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Homogenization results for ionic transport in periodic porous media

Claudia Timofte

University of Bucharest, Faculty of Physics, P.O. Box MG-11, Bucharest, Romania

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ABSTRACT

The effective behavior of the solution of a nonlinear system of coupled partial differential equations arising in the modeling of ionic transport phenomena in electrically charged periodic porous media is rigorously analyzed. Our model can be useful for biophysicists to describe the ionic transport through protein channels. Also, this setting proves to be relevant in the modeling of the flow of electrons and holes in semiconductor devices. The main tool for obtaining our macroscopic model is the use of the periodic unfolding method, which enables us to deal with a large class of heterogeneous media.

1. Introduction

The main purpose of this paper is to describe the effective behavior of the solution of a system of coupled partial differential equations arising in the modeling of ionic transfer phenomena, coupled with electrocapillary effects, in electrically charged periodic porous media. The so-called *Nernst–Planck–Poisson system* was originally proposed by W. Nernst and M. Planck (see [1]) for describing the potential difference in galvanic cells and has nowadays broad applicability in electrochemistry, in biology, in plasma physics or in the semiconductor device modeling, where this system is also known as *van Roosbroeck system* (see [2]). For more details about the physical aspects behind these models and for a review of the recent relevant literature, the interested reader is referred to [1–6].

We deal, at the microscale, with a periodic structure modeling a saturated electrically charged porous medium. In such a periodic microstructure, we shall consider the Poisson–Nernst–Planck system, with suitable boundary and initial conditions. The diffusion in the fluid phase is governed by the Nernst–Planck equations, while the electric potential which influences the ionic transfer is described by the Poisson equation. Moreover, we include in our analysis electrocapillarity effects (see (1)). Arguing in a similar manner as in [3] or [4], we get the well posedness of this problem in suitable spaces and we can obtain proper energy estimates. The increased complexity of the geometry and of the governing equations implies that an asymptotic procedure must be applied for describing the solution of such a problem. The complicated microstructure will be homogenized in order to obtain a model that captures its averaged properties.

Via the periodic unfolding method recently developed by D. Cioranescu, A. Damlamian, P. Donato, G. Griso and R. Zaki (see [7–9]), we can show that the effective behavior of the solution of our problem is described by a new coupled system of equations (see (3)–(5)). In particular, the evolution of the macroscopic electrostatic potential is governed by a new law, similar to Grahame's law (see [3,10]).

Apart from a significant simplification in the proofs, an advantage of using such an approach based on unfolding operators, which transform functions defined on oscillating domains into functions acting on fixed domains, is that we can avoid using

E-mail address: claudiatimofte@yahoo.com.

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extension operators and, thus, we can deal in a rigorous manner with a large class of heterogeneous media. Moreover, the homogenized equations being defined on a fixed domain Ω and having simpler coefficients will be easier to be handled numerically than the original equations. The dependence on the initial microstructure can be seen at the limit in the homogenized coefficients.

Related problems have been addressed, using different techniques, in [3,4,11,12] or [5]. As already mentioned, our approach relies on a new method. More precisely, we use the periodic unfolding method, which enables us to work with a large class of heterogeneous media. Another novelty brought by our paper resides in dealing with a general nonlinear boundary condition for the electrostatic potential and with nonlinear reaction terms. Some of the results we present here were announced, without detailed proofs, in [13]. In the present paper, we give detailed proofs and we are concerned with much more general situations (for example, we deal here with the case of more general nonlinear functions $G(x, v)$ or $F^{\pm}$). The case in which we deal with nonsymmetric matrices and the problem of obtaining corrector results will be treated in a forthcoming paper.

The rest of the paper is structured as follows: in Section 2, we formulate the microscopic problem and in Section 3 we give the main convergence result. Section 4 is devoted to the proof of the homogenization process. The paper ends with some concluding remarks and a few references.

2. Setting of the problem

Let us describe the geometry of the problem. We assume that the porous medium possesses a periodic microstructure. We consider a bounded connected smooth open set Ω in $\mathbb{R}^n$, with $|\partial\Omega| = 0$ and with $n \geq 2$. In particular, we are interested in dealing with the physically relevant cases $n = 2$ or $n = 3$. We denote by $Y = (0, 1)^n$ the reference cell, which is supposed to be decomposed in two parts, the fluid phase Y_f and, respectively, the solid phase Y_s. The sets Y_f and Y_s are considered to be open, nonempty and disjoint sets, with

$$Y = Y_f \cup \overline{Y_s}.$$

We suppose that $\overline{Y_s} \subset Y$, Y_f is connected and the boundary $\Gamma = \partial Y_s$ is Lipschitz continuous. To simplify the presentation, we assume that Y_s is also connected, but this assumption can be easily removed, since, exactly like in [14], we can deal with the case in which Y_s has a finite number of connected components.

The small real parameter $\varepsilon < 1$ is considered to take values in a sequence of strictly positive numbers that converges to zero. For each $\mathbf{k} \in \mathbb{Z}^n$, let

$$Y_s^k = \mathbf{k} + Y_s$$

and

$$K_\varepsilon = \{\mathbf{k} \in \mathbb{Z}^n \mid \varepsilon\overline{Y_s^k} \subset \Omega\}.$$

We denote by

$$\Omega_\varepsilon^s = \bigcup_{\mathbf{k}\in K_\varepsilon} \varepsilon Y_s^k$$

the solid part, by

$$\Omega_\varepsilon = \Omega \setminus \overline{\Omega_\varepsilon^s}$$

the fluid part and by

$$\theta = \left|Y \setminus \overline{Y_s}\right|$$

the porosity of the medium. Let $\Gamma_\varepsilon = \partial\Omega_\varepsilon^s$ be the inner boundary of the porous medium, i.e. the interface between the fluid and the solid phases. It follows that $\Gamma_\varepsilon \cap \partial\Omega = \emptyset$. Thus, by construction, the domain Ω is the union of two disjoint parts, Ω_ε^s and Ω_ε, and their common boundary Γ_ε.

Let us notice that, for simplicity, we restricted ourselves here to a case in which the solid part does not touch the outer boundary, but the results given in this paper still hold true, with minor changes, in the case in which we keep the assumption that the fluid part is connected, but the solid one is allowed to meet the exterior boundary $\partial\Omega$ (see, for instance, [8,11] or [3]). Also, let us remark that more general geometric situations can be treated with the aid of the periodic unfolding method (for examples of some special structures, for which the reference cell Y is no longer a parallelotope, the interested reader is referred to [7]).

In such a periodic microstructure, we shall consider the Poisson–Nernst–Planck system, with suitable boundary and initial conditions. The diffusion in the fluid phase is governed by the Nernst–Planck equations, while the electric potential which influences the ionic transfer is described by the Poisson equation. Moreover, we include electrocapillary effects in our analysis.