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Homogenization of the discrete diffusive coagulation–fragmentation equations in perforated domains

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A B S T R A C T

The asymptotic behavior of the solution of an infinite set of Smoluchowski's discrete coagulation–fragmentation–diffusion equations with non-homogeneous Neumann boundary conditions, defined in a periodically perforated domain, is analyzed. Our homogenization result, based on Nguetseng–Allaire two-scale convergence, is meant to pass from a microscopic model (where the physical processes are properly described) to a macroscopic one (which takes into account only the effective or averaged properties of the system). When the characteristic size of the perforations vanishes, the information given on the microscale by the non-homogeneous Neumann boundary condition is transferred into a global source term appearing in the limiting (homogenized) equations. Furthermore, on the macroscale, the geometric structure of the perforated domain induces a correction in the diffusion coefficients.

1. Introduction

This paper is devoted to the homogenization of an infinite set of Smoluchowski's discrete coagulation–fragmentation–diffusion equations in a periodically perforated domain. The system of evolution equations considered describes the dynamics of cluster growth, that is the mechanisms allowing clusters to coalesce to form larger clusters or break apart into smaller ones. These clusters can diffuse in space with a diffusion constant which depends on their size. Since the size of clusters is not limited *a priori*, the system of reaction–diffusion equations that we consider consists of an infinite number of equations. The structure of the chosen equations, defined in a perforated medium with a non-homogeneous Neumann condition on the boundary of the perforations, is useful for investigating several phenomena arising in porous media [14], [8], [13] or in the field of biomedical research [11].

Typically, in a porous medium, the domain consists of two parts: a fluid phase where colloidal species or chemical substances, transported by diffusion, are dissolved and a solid skeleton (formed by grains or

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pores) on the boundary of which deposition processes or chemical reactions take place. In recent years, the Smoluchowski equation has been also considered in biomedical research to model the aggregation and diffusion of β-amyloid peptide (Aβ) in the cerebral tissue, a process thought to be associated with the development of Alzheimer's disease. One can define a perforated geometry, obtained by removing from a fixed domain (which represents the cerebral tissue) infinitely many small holes (the neurons). The production of Aβ in monomeric form from the neuron membranes can be modeled by coupling the Smoluchowski equation for the concentration of monomers with a non-homogeneous Neumann condition on the boundaries of the holes.

The results of this paper constitute a generalization of some of the results contained in [14], [11], by considering an infinite system of equations where both the coagulation and fragmentation processes are taken into account. Unlike previous theoretical works, where existence and uniqueness of solutions for an infinite system of coagulation–fragmentation equations (with homogeneous Neumann boundary conditions) have been studied [19], [15], we focus in this paper on a distinct aspect, that is, the averaging of the system of Smoluchowski's equations over arrays of periodically-distributed microstructures.

Our homogenization result, based on Nguetseng–Allaire two-scale convergence [17], [1], is meant to pass from a microscopic model (where the physical processes are properly described) to a macroscopic one (which takes into account only the effective or averaged properties of the system).

1.1. Setting of the problem

Let Ω be a bounded open set in $\mathbb{R}^3$ with a smooth boundary $\partial\Omega$. Let Y be the unit periodicity cell $[0,1[^3$ (having the paving property). We perforate Ω by removing from it a set T_ϵ of periodically distributed holes defined as follows. Let us denote by T an open subset of Y with a smooth boundary Γ, such that $\overline{T} \subset \operatorname{Int} Y$. Set $Y^* = Y \setminus T$ which is called in the literature the solid or material part. We define $\tau(\epsilon\overline{T})$ to be the set of all translated images of $\epsilon\overline{T}$ of the form $\epsilon(k+\overline{T})$, $k \in \mathbb{Z}^3$. Then,

$$T_\epsilon := \Omega \cap \tau(\epsilon\overline{T}).$$

Introduce now the periodically perforated domain Ω_ϵ defined by

$$\Omega_\epsilon = \Omega \setminus \overline{T}_\epsilon.$$

For the sake of simplicity, we make the following standard assumption on the holes [6], [9]: there exists a 'security' zone around $\partial\Omega$ without holes, that is the holes do not intersect the boundary $\partial\Omega$, so that Ω_ϵ is a connected set.

The boundary $\partial\Omega_\epsilon$ of Ω_ϵ is then composed of two parts. The first one is the union of the boundaries of the holes strictly contained in Ω. It is denoted by Γ_ϵ and is defined by

$$\Gamma_\epsilon := \cup \left\{ \partial(\epsilon(k+\overline{T})) \mid \epsilon(k+\overline{T}) \subset \Omega \right\}.$$

The second part of $\partial\Omega_\epsilon$ is its fixed exterior boundary denoted by $\partial\Omega$. It is easily seen that (see [2], Eq. (3))

$$\lim_{\epsilon\to 0} \epsilon \mid \Gamma_\epsilon|_2 = |\Gamma|_2 \frac{|\Omega|_3}{|Y|_3}, \tag{1}$$

where $|\cdot|_N$ is the N-dimensional Hausdorff measure.

The previous definitions and Assumptions on Ω (and, T, Γ, Ω_ϵ, T_ϵ, Γ_ϵ, $\partial\Omega$) will be denoted in the rest of the paper as **Assumption 0**.