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ON THE HOMOGENIZATION OF A TRANSMISSION PROBLEM ARISING IN CHEMISTRY

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Abstract. The aim of this paper is to study the asymptotic behavior of the solution of a transmission problem in some chemical reactive flows through periodically perforated domains. The domain is considered to be a fixed bounded open subset $\Omega\subset\mathbf{R}^n$, in which identical and periodically distributed perforations (holes) of size ε are made. 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 associated to the homogenized medium.

Key words: homogenization, energy method, chemical reactive flows.

1. INTRODUCTION

The aim of this paper is to study the asymptotic behavior of the solution of a transmission problem in some chemical reactive flows through periodically perforated domains.

Let Ω be an open bounded set in $\mathbf{R}^n$ 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 (holes) are identical and periodically distributed and their size is of the order of ε. We shall consider that a granular material fills the holes and we shall be interested in studying the stationary reactive flow of a fluid confined in Ω^ε, of concentration u^ε, assuming that the reactive fluid is allowed to penetrate inside the grains, where chemical reactions take place (for the case in which the chemical reactions take place on the walls of the porous medium, see [4]-[6]). If we denote the concentration inside the grains by v^ε, a simplified setting of this kind of models is as follows:

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

where ν is the exterior unit normal to Ω^ε, $a > 0$, $\Pi^\varepsilon = \Omega \setminus \overline{\Omega^\varepsilon}$, S^ε is the boundary of the holes and $\partial\Omega$ is the external boundary of Ω. D_f and D_p are constant diffusion coefficients, characterizing the reactive fluid and, respectively, the granular material filling the holes.

We shall consider that the function f in (1) is a continuously differentiable function, monotonously non-decreasing and such that $f(0) = 0$.

The function in g is supposed to be given. We shall assume that g is continuous, monotone increasing and such that $g(0) = 0$. This general situation is well illustrated by the following two important practical examples:

a) $g(v) = \dfrac{\alpha v}{1 + \beta v}, \quad \alpha, \beta > 0$ (Langmuir kinetics)

b) $g(v) = |v|^{p-1} v, \quad 0 < p < 1$ (Freundlich kinetics)

The existence and uniqueness of a weak solution of (1) can be settled by using the classical theory of semilinear monotone problems (see [1] and [7]).

If we define θ^ε as being:

$$\theta^\varepsilon = \begin{cases} u^\varepsilon(x) & x \in \Omega^\varepsilon, \\ v^\varepsilon(x) & x \in \Pi^\varepsilon, \end{cases} \tag{2}$$

and we introduce

$$A = \begin{cases} D_f Id & \text{in } Y \setminus T, \\ D_p Id & \text{in } T, \end{cases}$$

then our main result of convergence for this model shows that θ^ε converges weakly in $H_0^1(\Omega)$ to the unique solution of the following homogenized problem:

$$\begin{cases} -\displaystyle\sum_{i,j=1}^{n} a_{ij}^0 \frac{\partial^2 u}{\partial x_i \partial x_j} + a \frac{|T|}{|Y \setminus T|} g(u) = f(u) & \text{in } \Omega, \\ \\ u = 0 & \text{on } \partial\Omega. \end{cases} \tag{3}$$

Here, $A^0 = ((a_{ij}^o))$ is the homogenized matrix, whose entries are defined as follows:

$$a_{ij}^{0} = \frac{1}{|Y|}\int_Y (a_{ij}(y) + a_{ik}(y)\frac{\partial \chi_j}{\partial y_k})dy \tag{4}$$

in terms of the functions χ_j, solutions of the so-called cell problems

$$\begin{aligned} &-\mathrm{div}_y (A(y)(D(\chi_j + y_j)) = 0, \quad \text{in } Y, \\ &\chi_j \text{ is } Y-\text{periodic.} \end{aligned} \tag{5}$$

The approach we used is the so-called energy method introduced by L. Tartar [9] for studying homogenization problems. It consists of constructing suitable test functions that are used in our variational problems. Also, let us mention that another possible way to get the limit problem (3) could be to use the two-scale convergence technique, coupled with periodic modulation (see [5] and the references therein).

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.

Finally, notice that throughout the paper, by C we shall denote a generic fixed strictly positive constant, whose value can change from line to line.

2. PRELIMINARIES AND THE MAIN RESULT

2.1. Notation and assumptions

Let Ω be a bounded connected open set in $\mathbf{R}^n$, with boundary $\partial\Omega$ of class C^2. Let $Y = [0, l_1[\times\{0, l_2[\times \ldots \times [0, l_n[$ be the representative cell in $\mathbf{R}^n$ and T an open subset of Y with boundary ∂T of class C^2, such that $\overline{T} \subset Y$. We shall refer to T as being *the elementary hole*. We shall denote by $T^{\varepsilon,k}$ the translated image of εT by εkl, $k \in \mathbf{Z}^n$. Also, we shall denote by T^{ε} the set of all the holes contained in Ω and by $\Omega^{\varepsilon} = \Omega \setminus \overline{T^{\varepsilon}}$. Hence, Ω^{ε} is a periodically perforated domain with holes of the same size as the period. Let us remark that the holes do not intersect the boundary $\partial\Omega$.

We shall also use the following notations:

$$Y^* = Y \setminus \overline{T}, \quad S^{\varepsilon} = \partial T^{\varepsilon}, \quad \theta = \frac{|Y^*|}{|Y|}.$$

Also, we shall denote by χ^{ε} the characteristic function of the domain Ω^{ε}.

2.2. 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:

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

Here, ν is the exterior unit normal to Ω^ε, $a > 0$, $\Pi^\varepsilon = \Omega \setminus \overline{\Omega^\varepsilon}$, S^ε is the boundary of the holes and $\partial\Omega$ is the external boundary of Ω. D_f and D_p are constant diffusion coefficients, , characterizing the reactive fluid and, respectively, the granular material filling the holes.

We shall consider that the function f in (6) is a continuously differentiable function, monotonously non-decreasing and such that $f(0) = 0$. We shall also suppose that there exist a positive constant C and an exponent q, with $0 \le q < n/(n-2)$, such that

$$\left| \frac{\partial f}{\partial u} \right| \le C(1 + |u|^q). \tag{7}$$

The function g in (6) is assumed to be given. We shall assume that g is continuous, monotone increasing and such that $g(0) = 0$. This general situation is well illustrated by the above mentioned important practical examples (Langmuir and Freundlich kinetics). Moreover, we shall suppose that there exist a positive constant C and an exponent q, with $0 \le q < n/(n-2)$, such that

$$|g(v)| \le C(1 + |v|^{q+1}). \tag{8}$$

Let us introduce the functional space

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

with

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

Also, let us consider the space

$$H^\varepsilon = \{ w^\varepsilon = (u^\varepsilon, v^\varepsilon) \mid u^\varepsilon \in V^\varepsilon, v^\varepsilon \in H^1(\Pi^\varepsilon), u^\varepsilon = v^\varepsilon \text{ on } S^\varepsilon \},$$

with the norm

$$\|w^\varepsilon\|^2_{H^\varepsilon} = \|\nabla u^\varepsilon\|^2_{L^2(\Omega^\varepsilon)} + \|\nabla v^\varepsilon\|^2_{L^2(\Pi^\varepsilon)}.$$

The variational formulation of problem (6) is the following one:

$$\begin{cases} \text{Find } w^{\varepsilon} \in H^{\varepsilon} \text{ such that} \\ D_f \int_{\Omega^{\varepsilon}} \nabla u^{\varepsilon} \cdot \nabla \varphi dx + D_p \int_{\Pi^{\varepsilon}} \nabla v^{\varepsilon} \cdot \nabla \psi dx + \\ + a \int_{\Pi^{\varepsilon}} g(v^{\varepsilon}) \psi dx = \int_{\Omega^{\varepsilon}} f(u^{\varepsilon}) \varphi dx, \ \forall (\varphi, \psi) \in H^{\varepsilon}. \end{cases} \tag{9}$$

Under the above structural hypotheses and the conditions fulfilled by H^{ε}, it is well-known by classical existence and uniqueness results (see [1] and [7]) that (9) is a well-posed problem.

Let us introduce again

$$A = \begin{cases} D_f Id & \text{in} \quad Y \setminus T, \\ D_p Id & \text{in} \quad T. \end{cases}$$

In order to describe the asymptotic behavior of the solution of problem (9), let us recall the following well-known extension results (see [2]-[3]):

Lemma 2.1. There exists a linear continuous extension operator $P^{\varepsilon} \in L(L^2(\Omega^{\varepsilon}); L^2(\Omega)) \cap L(V^{\varepsilon}; H_0^1(\Omega))$ and a positive constant C, independent of ε, such that

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

and

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

for any $v \in V^{\varepsilon}$.

An immediate consequence of the previous lemma is the following

Poincaré's inequality in V^{ε}:

Lemma 2.2. There exists a positive constant C, independent of ε, such that

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

for any $v \in V^{\varepsilon}$. Apart from these results, let us recall the following one (see [8]):

Lemma 2.3. There exists a positive constant C, independent of ε, such that

$$\left\| v \right\|^2_{L^2(S^{\varepsilon})} \leq C(\varepsilon^{-1} \left\| v \right\|^2_{L^2(\Omega^{\varepsilon})} + \varepsilon \left\| \nabla v \right\|^2_{L^2(\Omega^{\varepsilon})}),$$

for any $v \in V^{\varepsilon}$. Also,

$$\left\| v \right\|^2_{L^2(\Pi^{\varepsilon})} \leq C(\varepsilon \left\| v \right\|^2_{L^2(S^{\varepsilon})} + \varepsilon^2 \left\| \nabla v \right\|^2_{L^2(\Pi^{\varepsilon})}),$$

for every $v \in H^1(\Pi^{\varepsilon})$.

2.3. The main result

The main result of this paper is the following one:

Theorem 2.4. Let u^ε be the unique solution of the problem (6). Then, there exists an extension $P^\varepsilon u^\varepsilon$ of u^ε into all Ω, positive inside the holes, such that $P^\varepsilon u^\varepsilon \to u$ weakly in $H_0^1(\Omega)$ and u is the unique solution of:

$$\begin{cases} -\sum_{i,j=1}^{n} a_{ij}^0 \dfrac{\partial^2 u}{\partial x_i \partial x_j} + a\dfrac{|T|}{|Y^*|} g(u) = f(u) \quad \text{in} \quad \Omega, \\ u = 0 \quad \text{on} \quad \partial\Omega. \end{cases} \tag{10}$$

Here, $A^0 = ((a_{ij}^o))$ is the homogenized matrix, whose entries are defined as follows:

$$a_{ij}^0 = \frac{1}{|Y|}\int_Y (a_{ij}(y) + a_{ik}(y)\frac{\partial \chi_j}{\partial y_k})dy \tag{11}$$

in terms of the functions χ_j, solutions of the so-called cell problems

$$\begin{aligned} & -\operatorname{div}_y (A(y)(D(\chi_j + y_j)) = 0, \quad \text{in } Y, \\ & \chi_j \text{ is } Y-\text{periodic.} \end{aligned} \tag{12}$$

The constant matrix A^0 is symmetric and positive-definite.

3. PROOF OF THE MAIN RESULT

In order to describe the effective behavior of u^ε and v^ε, we need to prove some a priori estimates for them.

Proposition 3.1. Let u^ε and v^ε be the solutions of the problem (6). There exists a positive constant C, independent of ε, such that

$$\left\| P^\varepsilon u^\varepsilon \right\|_{H_0^1(\Omega)} \le C, \tag{13}$$

$$\left\| \tilde{v}^\varepsilon \right\|_{L^2(\Omega)} \le C, \tag{14}$$

$$\left\| \nabla w^\varepsilon \right\|_{L^2(\Omega^\varepsilon)\times L^2(\Pi^\varepsilon)} \le C, \tag{15}$$

$$\left\| P^\varepsilon u^\varepsilon - v^\varepsilon \right\|_{L^2(\Pi^\varepsilon)} \le C\varepsilon. \tag{16}$$

Proof. Let us take $(u^{\varepsilon}, v^{\varepsilon})$ as a test function in (9). Using the properties of f and g, Hölder and Poincaré's inequalities, the first three estimates come immediately. In order to get the fourth one, we shall make use of Lemma 2.3.:

$$\left\| P^{\varepsilon} u^{\varepsilon} - v^{\varepsilon} \right\|^2_{L^2(\Pi^{\varepsilon})} \leq C(\varepsilon \left\| u^{\varepsilon} - v^{\varepsilon} \right\|^2_{L^2(S^{\varepsilon})} + \varepsilon^2 \left\| \nabla (P^{\varepsilon} u^{\eta} - v^{\varepsilon}) \right\|^2_{L^2(\Pi^{\varepsilon})}) \leq$$

$$\leq C\varepsilon^2 (\left\| \nabla P^{\varepsilon} u^{\varepsilon} \right\|_{L^2(\Omega)} + \left\| \nabla v^{\varepsilon} \right\|^2_{L^2(\Pi^{\varepsilon})})^2 \leq$$

$$\leq C\varepsilon^2 (\left\| \nabla u^{\varepsilon} \right\|_{L^2(\Omega^{\varepsilon})} + \left\| \nabla v^{\varepsilon} \right\|^2_{L^2(\Pi^{\varepsilon})})^2 \leq C\varepsilon^2$$

and this concludes the proof.

Corollary 3.2. If u^{ε} and v^{ε} are the solutions of the problem (6), then, passing to a subsequence, still denoted by ε, there exist $u \in H^1_0(\Omega)$ and $v \in L^2(\Omega)$ such that

$$P^{\varepsilon} u^{\varepsilon} \to u \quad \text{weakly in } H^1_0(\Omega), \tag{17}$$

$$\tilde{v}^{\varepsilon} \to v \quad \text{weakly in } L^2(\Omega), \tag{18}$$

$$v = \frac{|T|}{|Y|} u. \tag{19}$$

Proof. The convergence results (17)-(19) are direct consequences of the estimates (13)-(16).

Finally, let us note that there exists a positive constant C, independent of ε, such that

$$\int_{\Omega} \left| \theta^{\varepsilon} \right|^2 dx \leq C$$

and

$$\int_{\Omega} \left| \nabla \theta^{\varepsilon} \right|^2 dx \leq C.$$

Hence, there exists $\theta \in H^1_0(\Omega)$ such that

$$\theta^{\varepsilon} \to \theta \quad \text{weakly in } H^1_0(\Omega)$$

and it is not difficult to see that $\theta = u$. This proves, in fact, the following

Corollary 3.3. Let θ^{ε} be defined by (2). Then, there exists $\theta \in H^1_0(\Omega)$ such that

$$\theta^\varepsilon \to \theta \quad \text{weakly in} \quad H_0^1(\Omega),$$

where θ is the unique solution of

$$\begin{cases} -\sum_{i,j=1}^n a_{ij}^0 \dfrac{\partial^2\theta}{\partial x_i \partial x_j} + a\dfrac{|T|}{|Y^*|} g(\theta) = f(\theta) & \text{in} \quad \Omega, \\ \theta = 0 & \text{on} \quad \partial\Omega. \end{cases}$$

and A^0 is given by (11)-(12), i.e. $\theta = u$, due to the well-posedness of problem (9).

Proof of Theorem 2.4. Set

$$\xi^\varepsilon = (\xi_1^\varepsilon, \xi_2^\varepsilon) = (D_f \nabla u^\varepsilon, D_p \nabla v^\varepsilon).$$

From (15) it follows that there exists a positive constant C such that

$$\|\xi_1^\varepsilon\|_{L^2(\Omega^\varepsilon)} \le C,$$

$$\|\xi_2^\varepsilon\|_{L^2(\Pi^\varepsilon)} \le C.$$

If we denote by ~ the zero extension to the whole of Ω of functions defined on Ω^ε or Π^ε, we see that $\tilde{\xi}_1^\varepsilon$ and $\tilde{\xi}_2^\varepsilon$ are bounded in $(L^2(\Omega))^n$ and, hence, there exist $\xi_1, \xi_2 \in (L^2(\Omega))^n$ such that

$$\tilde{\xi}_i^\varepsilon \to \xi_i \quad \text{weakly in} \quad (\mathrm{L}^2(\Omega))^n, \quad i = 1,2. \tag{20}$$

Let us now see which is the equation satisfied by ξ_1 and ξ_2. Let $\phi \in C_0^\infty(\Omega)$. Taking $(\phi|_{\Omega^\varepsilon}, \phi|_{\Pi^\varepsilon})$ as a test function in (9) we get

$$\int_\Omega \tilde{\xi}_1^\varepsilon \cdot \nabla\phi dx + \int_\Omega \tilde{\xi}_2^\varepsilon \cdot \nabla\phi dx + a\int_{\Pi^\varepsilon} g(v^\varepsilon)\phi dx = \int_\Omega \chi_{\Omega^\varepsilon} f(u^\varepsilon)\phi dx. \tag{21}$$

Now, we can pass to the limit, with $\varepsilon \to 0$, in all the terms of (21). For the first two, we have

$$\lim_{\varepsilon\to 0} \int_\Omega \tilde{\xi}_i^\varepsilon \cdot \nabla\phi dx = \int_\Omega \xi_i \cdot \nabla\phi dx,. \quad i = 1,2. \tag{22}$$

In order to pass to the limit in the third term, let us notice that, exactly like in [5], one can easily prove that for any $\phi \in C_0^\infty(\Omega)$ and for any $z^\varepsilon \to z$ weakly in $H_0^1(\Omega)$, we get

$$\phi g(z^{\varepsilon}) \to \phi g(z) \quad \text{strongly in } L^{\bar{q}}(\Omega), \tag{23}$$

where

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

In particular, we have

$$\phi g(\theta^{\varepsilon}) \to \phi g(\theta) \quad \text{strongly in } L^{\bar{q}}(\Omega), \tag{24}$$

Now, let us write $a\int_{\Pi^{\varepsilon}} g(v^{\varepsilon})\phi dx$ as

$$a\int_{\Pi^{\varepsilon}} g(v^{\varepsilon})\phi dx = a\int_{\Omega} g(\theta^{\varepsilon})\phi dx - a\int_{\Omega^{\varepsilon}} g(\theta^{\varepsilon})\phi dx.$$

Obviously

$$\lim_{\varepsilon \to 0} a\int_{\Omega} g(\theta^{\varepsilon})\phi dx = a\int_{\Omega} g(\theta)\phi dx = a\int_{\Omega} g(u)\phi dx.$$

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

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

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

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

Hence, we obtain:

$$\lim_{\varepsilon \to 0} a\int_{\Pi^{\varepsilon}} g(v^{\varepsilon})\phi dx = a\frac{|T|}{|Y|}\int_{\Omega} g(u)\phi dx. \tag{25}$$

It is not difficult to pass to the limit in the right-hand side of (21). We get

$$\lim_{\varepsilon \to 0} \int_{\Omega} \chi_{\Omega^{\varepsilon}} f(u^{\varepsilon})\phi dx = \frac{|Y^*|}{|Y|}\int_{\Omega} f(u)\phi dx. \tag{26}$$

Putting together (22), (25) and (26), we have

$$\int_\Omega \tilde{\xi}_1 \cdot \nabla\phi dx + \int_\Omega \tilde{\xi}_2 \cdot \nabla\phi dx + a\frac{|T|}{|Y|}\int_\Omega g(u)\phi dx =$$

$$= \frac{|Y^*|}{|Y|}\int_\Omega f(u)\phi dx, \forall\phi \in C_0^\infty(\Omega.$$

Hence

$$-\operatorname{div}(\xi_1 + \xi_2) + a\frac{|T|}{|Y|}g(u) = \frac{|Y^*|}{|Y|}f(u) \quad \text{in} \quad \Omega.$$

It remains now to identify $\xi_1 + \xi_2$. Introducing the auxiliary periodic problem (12) and following a standard procedure (see [5]), one easily gets

$$\xi_1 + \xi_2 = A^0\nabla u.$$

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 and Theorem 2.4. is proved.

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