On the Homogenization of a Semilinear Problem Arising in Chemistry

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Abstract: This paper deals with the homogenization of a nonlinear model for chemical reactive flows involving diffusion, adsorption and chemical reactions which take place at the boundary of a periodically perforated material. The effective behavior of such a reactive flow is described by a new elliptic boundary-value problem, containing an extra zero-order term which captures the effect of the adsorption and chemical reactions taking place on the boundaries of the perforations.

1. Introduction.

The aim of this paper is to study the effective behavior of chemical reactive flows involving diffusion, adsorption and chemical reactions which take place at the boundary of a periodically perforated material.

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. In fact, the domain Ω consists of two parts: a fluid phase Ω^ε and a solid skeleton (grains or pores), $\Omega \setminus \overline{\Omega}^\varepsilon$. We assume that chemical substances are dissolved in the fluid part Ω^ε. They are transported by diffusion and also, by adsorption, they can change from being dissolved in the fluid to residing on the surface of the pores. Here, on the boundary, chemical reactions take place. Hence, the model consists of a diffusion system in the fluid phase Ω^ε, a reaction system on the pore surface and a boundary condition coupling them (see (2)):

$$(V^\varepsilon) \begin{cases} \dfrac{\partial v^\varepsilon}{\partial t}(t,x) - D\Delta v^\varepsilon(t,x) = h(t,x), \quad x \in \Omega^\varepsilon,\, t > 0, \\ v^\varepsilon(t,x) = 0, \quad x \in \partial\Omega,\, t > 0, \\ v^\varepsilon(t,x) = v_1(x), \quad x \in \Omega^\varepsilon,\, t = 0, \end{cases} \tag{1}$$

$$-D\frac{\partial v^\varepsilon}{\partial \nu}(t,x) = \varepsilon f^\varepsilon(t,x), \quad x \in S^\varepsilon,\, t > 0, \tag{2}$$

and

$$(W^\varepsilon)\quad \begin{cases} \dfrac{\partial w^\varepsilon}{\partial t}(t,x) + a w^\varepsilon(t,x) = f^\varepsilon(t,x), \quad x \in S^\varepsilon,\, t > 0, \\ w^\varepsilon(t,x) = w_1(x), \quad x \in S^\varepsilon,\, t = 0, \end{cases} \tag{3}$$

where

$$f^\varepsilon(t,x) = \gamma(g(v^\varepsilon(t,x)) - w^\varepsilon(t,x)). \tag{4}$$

Here, ν is the exterior unit normal to Ω^ε, $a, \gamma > 0$, h is a given function representing an external source of energy, $v_1, w_1 \in H_0^1(\Omega)$ and S^ε is the boundary of our porous medium $\Omega \setminus \overline{\Omega^\varepsilon}$. Moreover, the fluid is assumed to be homogeneous and isotropic, with a constant diffusion coefficient $D > 0$. In (1)-(4), v^ε can be interpreted as being the concentration of the solute in the fluid region, w^ε as the concentration of the solute on the surface of the skeleton $\Omega \setminus \overline{\Omega^\varepsilon}$, v_1 as the initial concentration of the solute and w_1 as the initial concentration of the reactants on the surface S^ε of the skeleton; a and γ are called *the reaction factor* and *the adsorption factor*, respectively.

The semilinear boundary condition on S^ε in problem (1)-(4) describes the interchanges of chemical flows across the boundary S^ε. The function g in (2)-(4) is assumed to be given. We shall consider the case in which g is a monotone smooth function satisfying the condition $g(0) = 0$. For more general functions g, see [5]. This general situation is well illustrated by the following important practical example (see [5] and [7]):

$$g(v) = \frac{\alpha v}{1 + \beta v}, \quad \alpha, \beta > 0 \quad \text{(Langmuir kinetics)}.$$

The existence and uniqueness of a weak solution of the system (1)-(4) can be settled by using the classical theory of semilinear monotone problems (see, for instance, [1] and [9]). As a result, we know that there exists a unique weak solution $u^\varepsilon = (v^\varepsilon, w^\varepsilon)$.

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 F which has been appropriated rescaled and which is strictly included in Y, i.e. $\overline{F} \subset Y$.

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. If we denote by $\star$ the convolution with respect to time and if

$$r(\rho) = e^{-(a+\gamma)\rho}, \tag{5}$$

then we prove that the solution v^ε, properly extended to the whole of Ω, converges to the unique solution v (effective behavior) of the following problem:

$$(V)\quad \begin{cases} \dfrac{\partial v}{\partial t}(t,x) - D \displaystyle\sum_{i,j=1}^{n} q_{ij} \frac{\partial^2 v}{\partial x_i \partial x_j}(t,x) + F_0(t,x) = h(t,x), \quad t > 0,\ x \in \Omega, \\ v(t,x) = 0, \quad t > 0,\ x \in \partial\Omega, \\ v(t,x) = v_1(x), \quad t = 0,\ x \in \Omega, \end{cases} \tag{6}$$

with

$$F_0(t,x) = \frac{|\partial F|}{|Y \setminus \overline{F}|} \gamma \left[g(v(t,x)) - w_1(x) e^{-(a+\gamma)t} - \gamma r(\cdot) \star g(v(\cdot,x))(t) \right]. \tag{7}$$

In (6), $Q = ((q_{ij}))$ is the classical homogenized matrix, whose entries are defined as follows:

$$q_{ij} = \delta_{ij} + \frac{1}{\left|Y \setminus \overline{F}\right|} \int_{Y \setminus \overline{F}} \frac{\partial \chi_j}{\partial y_i} dy, \tag{8}$$

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

$$\begin{cases} -\Delta \chi_i = 0 \quad \text{in} \quad Y \setminus \overline{F}, \\ \dfrac{\partial(\chi_i + y_i)}{\partial \nu} = 0 \quad \text{on} \quad \partial F, \\ \chi_i \quad Y - \text{ periodic.} \end{cases} \tag{9}$$

Moreover, let us notice that the limit problem for the surface concentration w is

$$\begin{cases} \dfrac{\partial w}{\partial t}(t,x) + (a+\gamma) w(t,x) = \gamma g(v(t,x)), \quad t > 0,\, x \in \Omega, \\ w(t,x) = w_1(x), \quad t = 0,\, x \in \Omega \end{cases} \tag{10}$$

and obviously w can be written as

$$w(t,x) = w_1(x) e^{-(a+\gamma)t} + \gamma r(\cdot) \star g(v(\cdot, x))(t). \tag{11}$$

Also, notice that the influence of the adsorption and chemical reactions taking place on the boundaries of the perforations is reflected by the appearance of a zero-order extra-term.

In problem (1)-(4), the rate of chemical reactions on S^ε, namely a, and the adsorption coefficient γ were assumed to be constant. From a practical point of view, a more realistic model would be to assume that the surface ∂F is chemically and physically heterogeneous, which means that a and γ are rapidly oscillating functions. Moreover, one can consider a more general model, including the diffusion of the chemical species on the surface S^ε. In fact, the chemical substances can creep on the surface and this effect is similar to a surface-like diffusion. From a mathematical point of view, we can model this phenomenon by introducing a diffusion term in the law governing the evolution of the surface concentration w^ε. This new term is nothing but the Laplace-Beltrami operator properly rescaled. The limit problem in this case is almost the same as before, except that it involves the solution of a reaction-diffusion system with respect to an additional microvariable. Also, notice that the local behavior is no longer governed by an ordinary differential equation, but by a partial differential one (see (57)).

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 more simpler and we shall omit to treat it. In Chapter 2 we consider the simpler case of chemical flows just involving homogeneous adsorption and chemical reactions. After stating some notation and assumptions, we give a rigorous setting of the problem and we formulate the main convergence result, the proof of which is given in Chapter 3. The last part of Chapter 3 is devoted to treat a more general model, namely the case where the surface of the grains is heterogeneous and we have also diffusion thereon.

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.

In this chapter, we will be concerned with some preliminary notation and assumptions, as well as with the rigorous setting of our main model.

2.1. Notation and assumptions

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 F an open subset of Y with smooth boundary ∂F such that $\overline{F} \subset Y$. We shall refer to F as being *the elementary hole*. Also, let $[0, T]$, with $T > 0$, be the time interval of interest.

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 εF by the vector $kl = (k_1 l_1, ..., k_n l_n)$:

$$F_k^\varepsilon = \varepsilon(kl + F).$$

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

$$F^\varepsilon = \bigcup \left\{ F_k^\varepsilon \;\mid\; \overline{F_k^\varepsilon} \subset \mathbf{\Omega},\ \mathbf{k} \in \mathbb{Z}^{\mathbf{n}} \right\}.$$

Set

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

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

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

So

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

We shall also use the following notations:

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

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

and

$$Y^* = Y \setminus \overline{F}, \quad \theta = \frac{|Y^*|}{|Y|}.$$

In the sequel, we shall use the following notations:

$$H = L^2(\Omega),$$

with the classical scalar product and norm:

$$(u, v)_\Omega = \int_\Omega u(x)v(x)dx, \quad \|u\|_\Omega^2 = (u, u)_\Omega,$$

$$\mathcal{H} = L^2(0, T; H),$$

with

$$(u,v)_{\Omega,T} = \int_0^T (u(t),v(t))_\Omega dt, \quad \text{where } u(t)=u(t,\cdot), v(t)=v(t,\cdot),\ \|u\|^2_{\Omega,T} = (u,u)_{\Omega,T},$$

$$V = H^1(\Omega),$$

with

$$(u,v)_V = (u,v)_\Omega + (\nabla u, \nabla v)_\Omega,$$
$$\mathcal{V} = L^2(0,T;V),$$

with

$$(u,v)_{\mathcal{V}} = \int_0^T (u(t),v(t))_V dt,$$

$$\mathcal{W} = \left\{ v \in \mathcal{V} \,|\, \frac{dv}{dt} \in \mathcal{V}' \right\} \quad \text{where } \mathcal{V}' \text{ is the dual space of } \mathcal{V},$$

$$\mathcal{V}_0 = \{ v \in \mathcal{V} \,|\, v = 0 \text{ on } \partial\Omega \text{ a.e. on } (0,T) \},$$

$$\mathcal{W}_0 = \mathcal{V}_0 \bigcap \mathcal{W}.$$

Similarly, we define the spaces $V(\Omega^\varepsilon)$, $\mathcal{V}(\Omega^\varepsilon)$, $V(S^\varepsilon)$ and $\mathcal{V}(S^\varepsilon)$. Also, for the space of test functions we use the notation

$$\mathcal{D} = C_0^\infty((0,T)\times\Omega)).$$

Moreover, for an arbitrary function $\psi \in L^2(\Omega^\varepsilon)$, we shall denote by $\widetilde{\psi}$ its extension by zero inside the holes.

2.2. Setting of the problem

As already mentioned, we are interested in studying the behavior of the solution $u^\varepsilon = (v^\varepsilon, w^\varepsilon)$, in such a perforated domain, of the following problem:

$$(V^\varepsilon) \quad \begin{cases} \dfrac{\partial v^\varepsilon}{\partial t}(t,x) - D\Delta v^\varepsilon(t,x) = h(t,x), & x \in \Omega^\varepsilon,\ t>0, \\ v^\varepsilon(t,x) = 0, \quad x \in \partial\Omega,\ t>0, \\ v^\varepsilon(t,x) = v_1(x), \quad x \in \Omega^\varepsilon,\ t=0, \end{cases} \tag{12}$$

$$-D\frac{\partial v^\varepsilon}{\partial \nu}(t,x) = \varepsilon f^\varepsilon(t,x), \quad x \in S^\varepsilon,\ t>0, \tag{13}$$

and

$$(W^\varepsilon) \quad \begin{cases} \dfrac{\partial w^\varepsilon}{\partial t}(t,x) + a w^\varepsilon(t,x) = f^\varepsilon(t,x), & x \in S^\varepsilon,\ t>0, \\ w^\varepsilon(t,x) = w_1(x), \quad x \in S^\varepsilon,\ t=0, \end{cases} \tag{14}$$

where

$$f^\varepsilon(t,x) = \gamma(g(v^\varepsilon(t,x)) - w^\varepsilon(t,x)). \tag{15}$$

Here, ν is the exterior unit normal to Ω^ε, $a, \gamma > 0$, $h \in \mathcal{H}$, $v_1, w_1 \in H_0^1(\Omega)$ and S^ε is the boundary of our porous medium $\Omega \setminus \overline{\Omega^\varepsilon}$. Moreover, the fluid is assumed to be homogeneous and isotropic, with a constant diffusion coefficient $D > 0$.

The function g in (15) is assumed to be given. As already mentioned, we shall consider here the case in which g is a continuously differentiable function, monotonously nondecreasing and such that $g(v) = 0$ iff $v = 0$. Also, we shall suppose that there exist a positive constant C and an exponent q, with $0 \leq q < n/(n-2)$, such that

$$\left|\frac{\partial g}{\partial v}\right| \leq C(1 + |v|^q). \tag{16}$$

The weak formulation of problem (12)-(15) is:

$$\begin{cases} \text{Find } v^\varepsilon \in \mathcal{W}_0(\Omega^\varepsilon), v^\varepsilon(0) = v_1|_{\Omega^\varepsilon} \text{ such that} \\ -\left(v^\varepsilon, \dfrac{d\varphi}{dt}\right)_{\Omega^\varepsilon,T} + \varepsilon\left(f^\varepsilon, \varphi\right)_{\Omega^\varepsilon,T} = -D\left(\nabla v^\varepsilon, \nabla\varphi\right)_{\Omega^\varepsilon,T} + (h, \varphi)_{\Omega^\varepsilon,T}, \quad \forall \varphi \in \mathcal{W}_0(\Omega^\varepsilon) \end{cases} \tag{17}$$

and

$$\begin{cases} \text{Find } w^\varepsilon \in \mathcal{W}(S^\varepsilon), w^\varepsilon(0) = w_1|_{S^\varepsilon} \text{ such that} \\ -\left(w^\varepsilon, \dfrac{d\varphi}{dt}\right)_{S^\varepsilon,T} + a\left(w^\varepsilon, \varphi\right)_{S^\varepsilon,T} = \left(f^\varepsilon, \varphi\right)_{S^\varepsilon,T}, \quad \forall \varphi \in \mathcal{W}(S^\varepsilon). \end{cases} \tag{18}$$

By classical existence results (see [1] and [9]), there exists a unique weak solution $u^\varepsilon = (v^\varepsilon, w^\varepsilon)$ of the system (17)-(18).

Remark 2.1. *Let us notice that the solution of (14) can be written as*

$$w^\varepsilon(t, x) = w_1(x)e^{-(a+\gamma)t} + \gamma \int_0^t e^{-(a+\gamma)(t-s)} g(v^\varepsilon(s, x))ds \tag{19}$$

or, if we denote by $\star$ the convolution with respect to time, as

$$w^\varepsilon(\cdot, x) = w_1(x)e^{-(a+\gamma)t} + \gamma r(\cdot) \star g(v^\varepsilon(\cdot, x)), \tag{20}$$

where

$$r(\rho) = e^{-(a+\gamma)\rho}.$$

The solution v^ε of problem (V^ε) 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 [3] and [6]):

Lemma 2.2. *There exists a linear continuous extension operator $P^\varepsilon \in \mathcal{L}(L^2(\Omega^\varepsilon); L^2(\Omega)) \cap \cap \mathcal{L}(V^\varepsilon; H_0^1(\Omega))$ 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 $v \in V^\varepsilon$, where

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

with

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

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

Lemma 2.3. *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 $v \in V^\varepsilon$. $\blacksquare$

We also recall the following well-known result (see [4]):

Lemma 2.4. *There exists a positive constant C, independent of ε, such that*

$$\|v\|^2_{L^2(S^\varepsilon)} \leq C(\varepsilon^{-1} \|v\|^2_{L^2(\Omega^\varepsilon)} + \varepsilon \|\nabla v\|^2_{L^2(\Omega^\varepsilon)}), \tag{21}$$

for any $v \in V^\varepsilon$. $\blacksquare$

2.3. The main result

The main result of this paper is the following one:

Theorem 2.5. *One can construct an extension $P^\varepsilon v^\varepsilon$ of the solution v^ε of the problem (V^ε) such that*

$$P^\varepsilon v^\varepsilon \rightharpoonup v \quad \text{weakly in } \mathcal{V},$$

where v is the unique solution of the following limit problem:

$$\begin{cases} \dfrac{\partial v}{\partial t}(t,x) + F_0(t,x) - D \displaystyle\sum_{i,j=1}^{n} q_{ij} \frac{\partial^2 v}{\partial x_i \partial x_j}(t,x) = h(t,x), \quad t > 0,\ x \in \Omega, \\ v(t,x) = 0, \quad t > 0,\ x \in \partial\Omega, \\ v(t,x) = v_1(x), \quad t = 0,\ x \in \Omega, \end{cases} \tag{22}$$

with

$$F_0(t,x) = \frac{|\partial F|}{|Y^\star|}\gamma \left[g(v(t,x)) - w_1(x) e^{-(a+\gamma)t} - \gamma r(\cdot) \star g(v(\cdot,x))(t) \right].$$

In (22), $Q = ((q_{ij}))$ is the classical homogenized matrix, whose entries are defined as follows:

$$q_{ij} = \delta_{ij} + \frac{1}{|Y^*|} \int_{Y^*} \frac{\partial \chi_j}{\partial y_i} dy \tag{23}$$

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

$$\begin{cases} -\Delta \chi_i = 0 \quad in \quad Y^*, \\ \dfrac{\partial(\chi_i + y_i)}{\partial \nu} = 0 \quad on \quad \partial F, \\ \chi_i \quad Y- \ \ periodic. \end{cases} \tag{24}$$

The constant matrix Q is symmetric and positive-definite. Moreover, the limit problem for the surface concentration is:

$$\begin{cases} \dfrac{\partial w}{\partial t}(t,x) + (a+\gamma)w(t,x) = \gamma g(v(t,x)), \quad t>0,\, x\in\Omega, \\ w(t,x) = w_1(x), \quad t=0,\, x\in\Omega \end{cases} \tag{25}$$

and obviously, w can be written as

$$w(t,x) = w_1(x)e^{-(a+\gamma)t} + \gamma r(t)\star g(v(t,x)). \quad \blacksquare \tag{26}$$

Remark 2.6. *The weak formulation of problem (22) is:*

$$\begin{cases} \text{Find } v\in\mathcal{W}_0(\Omega), v(0)=v_1 \text{ such that} \\ -\left(v, \dfrac{d\varphi}{dt}\right)_{\Omega,T} + (F_0,\varphi)_{\Omega,T} = -D(Q\nabla v, \nabla\varphi)_{\Omega,T} + (h,\varphi)_{\Omega,T} \\ \forall\varphi\in\mathcal{W}_0(\Omega). \end{cases} \tag{27}$$

3. Proof of the main result.

In order to prove Theorem 2.5, let us first notice that there is at most one solution of the weak problem (27). Secondly, for describing the effective behavior of v^ε and w^ε, as $\varepsilon\to 0$, some a priori estimates on these solutions are required.

Proposition 3.1. *Let v^ε and w^ε be the solutions of the problem (12)-(15). There exists a positive constant C, independent of ε, such that*

$$\|w^\varepsilon(t)\|^2_{S^\varepsilon} \le (\|w^\varepsilon(0)\|^2_{S^\varepsilon} + \frac{\gamma}{\delta}\|g(v^\varepsilon)\|^2_{S^\varepsilon,t})e^{\gamma\delta t}, \quad \forall t\ge 0, \forall\delta>0, \tag{28}$$

$$\left\|\frac{\partial w^\varepsilon}{\partial t}\right\|^2_{S^\varepsilon,t} \le C(\|w^\varepsilon(0)\|^2_{S^\varepsilon} + \|g(v^\varepsilon)\|^2_{S^\varepsilon,t}), \quad \forall t\ge 0, \tag{29}$$

$$\|v^\varepsilon(t)\|^2_{\Omega^\varepsilon} \le C,\ \|\nabla v^\varepsilon(t)\|^2_{\Omega^\varepsilon,t} \le C \tag{30}$$

and

$$\left\|\frac{\partial v^\varepsilon}{\partial t}(t)\right\|^2_{\Omega^\varepsilon} \le C. \quad \blacksquare \tag{31}$$

Proof. From (14) we obtain

$$\int_{S^\varepsilon} \frac{\partial w^\varepsilon}{\partial t} w^\varepsilon d\sigma + \int_{S^\varepsilon} (a+\gamma)(w^\varepsilon)^2 d\sigma = \int_{S^\varepsilon} \gamma g(v^\varepsilon) w^\varepsilon d\sigma.$$

Therefore

$$\frac{1}{2}\frac{d}{dt}\|w^\varepsilon\|^2_{S^\varepsilon} + (a+\gamma)\|w^\varepsilon\|^2_{S^\varepsilon} \le \gamma\|g(v^\varepsilon)\|_{S^\varepsilon}\|w^\varepsilon\|_{S^\varepsilon} \le$$

$$\leq \gamma \left(\frac{\|g(v^\varepsilon)\|^2_{S^\varepsilon}}{2\delta} + \frac{\delta}{2} \|w^\varepsilon\|^2_{S^\varepsilon} \right), \quad \forall \delta > 0.$$

Integrating with respect to t and using Gronwall's inequality, we get

$$\|w^\varepsilon(t)\|^2_{S^\varepsilon} \leq \left(\|w^\varepsilon(0)\|^2_{S^\varepsilon} + \frac{\gamma}{\delta} \|g(v^\varepsilon)\|^2_{S^\varepsilon, t} \right) e^{\gamma \delta t}, \quad \forall t \geq 0, \forall \delta > 0. \tag{32}$$

In a similar manner we can obtain

$$\left\| \frac{\partial w^\varepsilon}{\partial t} \right\|^2_{S^\varepsilon, t} \leq C \left(\|w^\varepsilon(0)\|^2_{S^\varepsilon} + \|g(v^\varepsilon)\|^2_{S^\varepsilon, t} \right), \quad \forall t \geq 0. \tag{33}$$

Let us now prove (30). Multiplying (12) by v^ε, using (13)-(15) and integrating over Ω^ε, we have

$$\int_{\Omega^\varepsilon} \frac{\partial v^\varepsilon}{\partial t} v^\varepsilon dx + D \int_{\Omega^\varepsilon} \nabla v^\varepsilon \nabla v^\varepsilon dx + \varepsilon \int_{S^\varepsilon} \gamma (g(v^\varepsilon) - w^\varepsilon) v^\varepsilon d\sigma = \int_{\Omega^\varepsilon} h v^\varepsilon dx.$$

Therefore

$$\frac{1}{2} \frac{d}{dt} \|v^\varepsilon\|^2_{\Omega^\varepsilon} + D \|\nabla v^\varepsilon\|^2_{\Omega^\varepsilon} + \varepsilon \gamma \int_{S^\varepsilon} g(v^\varepsilon) v^\varepsilon d\sigma = \varepsilon \gamma \int_{S^\varepsilon} w^\varepsilon v^\varepsilon d\sigma + \int_{\Omega^\varepsilon} h v^\varepsilon dx \leq$$

$$\leq \varepsilon \gamma \|w^\varepsilon\|_{S^\varepsilon} \|v^\varepsilon\|_{S^\varepsilon} + C \|v^\varepsilon\|_{\Omega^\varepsilon} \leq$$
$$\leq \varepsilon \gamma \|w^\varepsilon\|_{S^\varepsilon} \|v^\varepsilon\|_{S^\varepsilon} + \frac{D}{2} \|\nabla v^\varepsilon\|^2_{\Omega^\varepsilon} + C.$$

Hence

$$\frac{1}{2} \frac{d}{dt} \|v^\varepsilon\|^2_{\Omega^\varepsilon} + \frac{D}{2} \|\nabla v^\varepsilon\|^2_{\Omega^\varepsilon} + \varepsilon \gamma \int_{S^\varepsilon} g(v^\varepsilon) v^\varepsilon d\sigma \leq \varepsilon \gamma \|w^\varepsilon\|_{S^\varepsilon} \|v^\varepsilon\|_{S^\varepsilon} + C.$$

Using Young's inequality and (28), we get

$$\frac{1}{2} \frac{d}{dt} \|v^\varepsilon\|^2_{\Omega^\varepsilon} + \frac{D}{2} \|\nabla v^\varepsilon\|^2_{\Omega^\varepsilon} + \varepsilon \gamma \int_{S^\varepsilon} g(v^\varepsilon) v^\varepsilon d\sigma \leq C_1 \varepsilon \|w^\varepsilon\|^2_{S^\varepsilon} + C_2 \varepsilon \|v^\varepsilon\|^2_{S^\varepsilon} + C \leq$$

$$\leq C_3 \varepsilon \|w^\varepsilon(0)\|^2_{S^\varepsilon} + C_4 \varepsilon \|g(v^\varepsilon)\|^2_{S^\varepsilon} + C_2 \varepsilon \|v^\varepsilon\|^2_{S^\varepsilon} + C.$$

Using Lemma 2.4 and our hypotheses for g and w_1, we easily get

$$\frac{1}{2} \frac{d}{dt} \|v^\varepsilon\|^2_{\Omega^\varepsilon} + \frac{D}{2} \|\nabla v^\varepsilon\|^2_{\Omega^\varepsilon} + \varepsilon \gamma \int_{S^\varepsilon} g(v^\varepsilon) v^\varepsilon d\sigma \leq C_5 \|v^\varepsilon\|^2_{\Omega^\varepsilon} + C_0 \varepsilon^2 \|\nabla v^\varepsilon\|^2_{\Omega^\varepsilon} + K.$$

Then

$$\frac{1}{2} \frac{d}{dt} \|v^\varepsilon\|^2_{\Omega^\varepsilon} + (\frac{D}{2} - C_0 \varepsilon^2) \|\nabla v^\varepsilon\|^2_{\Omega^\varepsilon} \leq C_5 \|v^\varepsilon\|^2_{\Omega^\varepsilon} + K.$$

Integrating with respect to time, we obtain

$$\|v^\varepsilon(t)\|^2_{\Omega^\varepsilon} + \frac{D}{2} \|\nabla v^\varepsilon\|^2_{\Omega^\varepsilon, t} \leq C.$$

Hence

$$\|v^\varepsilon(t)\|^2_{\Omega^\varepsilon} \leq C \tag{34}$$

and

$$\|\nabla v^\varepsilon(t)\|^2_{\Omega^\varepsilon,t} \leq C. \tag{35}$$

In a similar manner, we can get

$$\left\|\frac{\partial v^\varepsilon}{\partial t}(t)\right\|^2_{\Omega^\varepsilon} \leq C. \quad \blacksquare \tag{36}$$

The remaining step in the proof of Theorem 2.5 will be divided into three new steps.

First step. Let $v^\varepsilon \in \mathcal{W}_0(\Omega^\varepsilon)$ be the solution of the variational problem (17) and let $P^\varepsilon v^\varepsilon$ be the extension of v^ε inside the holes given by Lemma 2.2. Using our a priori estimates (30)-(31), we easily can see that there exists a constant C depending on T and the data, but independent of ε such that

$$\|P^\varepsilon v^\varepsilon(t)\|_\Omega + \|\nabla P^\varepsilon v^\varepsilon\|_{\Omega,t} + \|\partial_t(P^\varepsilon v^\varepsilon)(t)\|_\Omega \leq C, \tag{37}$$

for all $t \leq T$. Consequently, by passing to a subsequence, still denoted by $P^\varepsilon v^\varepsilon$, we can assume that there exists $v \in \mathcal{V}$ such that the following convergence properties hold:

$$P^\varepsilon v^\varepsilon \rightharpoonup v \quad \text{weakly in } \mathcal{V}, \tag{38}$$

$$\partial_t(P^\varepsilon v^\varepsilon) \rightharpoonup \partial_t v \quad \text{weakly in } \mathcal{H}, \tag{39}$$

$$P^\varepsilon v^\varepsilon \to v \quad \text{strongly in } \mathcal{H}. \tag{40}$$

It remains to identify the limit equation satisfied by v.

Second step. In order to get the limit equation satisfied by v we have to pass to the limit in (17). For getting the limit of the second term in the left hand side of (17), let us introduce, for any $h \in L^{s'}(\partial T)$, $1 \leq s' \leq \infty$, the linear form μ_h^ε on $W_0^{1,s}(\Omega)$ defined by

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

with $1/s + 1/s' = 1$. It is proved in [2] that

$$\mu_h^\varepsilon \to \mu_h \quad \text{strongly in } (W_0^{1,s}(\Omega))', \tag{41}$$

where

$$\langle \mu_h, \varphi \rangle = \mu_h \int\limits_\Omega \varphi dx,$$

with

$$\mu_h = \frac{1}{|Y|} \int\limits_{\partial F} h(y) d\sigma.$$

In the particular case in which $h \in L^\infty(\partial F)$ or even h is constant, we have

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

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

Moreover, if $z^\varepsilon \in H_0^1(\Omega)$ is such that $z^\varepsilon \rightharpoonup z$ weakly in $H_0^1(\Omega)$, then

$$\langle \mu_h^\varepsilon, z^\varepsilon|_{\Omega^\varepsilon} \rangle \to \mu_h \int_\Omega z dx. \tag{42}$$

Let us prove now that for any $\varphi \in C_0^\infty(\Omega)$ and for any $z^\varepsilon \rightharpoonup z$ weakly in $H_0^1(\Omega)$, we get

$$\varphi g(z^\varepsilon) \rightharpoonup \varphi g(z) \quad \text{weakly in } W_0^{1,\overline{q}}(\Omega), \tag{43}$$

where

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

To prove (43), let us first note that

$$\sup \|\nabla g(z^\varepsilon)\|_{L^{\overline{q}}(\Omega)} < \infty. \tag{44}$$

Indeed, from the growth condition (16) imposed to g, we get

$$\int_\Omega \left| \frac{\partial g}{\partial x_i}(z^\varepsilon) \right|^{\overline{q}} dx \le C \int_\Omega \left(1 + |z^\varepsilon|^{q\overline{q}}\right) \left| \frac{\partial z^\varepsilon}{\partial x_i} \right|^{\overline{q}} dx \le$$

$$\le C(1 + (\int_\Omega |z^\varepsilon|^{q\overline{q}\gamma}\, dx)^{1/\gamma})(\int_\Omega |\nabla z^\varepsilon|^{\overline{q}\delta}\, dx)^{1/\delta},$$

where we took γ and δ such that $\overline{q}\delta = 2$, $1/\gamma + 1/\delta = 1$ and $q\overline{q}\gamma = 2n/(n-2)$. Notice that, since $0 \le q < n/(n-2)$, we have $\overline{q} > 1$. Now, since

$$\sup \|z^\varepsilon\|_{L^{\frac{2n}{n-2}}(\Omega)} < \infty,$$

we get immediately (44). Hence, to get (43), it remains only to prove that

$$g(z^\varepsilon) \to g(z) \quad \text{strongly in } L^{\overline{q}}(\Omega). \tag{45}$$

But this is just a consequence of the following well-known result (see [8]):

Theorem 3.2. *Let $G : \Omega \times \mathbb{R} \to \mathbb{R}$ be a Carathéodory function, i.e.*

a) for every z the function $G(\cdot, z)$ is measurable with respect to $x \in \Omega$.

b) for every (a.e.) $x \in \Omega$, the function $G(x, \cdot)$ is continuous with respect to z.

Moreover, if we assume that there exists a positive constant C such that

$$|G(x,z)| \le C\left(1 + |z|^{r/t}\right),$$

with $r \ge 1$ and $t < \infty$, then the map $z \in L^r(\Omega) \mapsto G(x, z(x)) \in L^t(\Omega)$ is continuous in the strong topologies. ∎

Indeed, since

$$|g(z)| \le C(1 + |z|^{q+1}),$$

applying the above theorem for $G(x,z) = g(z)$, $t = \overline{q}$ and $r = (2n/(n-2)) - r'$, with $r' > 0$ such that $q + 1 < r/t$ and using the compact injection $H^1(\Omega) \hookrightarrow L^r(\Omega)$ we easily get (47).

Finally, from (41) (with $h = 1$) and (43) written for $z^\varepsilon = P^\varepsilon v^\varepsilon(t)$, we conclude

$$\langle \mu^\varepsilon, \varphi g(P^\varepsilon v^\varepsilon(t))\rangle \to \frac{|\partial F|}{|Y|} \int_\Omega \varphi g(v(t)) dx \quad \forall \varphi \in \mathcal{D}. \tag{46}$$

We are now in a position to use Lebesgue's convergence theorem. To this end, we use the above pointwise convergence, the a priori estimates (30) and the growth condition (16). As a result, we get

$$\lim_{\varepsilon \to 0} \varepsilon \gamma(g(v^\varepsilon), \varphi)_{S^\varepsilon, T} = \frac{|\partial F|}{|Y|} \gamma(g(v), \varphi)_{\Omega, T}, \tag{47}$$

which is the desired result. This ends the second step of the proof.

Third step. Let ξ^ε be the gradient of v^ε in Ω^ε and let us denote by $\widetilde{\xi^\varepsilon}$ its extension with zero to the whole of Ω. Obviously, $\widetilde{\xi^\varepsilon}$ is bounded in $(\mathcal{H}(\Omega))^n$ and hence there exists $\xi \in (\mathcal{H}(\Omega))^n$ such that

$$\widetilde{\xi^\varepsilon} \rightharpoonup \xi \quad \text{weakly in } (\mathcal{H}(\Omega))^n. \tag{48}$$

Let us see which is the equation satisfied by ξ. Take $\varphi \in \mathcal{D}$. From (17) we get

$$-\left(\chi_{\Omega^\varepsilon} P^\varepsilon v^\varepsilon, \frac{d\varphi}{dt}\right)_{\Omega, T} + D(\widetilde{\xi^\varepsilon}, \nabla \varphi)_{\Omega, T} + \varepsilon (f^\varepsilon, \varphi)_{S^\varepsilon, T} = (\chi_{\Omega^\varepsilon} h, \varphi)_{\Omega, T}. \tag{49}$$

Now, we can pass to the limit, with $\varepsilon \to 0$, in all the terms of (49). We have:

$$-\frac{|Y^\star|}{|Y|}\left(v, \frac{d\varphi}{dt}\right)_{\Omega, T} + D(\xi, \nabla\varphi)_{\Omega, T} + \frac{|Y^\star|}{|Y|}(F_0, \varphi)_{\Omega, T} = \frac{|Y^*|}{|Y|}(h, \varphi)_{\Omega, T} \quad \forall \varphi \in \mathcal{D}(\Omega).$$

Hence ξ verifies

$$\frac{|Y^*|}{|Y|}\frac{\partial v}{\partial t} - D \operatorname{div} \xi + \frac{|Y^*|}{|Y|} F_0 = \frac{|Y^*|}{|Y|} h, \quad t > 0,\ x \in \Omega. \tag{50}$$

It remains now to identify ξ. Following a standard procedure and using (23)-(24) (see, for instance, [5] and [7]), we get

$$D\frac{|Y^*|}{|Y|}\sum_{i,j=1}^n q_{ij} \frac{\partial^2 v}{\partial x_i \partial x_j} = D \operatorname{div} \xi = \frac{|Y^*|}{|Y|}\frac{\partial v}{\partial t} + \frac{|Y^*|}{|Y|} F_0 - \frac{|Y^*|}{|Y|} h,$$

which means that v satisfies

$$\frac{\partial v}{\partial t} - D \sum_{i,j=1}^n q_{ij} \frac{\partial^2 v}{\partial x_i \partial x_j} + F_0(t,x) = h, \quad t > 0,\ x \in \Omega.$$

Since $v \in \mathcal{W}_0(\Omega)$ (i.e. $v = 0$ on $\partial\Omega$) and v is uniquely determined, the whole sequence $P^\varepsilon v^\varepsilon$ converges to v and Theorem 2.5 is proved. ▪

In a similar manner we can treat the case in which the surface ∂F is physically and chemically heterogeneous and more precisely, the case in which the reaction and the adsorption coefficients a and γ, respectively, are rapidly oscillating functions, i.e.

$$a^\varepsilon(x) = a(\frac{x}{\varepsilon}),\ \gamma^\varepsilon(x) = \gamma(\frac{x}{\varepsilon}),$$

with a and γ positive functions in $W^{1,\infty}(\Omega)$ which are Y-periodic (for linear adsorption rates, see [7]). If we denote by $y = \frac{x}{\varepsilon}$, we have:

Theorem 3.3. *The effective behavior of v and w is governed by the following system:*

$$\begin{cases} \dfrac{\partial v}{\partial t}(t,x) + G_0(t,x) - D\displaystyle\sum_{i,j=1}^{n} q_{ij}\frac{\partial^2 v}{\partial x_i \partial x_j} = h(t,x), \quad t>0,\ x\in\Omega, \\ v(t,x) = 0 \quad t>0,\ x\in\partial\Omega, \\ v(t,x) = v_1(x) \quad t=0,\ x\in\Omega, \end{cases} \tag{51}$$

and

$$\begin{cases} \dfrac{\partial w}{\partial t}(t,x,y) + (a(y)+\gamma(y))w(t,x,y) = \gamma(y)g(v(t,x)), \quad t>0,\ x\in\Omega,\ y\in\partial F \\ w(t,x,y) = w_1(x) \quad t=0,\ x\in\Omega,\ y\in\partial F, \end{cases} \tag{52}$$

where

$$G_0(t,x) = \frac{1}{|Y^\star|}\int_{\partial F} f_0(t,x,y)d\sigma \tag{53}$$

and

$$f_0 = \gamma(y)(g(v(t,x)) - w(t,x,y)). \tag{54}$$

Here, $Q = ((q_{ij}))$ is the homogenized matrix, whose entries were defined by (23)-(24). ▪

Obviously, the solution of (52) can be found using the method of "variation of constants". Hence, we get

$$w(t,x,y) = w_1(x)e^{-(a(y)+\gamma(y))t} + \gamma(y)\int_0^t e^{-(a(y)+\gamma(y))(t-s)}g(v(s,x))ds,$$

or, using the convolution notation

$$w(t,x,y) = w_1(x)e^{-(a(y)+\gamma(y))t} + \gamma(y)r(\cdot,y)\star g(v(\cdot,x))(t),$$

with

$$r(\tau,y) = e^{-(a(y)+\gamma(y))\tau}.$$

Moreover, let us notice that (51)-(54) imply that $v(t,x)$ satisfies the following equation

$$\frac{\partial v}{\partial t}(t,x) - D\sum_{i,j=1}^{n} q_{ij}\frac{\partial^2 v}{\partial x_i \partial x_j}(t,x) + \overline{F}_0(t,x) = h(t,x), \quad t>0,\ x\in\Omega, \tag{55}$$

with

$$\overline{F}_0(t,x) = \frac{1}{|Y^\star|} \int\limits_{\partial F} \Big\{ \gamma(y)[g(v(t,x)) - w_1(x) e^{-(a(y)+\gamma(y))t} - \gamma(y) r(\cdot, y) \star g(v(\cdot, x))(t)] \Big\} \, d\sigma. \tag{56}$$

Proof. We shall not go into the details of the proof of this theorem, since it follows exactly the same steps in the proof of Theorem 2.5. The only difference we have to tackle is the way we treat the coefficients a^ε and γ^ε. To get rid of the difficulties coming from the fact that they are rapidly oscillating let us notice that in fact they are both uniformly bounded in $L^\infty(\Omega)$ and converge strongly therein. ▪

Remark 3.4. *The above adsorption model can be slightly generalized by allowing surface diffusion on S^ε. This implies that the first equation in (14) has to be replaced by*

$$\frac{\partial w^\varepsilon}{\partial t}(t,x) - \varepsilon^2 E \Delta^\varepsilon w^\varepsilon(t,x) + a^\varepsilon(x) w^\varepsilon(t,x) = f^\varepsilon(t,x) \quad x \in S^\varepsilon,\ t > 0,$$

where $E > 0$ is the diffusion constant on the surface S^ε and Δ^ε is the Laplace-Beltrami operator on S^ε.

In this case, the homogenized limit is almost the same as before, the only difference being that now, instead of (52), we get the following local partial differential equation:

$$\frac{\partial w}{\partial t}(t,x,y) - E \Delta_y^{\partial F} w(t,x,y) + (a(y) + \gamma(y)) w(t,x,y) =$$
$$= \gamma(y) g(v(t,x)),\ t > 0,\ x \in \Omega,\ y \in \partial F, \tag{57}$$

where $\Delta^{\partial F}$ denotes the Laplace-Beltrami operator on ∂F and the subscript y indicates the fact that the derivatives are taken with respect to the local variable y.

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