J. Math. Anal. Appl. ••• (••••) •••–•••

Contents lists available at ScienceDirect

Journal of Mathematical Analysis and Applications

www.elsevier.com/locate/jmaa

Upscaling of a parabolic system with a large nonlinear surface reaction term

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ARTICLE INFO

Article history:
Received 18 May 2018
Available online xxxx
Submitted by H.-M. Yin

Keywords:
Homogenization
Fast reaction
Nonlinear transmission conditions

ABSTRACT

Motivated by the study of the dynamics of calcium ions in biological cells, the authors derived in [33], via periodic homogenization, a macroscopic bidomain model, by considering in the corresponding microscopic two-component problem a properly scaled nonlinear exchange term. We study here, at the microscopic scale, a similar parabolic system, with a large nonlinear interfacial reaction term. At the macroscopic scale, the nonlinear effect of this reaction term is recovered in the homogenized diffusion matrix, which is not anymore constant. This nonstandard phenomenon shows the fine interplay between reaction and diffusion in such processes.

1. Introduction

The study of the dynamics of calcium ions, acting as messengers between the endoplasmic reticulum and the cytosol inside living cells, represents a topic of huge interest in biology, which still requires special attention. The endoplasmic reticulum is a complex highly heterogeneous structure, which spreads throughout the cytoplasm (see [36]). In order to describe the dynamics of calcium ions in a living cell, it is natural to model such a cell as a domain Ω, which is a periodic structure made up of two connected constituents Ω_1^ε and Ω_2^ε, both reaching the external fixed boundary of the domain Ω and separated by an interface Γ^ε. Here, ε is a real positive small parameter, related to the characteristic dimension of the two constituents. In this model, the constituent Ω_1^ε represents the cytosol, while the constituent Ω_2^ε is the endoplasmic reticulum.

Our goal in this paper is to rigorously analyze, in such a geometry, the effective behavior of a parabolic coupled nonlinear system of reaction–diffusion equations describing the evolution of the concentrations of the calcium ions in the cell Ω. We consider, at the microscale, two equations governing the concentration of calcium ions in the cytosol and, in the endoplasmic reticulum, respectively, coupled through a large exchange term.

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https://doi.org/10.1016/j.jmaa.2018.09.028

More precisely, our aim is to study the asymptotic behavior, as the small parameter ε tends to zero, of the solution $u^\varepsilon = (u_1^\varepsilon, u_2^\varepsilon)$ of problem (1) below. This problem was studied in [33] for $\gamma \geq 0$ and $g^\varepsilon \equiv 0$. We recall that the significant case for biological applications, corresponding to $\gamma = 1$ and leading after homogenization to a bidomain model, was there fully addressed. Our main goal here is to extend the study in [33] to the case $\gamma < 0$, for a special nonlinear function H satisfying relation (3) (see also Remark 2.2), where the function h introduced in (3) verifies the hypotheses (H3). For $\gamma < 0$, the most challenging case, from a mathematical point of view, is the one corresponding to $\gamma = -1$. This models a fast nonlinear reaction taking place on the active interface Γ^ε. Similar fast surface reaction terms, giving significant effects at the macroscale, appear in the literature in several recent works, as for instance in [12], [7], [4], and [38]. Large nonlinear terms arise also in the context of problems involving flux jump (see [5], [6], and [38]), as well as in problems involving fast nonlinear volume reaction terms ([8], [48], and [25]). The non-zero function g^ε in (1), meaning that the flux is not continuous across Γ^ε, models the imperfect character of the biological membranes. For similar problems with jump in flux, we refer the reader to [28], [29], [5], [6], [39], [38], [15], [16], [17], [18], and [9].

In order to pass to the limit in problem (1), we choose to use the periodic unfolding operators from [22], adapted to time-dependent functions. The main difficulty of our study consists in the passage to the limit in the nonlinear terms defined on the oscillating interface Γ^ε. The convergence result for these terms is stated in Proposition 3.4. After passage to the limit in problem (1), we obtain system (26). We remark in this system the nonstandard form of the homogenized matrix given in (27), which is not constant, depending on the solution u itself, via $h'(u)$, the derivative of the nonlinear function h modeling the large exchange term across the interface Γ^ε. Such a phenomenon was announced in [50]. Up to our knowledge, this kind of dependence of the homogenized matrix on the derivative of h is new for problems in composite media with two connected constituents and with discontinuous solution across their common boundary, but it appears, in other contexts and for functions h explicitly given, in [7] and [38] (see Remark 3.7). For the dependence of the homogenized matrix on the solution u of the limit problem, we refer the reader to the recent papers [4], [5], [6], [24], [31], [46], and [20]. From a more physical point of view, this nonstandard form of the homogenized matrix shows that the large nonlinear reaction term present at the microscopic scale on the interface Γ^ε gives rise at the macroscopic scale to a modified diffusion matrix.

The layout of the paper is as follows: in Section 2, we set the microscopic problem and we give some properties of its solution. In Section 3, we state and prove the homogenization results. In Appendix, we give the definition and some properties of the periodic unfolding operators used throughout the paper and we recall some key results used in our proofs. We end the paper with some references.

2. Setting of the problem

For reader's convenience, we present the study of problem (1) in the domain $\Omega = (0,1)^N \subset \mathbb{R}^N$ $(N \geqslant 3)$, but we point out that more general domains Ω can be considered. We refer to [14] and [[34], Section 3.2] for such domains, for which all the extension results, whose use is crucial in Section 3 below, hold true. Roughly speaking, the domain Ω is the union of two sub-domains, both connected and reaching the boundary $\partial\Omega$ of Ω. The precise mathematical description of the domain is given below. Let $Y = (0,1)^N$ be the reference cell. We assume that Y_1 and Y_2 are two disjoint connected open subsets of the reference cell $Y = (0,1)^N$, with a common boundary Γ and such that both reach the boundary ∂Y of Y. We set $\partial Y_1 = \Gamma \cup \Gamma_1$ and $\partial Y_2 = \Gamma \cup \Gamma_2$, where Γ_α, for $\alpha \in \{1,2\}$, are the intersections of ∂Y_α with ∂Y. We suppose that Γ_α are identically reproduced on the opposite faces of Y. Also, for each $k \in \mathbb{Z}^N$, we denote $Y_\alpha^k = k + Y_\alpha$, for $\alpha \in \{1,2\}$. Let $\varepsilon \in (0,1)$ be a small parameter related to the characteristic dimension of the periodic structure, taking values in a positive real sequence tending to zero, such that the stretched domain $\varepsilon^{-1}\Omega$ can be represented as a finite union of axis-parallel cuboids having corner coordinates in $\mathbb{Z}^N$. For each ε, we define $\mathbb{Z}_\varepsilon = \left\{k \in \mathbb{Z}^N \,|\, \varepsilon Y_\alpha^k \cap \Omega \neq \emptyset,\ \alpha \in \{1,2\}\right\}$ and we set $\Omega_2^\varepsilon = \Omega \setminus \bigcup_{k\in\mathbb{Z}_\varepsilon} \left(\varepsilon \overline{Y_1^k}\right)$, $\Omega_1^\varepsilon = \Omega \setminus \overline{\Omega_2^\varepsilon}$ and $\Gamma^\varepsilon = \partial\Omega_1^\varepsilon \cap \Omega = \partial\Omega_2^\varepsilon \cap \Omega$. This geometry covers, for instance, the so-called "pipe-model" (see [14] for details