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Upscaling of Chemical Reactive Flows in Porous Media

by

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- Dedicated to Acad. Lazar Dragos at his 75th birthday anniversary -

Abstract

The aim of this paper is to study the asymptotic behavior of the solution of a nonlinear problem arising in the modeling of chemical reactive flows through periodically perforated domains. The asymptotic behavior of the solution of such a problem is governed by a new elliptic boundary-value problem with an extra zero-order term that captures the effect of the chemical reactions.

Key words and phrases: upscaling, reactive flows, Langmuir kinetics.
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1 Introduction

The aim of this paper is to study the asymptotic behavior of the solution of a nonlinear problem arising in the modelling of chemical reactive flows through periodically perforated domains. More precisely, we shall focus on the so-called Langmuir model (see [5]-[6] and the references therein). Let Ω be an open bounded set in $\mathbb{R}^n$ and let us perforate it by holes. As a result, we obtain an open set Ω^ε which will be referred to as being the *perforated domain* ; ε represents a small parameter related to the characteristic size of the perforations. We shall deal with the case in which the perforations are identical and periodically distributed and their size is of the order of ε. In these perforations we shall introduce a set of reactive solid grains (reactive obstacles).

The nonlinear problem studied in this paper concerns the stationary reactive flow of a fluid confined in Ω^ε, of concentration u^ε, reacting on the boundary of the perforations:

$$\begin{cases} -D_f \Delta u^\varepsilon + \beta(u^\varepsilon) = f \quad \text{in } \Omega^\varepsilon, \\ \\ -D_f \dfrac{\partial u^\varepsilon}{\partial \nu} = a\varepsilon g(u^\varepsilon) \quad \text{on } S^\varepsilon, \\ \\ u^\varepsilon = 0 \quad \text{on } \partial\Omega. \end{cases} \tag{1}$$

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Here, ν is the exterior unit normal to Ω^ε, $a > 0$, $f \in L^2(\Omega)$, S^ε is the boundary of the obstacles and $\partial\Omega$ is the fixed external boundary of Ω. Moreover, the fluid is assumed to be homogeneous and isotropic, with a constant diffusion coefficient $D_f > 0$.

We shall consider that the functions β and g in (1) are continuously differentiable functions, monotonously non-decreasing and such that $\beta(0) = 0$, $g(0) = 0$. This general situation is well illustrated by the following important practical examples, arising in the so-called Langmuir model:

$$\beta(v) = \frac{\lambda v}{1 + \mu v}, \quad \lambda, \mu > 0$$

and

$$g(v) = \frac{\delta v}{1 + \gamma v}, \quad \delta, \gamma > 0.$$

The existence and uniqueness of a weak solution of (1) can be settled by using the classical theory of semilinear monotone problems (see, for instance, [1] and [7]). As a result, we know that there exists a unique weak solution $u^\varepsilon \in V^\varepsilon \bigcap H^2(\Omega^\varepsilon)$, where

$$V^\varepsilon = \{v \in H^1(\Omega^\varepsilon) \mid v = 0 \text{ on } \partial\Omega\}.$$

From a geometrical point of view, we shall just consider periodic structures obtained by removing periodically from Ω, with period εY (where Y is a given hyper-rectangle in $\mathbb{R}^n$), an elementary hole T which has been appropriated rescaled and which is strictly included in Y, i.e. $\overline{T} \subset Y$.

As usual in homogenization, we shall be interested in obtaining a suitable description of the asymptotic behavior, as ε tends to zero, of the solution u^ε in such domains.

We shall see that the solution u^ε, properly extended to the whole of Ω, converges weakly in $H_0^1(\Omega)$ to the unique solution of the following homogenized problem:

$$\begin{cases} \displaystyle\sum_{i,j=1}^{n} q_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} + a \frac{|\partial T|}{\left|Y \setminus \overline{T}\right|} g(u) + \beta(u) = f \quad \text{in } \Omega, \\ u = 0 \quad \text{on } \partial\Omega. \end{cases} \tag{2}$$

Here, $Q = ((q_{ij}))$ is the classical homogenized matrix, whose entries are defined as follows:

$$q_{ij} = D_f \left(\delta_{ij} + \frac{1}{|Y \setminus T|} \int_{Y \setminus T} \frac{\partial \chi_j}{\partial y_i} dy \right) \tag{3}$$

in terms of the functions χ_i, $i = 1, ..., n$, solutions of the so-called cell problems

$$\begin{cases} -\Delta \chi_i = 0 \ \text{ in } \ Y \setminus \overline{T}, \\ \dfrac{\partial(\chi_i + y_i)}{\partial \nu} = 0 \ \text{ on } \ \partial T, \\ \chi_i \ \ Y - \text{ periodic.} \end{cases} \tag{4}$$

The approach we used is the so-called energy method introduced by L. Tartar [8] for studying homogenization problems. The structure of our paper is as follows: first, let us mention that we shall just focus on the case $n \geq 3$, which will be treated explicitly. The case $n = 2$ is much simpler and we shall omit to treat it here. In Chapter 2 we introduce some useful notations and assumptions and we give the main result. In Chapter 3 we give the proof of the main convergence result of this paper.

2 Preliminaries and the Main Result

Let Ω be a smooth bounded connected open subset of $\mathbb{R}^n$ $(n \geq 3)$ and let $Y = [0, l_1[\times ...[0, l_n[$ be the representative cell in $\mathbb{R}^n$. Denote by T an open subset of Y with smooth boundary ∂T such that $\overline{T} \subset Y$. We shall refer to T as being *the elementary hole.*
Let ε be a real parameter taking values in a sequence of positive numbers converging to zero. For each ε and for any integer vector $k \in \mathbb{Z}^n$, set T_k^ε the translated image of εT by the vector $kl = (k_1 l_1, ..., k_n l_n)$:

$$T_k^\varepsilon = \varepsilon(kl + T).$$

The set T_k^ε represents the holes in $\mathbb{R}^n$. Also, let us denote by T^ε the set of all the holes contained in Ω, i.e.

$$T^\varepsilon = \bigcup \left\{ T_k^\varepsilon \ \mid \ \overline{T_k^\varepsilon} \subset \Omega, \ k \in \mathbb{Z}^n \right\}.$$

Set

$$\Omega^\varepsilon = \Omega \setminus \overline{T^\varepsilon}.$$

Hence, Ω^ε is a periodically perforated domain with holes of size of the same order as the period. Remark that the holes do not intersect the boundary $\partial\Omega$.
Let

$$S^\varepsilon = \cup \{ \partial T_k^\varepsilon \mid \overline{T_k^\varepsilon} \subset \Omega, \ k \in \mathbb{Z}^n \}.$$

So

$$\partial\Omega^\varepsilon = \partial\Omega \cup S^\varepsilon.$$

We shall also use the following notations:

$$|\omega| = \text{ the Lebesgue measure of any measurable subset } \omega \text{ of } \mathbb{R}^n,$$

$$\chi_\omega = \text{ the characteristic function of the set } \omega,$$

$$Y^* = Y \setminus \overline{T},$$

and

$$\rho = \frac{|Y^*|}{|Y|}. \tag{5}$$

2.1 Setting of the problem

As already mentioned, we are interested in studying the behavior of the solution, in such a perforated domain, of the following problem:

$$\begin{cases} -D_f \Delta u^\varepsilon + \beta(u^\varepsilon) = f \quad \text{in } \Omega^\varepsilon, \\ -D_f \dfrac{\partial u^\varepsilon}{\partial \nu} = a\varepsilon g(u^\varepsilon) \quad \text{on } S^\varepsilon, \\ u^\varepsilon = 0 \quad \text{on } \partial\Omega. \end{cases} \tag{6}$$

Here, ν is the exterior unit normal to Ω^ε, $a > 0$, $f \in L^2(\Omega)$, S^ε is the boundary of the obstacles and $\partial\Omega$ is the fixed external boundary of Ω. Moreover, the fluid is assumed to be homogeneous and isotropic, with a constant diffusion coefficient $D_f > 0$.
We shall consider that the functions β and g in (6) are continuously differentiable functions, monotonously non-decreasing and such that $\beta(0) = 0$, $g(0) = 0$. We shall also suppose that there exist a positive constant C and an exponent q, with $0 \le q < n/(n-2)$, such that

$$\left| \frac{d\beta}{dv} \right| \le C(1 + |v|^q)$$

and

$$\left| \frac{dg}{dv} \right| \le C(1 + |v|^q).$$

This general situation is well illustrated by the above mentioned important practical examples (Langmuir model).
Let us introduce the functional space

$$V^\varepsilon = \{v \in H^1(\Omega^\varepsilon) \mid v = 0 \text{ on } \partial\Omega\},$$

with the norm

$$\|v\|_{V^\varepsilon} = \|\nabla v\|_{L^2(\Omega^\varepsilon)}.$$

The weak formulation of problem (6) is:

$$\begin{cases} \text{Find } u^\varepsilon \in V^\varepsilon \text{ such that} \\ D_f \displaystyle\int_{\Omega^\varepsilon} \nabla u^\varepsilon \cdot \nabla\varphi dx + a\varepsilon \int_{S^\varepsilon} g(u^\varepsilon)\varphi d\sigma + \\ + \displaystyle\int_{\Omega^\varepsilon} \beta(u^\varepsilon)\varphi dx = \int_{\Omega^\varepsilon} f\varphi dx \quad \forall \varphi \in V^\varepsilon. \end{cases} \tag{7}$$

By classical existence results (see [1]), there exists a unique weak solution $u^\varepsilon \in V^\varepsilon \cap H^2(\Omega^\varepsilon)$ of problem (7).
The solution u^ε of problem (7) being defined only on Ω^ε, we need to extend it to the whole of Ω to be able to state the convergence result. In order to do that, let us recall the following well-known extension result (see [4]):

LEMMA **1** *There exists a linear continuous extension operator* $P^\varepsilon \in \mathcal{L}(L^2(\Omega^\varepsilon); L^2(\Omega)) \cap \mathcal{L}(V^\varepsilon; H_0^1(\Omega))$ *and a positive constant* C*, independent of* ε*, such that*

$$\|P^\varepsilon v\|_{L^2(\Omega)} \leq C\,\|v\|_{L^2(\Omega^\varepsilon)}$$

and

$$\|\nabla P^\varepsilon v\|_{L^2(\Omega)} \leq C\,\|\nabla v\|_{L^2(\Omega^\varepsilon)}\,,$$

for any $v \in V^\varepsilon$. ▪

An immediate consequence of the previous lemma is the following Poincaré's inequality in V^ε :

LEMMA **2** *There exists a positive constant* C*, independent of* ε*, such that*

$$\|v\|_{L^2(\Omega^\varepsilon)} \leq C\,\|\nabla v\|_{L^2(\Omega^\varepsilon)}\,,$$

for any $v \in V^\varepsilon$. ▪

2.2 The main result

The main result of this paper is the following one:

THEOREM **1** *One can construct an extension* $P^\varepsilon u^\varepsilon$ *of the solution* u^ε *of the variational problem (7) such that*

$$P^\varepsilon u^\varepsilon \rightharpoonup u \quad \textit{weakly in } \ H_0^1(\Omega),$$

where u *is the unique solution of*

$$\begin{cases} -\displaystyle\sum_{i,j=1}^{n} q_{ij}\frac{\partial^2 u}{\partial x_i \partial x_j} + a\frac{|\partial T|}{|Y^*|}g(u) + \beta(u) = f \quad \textit{in } \Omega, \\ \\ u = 0 \quad \textit{on } \partial\Omega. \end{cases} \tag{8}$$

Here, $Q = ((q_{ij}))$ *is the classical homogenized matrix, whose entries are defined as follows:*

$$q_{ij} = D_f(\delta_{ij} + \frac{1}{|Y^*|}\int\limits_{Y^*}\frac{\partial \chi_j}{\partial y_i}dy), \tag{9}$$

in terms of the functions χ_i*,* $i = 1, ..., n$*, solutions of the so-called cell problems*

$$\begin{cases} -\Delta \chi_i = 0 \quad \textit{in } \ Y^*, \\ \\ \dfrac{\partial(\chi_i + y_i)}{\partial \nu} = 0 \quad \textit{on } \ \partial T, \\ \\ \chi_i \quad Y- \ \textit{periodic.} \end{cases} \tag{10}$$

The constant matrix Q *is symmetric and positive-definite.* ▪

3 Proof of the main result

Proof of Theorem 1. We divide the proof into three steps.

First step. Let $u^\varepsilon \in V^\varepsilon$ be the solution of the variational problem (7) and let $P^\varepsilon u^\varepsilon$ be the extension of u^ε inside the obstacles given by Lemma 1. Taking $\varphi = u^\varepsilon$ as a test function in (7), we easily get

$$\|P^\varepsilon u^\varepsilon\|_{H_0^1(\Omega)} \leq C.$$

Consequently, by passing to a subsequence, still denoted by $P^\varepsilon u^\varepsilon$, we can assume that there exists $u \in H_0^1(\Omega)$ such that

$$P^\varepsilon u^\varepsilon \rightharpoonup u \quad \text{weakly in } H_0^1(\Omega). \tag{11}$$

It remains to identify the limit equation satisfied by u.

Second step. For getting the effective behavior of our solution we have to pass to the limit in (7). In order to do this, following [3] and [6], let us introduce, for any $h \in L^p(\partial T)$, $1 \leq p \leq \infty$, the linear form μ_h^ε on $W_0^{1,s}(\Omega)$ defined by

$$\langle \mu_h^\varepsilon, \varphi \rangle = \varepsilon \int_{S^\varepsilon} h(\frac{x}{\varepsilon})\varphi d\sigma \quad \forall \varphi \in W_0^{1,s}(\Omega),$$

with $1/s + 1/p = 1$. From [3] we know that

$$\mu_h^\varepsilon \to \mu_h \quad \text{strongly in } (W_0^{1,s}(\Omega))', \tag{12}$$

where

$$\langle \mu_h, \varphi \rangle = \mu_h \int_\Omega \varphi dx,$$

with

$$\mu_h = \frac{1}{|Y|} \int_{\partial T} h(y) d\sigma.$$

Moreover, if h is constant, we have

$$\mu_h^\varepsilon \to \mu_h \quad \text{strongly in } W^{-1,\infty}(\Omega) \tag{13}$$

and we shall denote μ^ε the above introduced measure in the particular case in which $h = 1$. Notice that in this case μ_h becomes $\mu_1 = \dfrac{|\partial T|}{|Y|}$.

On the other hand, let us notice that, exactly like in [6], one can easily prove that for any $\varphi \in C_0^\infty(\Omega)$ and for any $z^\varepsilon \rightharpoonup z$ weakly in $H_0^1(\Omega)$, we get

$$\varphi g(z^\varepsilon) \rightharpoonup \varphi g(z) \quad \text{weakly in } W_0^{1,\overline{q}}(\Omega) \tag{14}$$

and

$$\varphi \beta(z^\varepsilon) \rightharpoonup \varphi \beta(z) \quad \text{weakly in } W_0^{1,\overline{q}}(\Omega), \tag{15}$$

where

$$\overline{q} = \frac{2n}{q(n-2)+n}.$$

Now, from (13) (with $h = 1$) and (14) written for $z^\varepsilon = P^\varepsilon u^\varepsilon$, we obtain

$$\langle \mu^\varepsilon, \varphi g(P^\varepsilon u^\varepsilon)\rangle \to \frac{|\partial T|}{|Y|} \int_\Omega \varphi g(u) dx \quad \forall \varphi \in C_0^\infty(\Omega). \tag{16}$$

Third step. Let ξ^ε be the gradient of u^ε in Ω^ε and let us denote by $\widetilde{\xi^\varepsilon}$ its extension with zero to the whole of Ω, i.e.

$$\widetilde{\xi^\varepsilon} = \begin{cases} \xi^\varepsilon & \text{in} \quad \Omega^\varepsilon, \\ 0 & \text{in} \quad \Omega \setminus \overline{\Omega^\varepsilon}. \end{cases}$$

Obviously, $\widetilde{\xi^\varepsilon}$ is bounded in $(L^2(\Omega))^n$ and hence there exists $\xi \in (L^2(\Omega))^n$ such that

$$\widetilde{\xi^\varepsilon} \rightharpoonup \xi \quad \text{weakly in } (L^2(\Omega))^n. \tag{17}$$

Let us see now which is the equation satisfied by ξ. Take $\varphi \in C_0^\infty(\Omega)$. From (7) we get

$$D_f \int_\Omega \widetilde{\xi^\varepsilon} \cdot \nabla \varphi dx + a\varepsilon \int_{S^\varepsilon} g(u^\varepsilon)\varphi d\sigma +$$

$$+ \int_\Omega \chi_{\Omega^\varepsilon} \beta(P^\varepsilon u^\varepsilon)\varphi dx = \int_\Omega \chi_{\Omega^\varepsilon} f \varphi dx. \tag{18}$$

Now, we can pass to the limit, with $\varepsilon \to 0$, in all the terms of (18). For the first one, we have

$$D_f \lim_{\varepsilon \to 0} \int_\Omega \widetilde{\xi^\varepsilon} \cdot \nabla \varphi dx = D_f \int_\Omega \xi \cdot \nabla \varphi dx. \tag{19}$$

For the second term, using (16), we get

$$\lim_{\varepsilon \to 0} a\varepsilon \int_{S^\varepsilon} g(u^\varepsilon)\varphi d\sigma = a \frac{|\partial T|}{|Y|} \int_\Omega g(u)\varphi dx. \tag{20}$$

On the other hand, we know that $\chi_{\Omega^\varepsilon} \rightharpoonup \dfrac{|Y^*|}{|Y|}$ weakly in any $L^\sigma(\Omega)$, with $\sigma \geq 1$. In particular, defining q^* such that

$$\frac{1}{\overline{q}} + \frac{1}{q^*} = 1,$$

we see that $q^* \geq 1$ and, consequently,

$$\chi_{\Omega^\varepsilon} \rightharpoonup \frac{|Y^*|}{|Y|}, \text{ weakly in } L^{q^*}(\Omega).$$

Hence, we obtain

$$\lim_{\varepsilon\to 0}\int_{\Omega}\chi_{\Omega^\varepsilon}\beta(u^\varepsilon)\varphi dx = \frac{|Y^*|}{|Y|}\int_{\Omega}\beta(u)\varphi dx. \tag{21}$$

It is not difficult to pass to the limit in the right-hand side of (18). Indeed, we obtain

$$\lim_{\varepsilon\to 0}\int_{\Omega}\chi_{\Omega^\varepsilon} f\varphi dx = \frac{|Y^*|}{|Y|}\int_{\Omega} f\varphi dx. \tag{22}$$

Putting together (19)-(22), we have

$$D_f\int_{\Omega}\xi\cdot\nabla\varphi dx + a\frac{|\partial T|}{|Y|}\int_{\Omega} g(u)\varphi dx +$$

$$+\frac{|Y^*|}{|Y|}\int_{\Omega}\beta(u)\varphi dx = \frac{|Y^*|}{|Y|}\int_{\Omega} f\varphi dx, \quad \forall\varphi\in\mathcal{D}(\Omega).$$

Hence ξ verifies

$$-D_f \operatorname{div}\xi + a\frac{|\partial T|}{|Y|}g(u) + \frac{|Y^*|}{|Y|}\beta(u) = \frac{|Y^*|}{|Y|}f \quad \text{ in } \Omega. \tag{23}$$

It remains now to identify ξ. Introducing the auxiliary periodic problem (10) and following a standard procedure (see, for instance, [6]), one easily gets

$$D_f \operatorname{div}\xi = \frac{|Y^*|}{|Y|}\sum_{i,j=1}^{n} q_{ij}\frac{\partial^2 u}{\partial x_i\partial x_j}.$$

Hence, we get exactly the limit equation (8). Since $u\in H_0^1(\Omega)$ (i.e. $u=0$ on $\partial\Omega$) and u is uniquely determined, the whole sequence $P^\varepsilon u^\varepsilon$ converges to u and Theorem 1 is proved. ∎

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