\[ u_1(x, y) = u_1^1(x, y) + u_1^2(x, y) = - \sum_j \zeta_j^1(y) \partial_x \tilde{p}_0(x) + \zeta_j^2(y) \partial_x u_0(x) + C(x) \] (27)
with partial solutions
\[ u_1^1(x, y) = - \sum_j \zeta_j^1(y) \partial_x \tilde{p}_0(x) + C_1^1(x), \]
\[ u_1(x, y) = - \sum_j \zeta_j^2(y) \partial_x u_0(x) + C^2(x). \]
Hereby, \( C, C_1, C_2 \) are constants dependent upon the slow variable \( x \).

As a consequence of representation (27), the following cell problems in \( \zeta_j^1, \zeta_j^2 \) for \( j = 1, 2 \)
arise.
\[ -\nabla_y \cdot (e^{-\Phi_0} \nabla_y \zeta_j^1) = \nabla_y \cdot (e^{-\Phi_0} w_j^1 u_0) \quad \text{in } Y_{l,0}(t, x), \] (28a)
\[ (e^{-\Phi_0} \nabla_y \zeta_j^1) \cdot \nu_0 = -e^{-\Phi_0} w_j^1 u_0 \quad \text{on } \Gamma_{l,0}(t, x), \] (28b)
\[ \zeta_j^1 \text{ periodic in } y, \] (28c)
\[ -\nabla_y \cdot (e^{-\Phi_0} \nabla_y \zeta_j^2) = \nabla_y \cdot (e^{-\Phi_0} w_j^2 u_0 + e^{\Phi_0} e_j) \quad \text{in } Y_{l,0}(t, x), \] (29a)
\[ (e^{-\Phi_0} \nabla_y \zeta_j^2) \cdot \nu_0 = (-e^{-\Phi_0} w_j^2 u_0 e^{\Phi_0} e_j) \cdot \nu_0 \quad \text{on } \Gamma_{l,0}(t, x), \] (29b)
\[ \zeta_j^2 \text{ periodic in } y, \] (29c)

**Remark 5** Summarizing the results, we have obtained a macroscopic equation (Darcy’s law) describing the averaged fluid flow. Similar to (4), it involves the interaction potential in leading order. Darcy’s law is supplemented by cell problems (24) and (25), which enable us to calculate the time- and space-dependent permeability tensors \( K_1 \) and \( K_2 \). Moreover, we established the representation (27) of the first orders’ correction of the new principle variable, i.e. the transformed concentration \( u_1 \). Additionally, supplementary cell problems (28), and (29) are defined.

### 5.3 Zero order problems

Finally, we investigate the zero order equation of (2a) and (3a). As a consequence, for the transport equation, we consider
\[ \partial_t c_0 - \nabla_x \cdot (-v_0 c_0 + \nabla_x c_0 + \nabla_y c_1 + c_0 \nabla_x \Phi_0 + c_0 \nabla_y \Phi_1 + c_1 \nabla_y \Phi_0) \\
- \nabla_y \cdot (-v_1 c_0 - v_0 c_1 + \nabla_x c_1 + \nabla_y c_2 + c_0 \nabla_x \Phi_1 + c_1 \nabla_x \Phi_0 + c_1 \nabla_y \Phi_1 \\
+ c_2 \nabla_y \Phi_0 + c_0 \nabla_y \Phi_2) = 0. \]
The corresponding boundary condition is of order $\varepsilon^1$ and with the additional terms due to the evolving pore geometry [22] it reads:

\[
\begin{align*}
& (-v_1 c_0 - v_0 c_0 + \nabla x c + \nabla y c_2) \cdot v_0 \\
& + (c_0 \nabla x \Phi_0 + c_1 \nabla x \Phi_0 + c_2 \nabla y \Phi_0 + c_0 \nabla y \Phi_2) \cdot v_0 \\
& + (-v_0 e^{-\Phi_0} u_0 + e^{-\Phi_0} \nabla y (u_1 + u_0 \Phi_1) + e^{-\Phi_0} \nabla x u_0) \cdot v_1 \\
& + y \cdot \nabla x (-v_0 e^{-\Phi_0} u_0 + e^{-\Phi_0} \nabla y (u_1 + u_0 \Phi_1) + e^{-\Phi_0} \nabla x u_0) \cdot v_0 \\
& + \lambda \nu_0 \cdot \nabla y (-v_0 e^{-\Phi_0} u_0 + e^{-\Phi_0} \nabla y (u_1 + u_0 \Phi_1) + e^{-\Phi_0} \nabla x u_0) \cdot v_0 \\
& - \alpha f(c_0, \rho)(c_0 - \rho) = 0.
\end{align*}
\]

From these equations we want to derive a macroscopic description of the transport processes in the new principle variable. Defining $G = -v_0 c_0 + \nabla x c + c_0 \nabla x \Phi_0 + c_0 \nabla y \Phi_1 + c_1 \nabla y \Phi_0$, integrating with respect to $y$, applying the boundary condition

\[
\begin{align*}
& \int_{Y_{t,x}} \partial_t (e^{-\Phi_0} u_0) dy + \int_{\Gamma_{t,x}} \nabla_x \cdot G dy \\
& + \int_{\Gamma_{0(t,x)}} G \cdot \nu_1 + y \cdot \nabla_x (G \cdot \nu_0) + \lambda \nu_0 \cdot \nabla_y (G \cdot \nu_0) do_y \\
& - \int_{\Gamma_{0(t,x)}} \alpha f(e^{-\Phi_0} u_0, \rho)(e^{-\Phi_0} u_0 - \rho) do_y = 0.
\end{align*}
\]

Applying the transport theorem in order to interchange integration and spatial derivation, we obtain

\[
\begin{align*}
& \int_{Y_{t,x}} \partial_t (e^{-\Phi_0} u_0) dy + \nabla x \cdot \int_{Y_{t,x}} G dy - \int_{\Gamma_{0(t,x)}} \frac{\nabla x L_0}{\nabla y L_0} G do_y \\
& + \int_{\Gamma_{0(t,x)}} G \cdot \nu_1 + y \cdot \nabla_x (G \cdot \nu_0) + \lambda \nu_0 \cdot \nabla_y (G \cdot \nu_0) do_y \\
& - \int_{\Gamma_{0(t,x)}} \alpha f(e^{-\Phi_0} u_0, \rho)(e^{-\Phi_0} u_0 - \rho) do_y = 0.
\end{align*}
\]

With (8) and the lemmata 3.1 and 3.2 in [22], which can be applied directly, several terms cancel and we obtain

\[
\int_{Y_{t,x}} \partial_t (e^{-\Phi_0} u_0) dy + \nabla x \cdot \int_{Y_{t,x}} G dy = \int_{\Gamma_{0(t,x)}} \alpha f(e^{-\Phi_0} u_0, \rho)(e^{-\Phi_0} u_0 - \rho) do_y.
\]

Using the transport theorem for the time derivative and the boundary condition for the normal velocity we obtain

\[
\partial_t \left( \int_{Y_{t,x}} e^{-\Phi_0} u_0 dy \right) + \nabla x \cdot \int_{Y_{t,x}} G dy = - \int_{\Gamma_{0(t,x)}} f(e^{-\Phi_0} u_0, \rho) do_y.
\]
Here the transformations and the cell problems (28) and (29) may be inserted, and, in particular with (27), we obtain

\[
G = -v_0 c_0 + \nabla_x c_0 + \nabla_y c_1 + c_0 \nabla_x \Phi_0 + c_0 \nabla_y \Phi_1 + c_1 \nabla_y \Phi_0
\]

\[
= -v_0 c_0 + e^{-\Phi_0} \nabla_x u_0 + e^{-\Phi_0} \nabla_y u_1
\]

\[
= \left( \sum_j w_j(y) \partial_x \tilde{p}_0(x) + w_1^2(y) \partial_x u_0(x) \right) e^{-\Phi_0} u_0 + e^{-\Phi_0} \sum_j e_j \partial_x u_0
\]

\[
- e^{-\Phi_0} \left( \sum_j \zeta_j(y) \partial_x \tilde{p}_0(x) + \zeta_1(y) \partial_x u_0(x) \right)
\]

\[
= \left( \sum_j w_j(y) e^{-\Phi_0} u_0 - e^{-\Phi_0} \zeta_j(y) \right) \partial_x \tilde{p}_0(x)
\]

\[
+ \left( \sum_j w_j(y) e^{-\Phi_0} u_0 + e^{-\Phi_0} e_j - e^{-\Phi_0} \zeta_j(y) \right) \partial_x u_0(x)
\]

In summary, we derive

\[
\partial_t A u_0 + \nabla_x \cdot (D^1 \nabla_x \tilde{p}_0 + D^2 \nabla_x u_0) = - \int_{\Gamma_0(t,x)} \alpha f(e^{-\Phi_0} u_0, \rho) \rho \, d\sigma.
\]  

(30)

Finally, analyzing (3), the leading order level set \( L_0 \) fulfills

\[
\partial_t L_0 - \alpha f(e^{-\Phi_0} u_0, \rho) |\nabla_y L_0| = 0 \text{ in } Y \times \Omega.
\]  

(31)

**Remark 6** In summary, we proposed a macroscopic equation describing transport in the new leading order variable \( u_0 \), c.f. (30). It includes gradients of the new principle variables and also time- and space-dependent macroscopic coefficient functions. More precisely, the cell problems (28) and (29) enable calculating the diffusion tensors \( D^1, D^2 \). Moreover, the level set equation (31) changes again to an equation comprising micro-macro structure.

### 6 Discussion and conclusion

In this paper, a flow and transport model including a general interaction potential and an evolving solid-liquid interface has been investigated in a multi-scale context. The purpose of the current study was to establish a comprehensive and mathematically well-founded macroscopic model description of the underlying physical phenomena. To this end, two-scale asymptotic expansion in a level set framework was applied to the corresponding system of partial differential equations. Thereby, to different cases of interaction potential have been discussed and the respective upscaling results have been summarized in Theorem 3.1 and Theorem 3.2.

First, a purely macroscopic interaction potential was analyzed. There, the structure of the original partial differential equations describing transport and level set was reproduced and
coupling among the describing model equations were maintained throughout the upscaling procedure. However, due to the evolving microstructure, the upscaled level set equation additionally comprises a micro-macro structure. What is more, the transport equation is supplemented by cell problems that determine time- and space-dependent coefficients such as porosity and diffusion tensor. Likewise, the time- and space-dependent permeability tensor is characterized by means of the solution of certain cell problems. Admittedly, it is well known that Stokes’ equations transform into Darcy’s law while carrying out upscaling procedure. Nevertheless, new findings emerge from our study since, apart from the pressure gradient, the interaction force density is directly involved in Darcy’s law.

Second, and more interestingly, an interaction potential including microscopic components was analyzed. In doing so, two main features of our investigation should be highlighted. On the one hand, the application of the concentration’s transformation including the interaction potential was formalized, which was not necessary in the case of the purely macroscopic interaction potential. On the other hand, new principle variables have been introduced. This procedure enabled us at first to balance pressure and interaction forces and to define a similar Darcy’s law for the case of purely macroscopic interaction potential. Contrary to that case, two different permeability tensors and corresponding cell problems - one for each of the forcing terms - were defined. The second advantage of the new principle variables is that a macroscopic transport equation in the new macroscopic quantity was able to be defined.

As far as the upscaled transport equation is concerned, coupled supplementary cell problems determining diffusion tensor and porosity as time- and space-dependent averaged coefficient functions were defined. Similar to Darcy’s law, one family of cell problems for each forcing term emerges. Such complex couplings of cell problems have already been investigated in [2, 8] where linearized problems including electrostatics in rigid porous media were considered. In comparison to their work, additional complexity arose in this research due to the couplings generated by the changing geometry. Because of the nonlinear structure of the transformation (20) and its \( y \)-dependency, a trivial back-transformation from the new principle variables to the original variables is not possible. Instead, we point out that, in the case of a general interaction potential without explicit \( y \)-dependency, both of the previously discussed cases coincide. Moreover, in case of no interaction, i.e. \( \Phi \equiv 0 \), and also of no evolving microstructure, i.e. \( v_n \equiv 0, c_0 \equiv u_0 \) holds and the well-known averaged coefficient functions

\[
A = |Y_l|, \quad \bar{v}_0 = \int_{Y_l} v_0 \, dy, \quad \text{and} \quad D_{ij} = \int_{Y_l} (\partial_{y_i} \zeta_j^2 + \delta_{ij}) \, dy
\]

are reproduced. In this sense, the derived model is consistent with the standard model, c.f. [7].

In conclusion, we have investigated the consistent extension of a well-established multi-scale problem, i.e. a comprehensive model including general interaction potential and evolving microstructure consisting of the fully nonlinear partial differential equation (1), (2), and (3). For that reason, a wide range of applications including, but not limited to, electrostatics is accessible. Further research might numerically compare our results with those for lin-
earized systems with electrostatic interaction or to numerically illustrate the interplay of different interaction potentials such as electrostatic and van-der-Waals. In general, highly sophisticated numerical discretization is required to capture the numerous couplings and micro-macro structure of the problem. Such a thorough, numerical investigation with radially symmetrical geometry and circumstantial fluid flow and simple interaction potential has already been done in [17]. However, considerably more work must continue in that direction for new approaches to be developed and to make the results obtained mathematically more rigorous.

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