

# THE EFFECTIVENESS FACTOR OF REACTION-DIFFUSION EQUATIONS: HOMOGENIZATION AND EXISTENCE OF OPTIMAL PELLET SHAPES

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*Dedicated to an exceptional mathematician, David Kinderlehrer, with admiration.*

ABSTRACT. We study the asymptotic behaviour of the so-called *effectiveness factor*  $\eta_\varepsilon$  of a nonlinear diffusion equation that occurs on the boundary of periodically distributed inclusions (or particles) in an  $\varepsilon$ -periodic medium in  $\mathbb{R}^N$ ,  $N \geq 3$ . Here,  $\varepsilon$  is a small parameter related to the characteristic size of the inclusions, which, in the homogenization process, will tend to 0. The inclusions are modeled as homothety of a fixed pellet  $T$ , rescaled by a factor  $r(\varepsilon)$ . We study the cases in which  $r(\varepsilon) = O(\varepsilon^\alpha)$ , known as *big holes*, for  $\alpha = 1$ , as well as *non-critical small holes*, for  $1 < \alpha < \frac{N}{N-2}$ . We will prove the existence of some convex shapes which maximize the effectiveness of the homogenized problem. In particular, we deduce that for small holes the sphere is the domain of highest effectiveness.

## 1. INTRODUCTION

We study the asymptotic behaviour of the so-called *effectiveness factor*  $\eta_\varepsilon$  of nonlinear diffusion equations for which a reaction occurs on the boundary of periodically distributed inclusions (or particles) in an  $\varepsilon$ -periodic medium.

To be more precise, let  $\Omega \subset \mathbb{R}^N$ , with  $N \geq 3$ , be a bounded connected open set such that  $|\partial\Omega| = 0$  and let  $Y = (-\frac{1}{2}, \frac{1}{2})^N$  be the reference cell in  $\mathbb{R}^N$ . Let  $T$  be another open bounded subset of  $\mathbb{R}^N$ , with the boundary  $\partial T$  of class  $C^2$ .  $T$  will be called *the elementary particle*. We assume that 0 belongs to  $T$  and that  $T$  is star-shaped with respect to 0. Since  $T$  is bounded, without loss of generality, we can assume that  $\overline{T} \subset Y$ . We point out that, even though the usual term in homogenization theory for inclusions is *holes* (in order to give the idea that something has been removed from the domain), here we will avoid this terminology. For us, these inclusions will be pellets, for example the ones that can be found in fixed bed chemical reactors and towers. Therefore, we will refer to these *holes* as *pellets*, *particles* or even *inclusions* and *obstacles*.

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Let  $\varepsilon$  be a real parameter taking values in a sequence of positive numbers converging to zero. Here  $\varepsilon$  represents a small parameter related to the characteristic size of the particles. For each  $\varepsilon$  and for any vector  $\mathbf{i} \in \mathbb{Z}^N$ , we shall denote by  $T_{\mathbf{i}}^\varepsilon$  the translated image of  $r(\varepsilon)T$  by the vector  $\varepsilon\mathbf{i}$ :  $T_{\mathbf{i}}^\varepsilon = \varepsilon\mathbf{i} + r(\varepsilon)T$ . Also, let us denote by  $T^\varepsilon$  the set of all the pellets contained in  $\Omega$ , i.e.

$$T^\varepsilon = \bigcup \{T_{\mathbf{i}}^\varepsilon \mid \overline{T_{\mathbf{i}}^\varepsilon} \subset \Omega, \mathbf{i} \in \mathbb{Z}^N\}$$

and  $n(\varepsilon) = \#\{\mathbf{i} \in \mathbb{Z}^N : \overline{T_{\mathbf{i}}^\varepsilon} \subset \Omega\}$  be let the number of pellets. Set  $\Omega^\varepsilon = \Omega \setminus \overline{T^\varepsilon}$ . Therefore,  $\Omega^\varepsilon$  is a periodically perforated structure with pellets of the size  $r(\varepsilon)$ . Let us notice that the inclusions do not intersect the fixed boundary  $\partial\Omega$ . Let  $S^\varepsilon = \cup\{\partial T_{\mathbf{i}}^\varepsilon \mid \overline{T_{\mathbf{i}}^\varepsilon} \subset \Omega, \mathbf{i} \in \mathbb{Z}^N\}$ . Hence, we can write  $\partial\Omega^\varepsilon = \partial\Omega \cup S^\varepsilon$ .

We shall consider the homogenization of problems in which the reaction takes place on the boundary of the particles. More precisely, we shall start from the family of problems

$$(1.1) \quad \begin{cases} -\Delta u^\varepsilon = f & \text{in } \Omega^\varepsilon, \\ \frac{\partial u^\varepsilon}{\partial \nu} + \mu(\varepsilon)g(u^\varepsilon) = 0 & \text{on } S^\varepsilon, \\ u^\varepsilon = 1 & \text{on } \partial\Omega, \end{cases}$$

where  $\nu$  is the exterior unit normal to  $S^\varepsilon$ ,  $g$  is a non-decreasing function and the rest of the data  $\mu(\varepsilon)$  and  $f$  will be specified later.

We shall assume that  $r(\varepsilon) = \varepsilon^\alpha$ . Particles that scale with  $\alpha = 1$  are called *big particles* and the ones corresponding to the case  $\alpha > 1$  are called *small particles*. There is a special case,  $\alpha = \frac{N}{N-2}$ , which is known as the *critical case*, in which the limit behaviour of the solution of problem (1.1) changes (see, e.g. [16]). We shall deal here only with the cases  $1 \leq \alpha < \frac{N}{N-2}$ . The case  $\alpha = \frac{N}{N-2}$  will be the subject of a forthcoming paper. The case  $\alpha > \frac{N}{N-2}$  is not interesting, since the reaction term disappears at the limit and, therefore, the solution of problem (1.1) converges to  $u_0 \equiv 1$  in  $\Omega$ .

We address here the relevant cases in which  $\mu(\varepsilon)|S^\varepsilon| = O(1)$ . In fact, if  $r(\varepsilon) = \varepsilon^\alpha$ , then  $\mu(\varepsilon) = \varepsilon^{-\gamma}$ , with  $\gamma = \alpha(N-1) - N$ . In particular, for big holes, since  $\alpha = 1$ , it follows that  $\gamma = -1$ .

The problem (1.1) will be analyzed for a broad class of nonlinear monotone kinetics such that

$$(1.2) \quad g \text{ is a maximal monotone graph (single-valued or even multivalued), with } g(0) = 0,$$

and for

$$(1.3) \quad f \in L^2(\Omega), \quad f \geq 0.$$

We recall that, in the Chemical Engineering context, it is typically assumed that  $g(1) = 1$ , and hence the above conditions guaranty that  $0 \leq u^\varepsilon \leq 1$ , which is the natural setting for chemical concentrations.

A particular case we shall discuss is the Freundlich isotherm kinetics

$$(1.4) \quad g(u) = |u|^{p-1}u, \quad p \in (0, 1].$$

Also, we can consider the limit case of *zero order reactions*:

$$(1.5) \quad g(u) = \begin{cases} 0 & u < 0, \\ [0, 1] & u = 0, \\ 1 & u > 0. \end{cases}$$

in the context of maximal monotone graphs of  $\mathbb{R}^2$  (see, e.g., [3, 22]).

Problems of the form (1.1) have been extensively studied in the literature. The case of big inclusions, i.e. the case in which  $\alpha = 1$ , with nonhomogeneous constant Dirichlet conditions on the boundary of the inclusions, was addressed in [8]. For nonlinear problems, various techniques, such as the method of oscillating test function (see [9]) and, more recently, the periodic unfolding method (see [7]), have been used.

For small inclusions, i.e. for  $\alpha > 1$ , the linear Neumann homogeneous problem was studied in [24], the Neumann nonhomogeneous problem in [11] and the nonlinear problem was analyzed, by different techniques, in [20, 27]. The case where the inclusions are substituted by a connected set can also be analyzed.

We shall work here with relatively smooth nonlinear kinetics  $g$ , for which  $g(0) = 0$  and which satisfy suitable growth conditions (see (1.8) and (1.12)) but, as indicated before, it seems that our results could be extended even to the case in which  $g$  is a multivalued maximal monotone graph on  $\mathbb{R}^2$  (see Remark 1 below). Inspired by the definition given in the linear case ( $p = 1$ ) by the chemical engineer R. Aris (see [1]), we define the notion of *effectiveness* of the pellet in this more general setting as follows:

$$(1.6) \quad \eta_\varepsilon(T) = \frac{1}{|S_\varepsilon|} \int_{S_\varepsilon} g(u_\varepsilon) d\sigma.$$

This is well defined since, for  $g$  smooth and satisfying (1.8) or (1.12),  $g(u^\varepsilon) \in W^{1,\bar{q}}(\Omega^\varepsilon)$ , with  $\bar{q} = \frac{2N}{q(N-2)+N}$ . Definition (1.6) can be naturally extended to the homogenized case (which will be studied below), by putting

$$(1.7) \quad \eta(T) = \frac{1}{|\Omega|} \int_{\Omega} g(u) dx.$$

It is known that there exists an extension  $P^\varepsilon u^\varepsilon$  of the solution  $u^\varepsilon$  to the unperforated domain  $\Omega$  such that  $P^\varepsilon u^\varepsilon \rightharpoonup u_0$  in  $H^1(\Omega)$ . The limit  $u_0$  is the solution of a different elliptic problem, defined over the whole domain  $\Omega$ , in which the reaction term appears in the interior equation and an effective diffusion matrix which is not the identity arises for the case  $\alpha = 1$ , but not for  $\alpha > 1$ .

We recall some previous homogenization results. For the case of big holes we assume that  $r(\varepsilon) = \varepsilon$  and consider either a smooth kinetic

$$(1.8) \quad |g'(v)| \leq C(1 + |v|^q), \quad 0 \leq q < \frac{N}{N-2},$$

or a not necessarily smooth one, but with bounded growth

$$(1.9) \quad |g(v)| \leq C(1 + |v|^q), \quad 0 \leq q < \frac{N}{N-2}.$$

Following the theory in [9] and [10], the solution  $u^\varepsilon$  of problem (1.1), properly extended to the whole of  $\Omega$ , converges weakly in  $H^1(\Omega)$ , as  $\varepsilon \rightarrow 0$ , to  $u \in H^1(\Omega)$ , i.e.  $P^\varepsilon u^\varepsilon \rightharpoonup u$ , where

$u$  is the unique solution of the following homogenized problem:

$$(1.10) \quad \begin{cases} -\operatorname{div}(a_0(T)\nabla u) + \frac{|\partial T|}{|Y \setminus T|} g(u) = f & \text{in } \Omega, \\ u = 1 & \text{on } \partial\Omega. \end{cases}$$

The proof of the existence and uniqueness of a weak solution for this problem can be found, e.g., in [13]. Here,  $a_0(T) \in \mathcal{M}_N(\mathbb{R})$  (the set of  $N \times N$  matrices) is the classical homogenized matrix (see, e.g., [9]). If we write  $a_0(T) = (q_{ij})$ , then

$$q_{ij} = \delta_{ij} + \frac{1}{|Y \setminus T|} \int_{Y \setminus T} \frac{\partial \chi_j}{\partial y_i} dy,$$

where  $\chi_i$  are the solutions of the so-called *cell problems*:

$$(1.11) \quad \begin{cases} -\Delta \chi_i = 0 & \text{in } Y \setminus T, \\ \frac{\partial(\chi_i + y_i)}{\partial \nu} = 0 & \text{on } \partial T, \\ \chi_i & Y\text{-periodic.} \end{cases}$$

For the case of small non-critical holes ( $1 < \alpha < \frac{N}{N-2}$ ), under the assumption that for the nonlinear function  $g$  there exist two constants  $k_1, k_2$  such that

$$(1.12) \quad 0 < k_1 \leq g'(u) \leq k_2,$$

Zubova and Shaposhnikova showed in [27] that

$$(1.13) \quad \|\nabla u_\varepsilon - \nabla u_0\|_{L^2(\Omega^\varepsilon)^N} + \varepsilon^{-\gamma} \|u_\varepsilon - u_0\|_{L^2(S_\varepsilon)} \rightarrow 0,$$

where, for  $r(\varepsilon) = C\varepsilon^\alpha$ ,  $u_0$  is the solution of

$$(1.14) \quad \begin{cases} -\Delta u_0 + C^{N-1} |\partial T| g(u_0) = f & \text{in } \Omega, \\ u_0 = 1, & \text{on } \partial\Omega. \end{cases}$$

This paper (which develops a previous short presentation [17]) is organized as follows: in Section 2, we present the main results of the paper, which we prove in the remaining sections. Section 3 is devoted to the proof Theorem 1, in which we compute the limit  $\eta$  of the effectiveness factor  $\eta_\varepsilon$  as  $\varepsilon \rightarrow 0$ . In Section 4, we prove Theorem 2, in which we show the existence of optimal shapes, and Theorem 3, which contains their characterization for small holes.

## 2. STATEMENT OF THE MAIN RESULTS

In order to perform the homogenization process, we need to impose some regularity conditions for  $g$ .

**Assumption 1.** Let the following regularity hold:

- If  $\alpha = 1$ , (1.8),
- If  $1 < \alpha < \frac{N}{N-2}$ , (1.12).

We state here the main results of this paper. The first one is a homogenization result for the effectiveness.

**Theorem 1.** Let  $1 \leq \alpha < \frac{N}{N-2}$  and Assumption 1 hold. Then,

$$(2.1) \quad \eta_\varepsilon(T) \rightarrow \eta(T), \quad \text{as } \varepsilon \rightarrow 0.$$

**Remark 1.** It is an open problem whether or not this convergence remains true under more general nonlinearities  $g$ . Our proof of the convergence for  $\alpha = 1$  relies on [6], in which one requires differentiability of  $g(u^\varepsilon)$ . We could, however, define the effectiveness  $\eta_\varepsilon$  by means of  $g(\text{tr}_{S_\varepsilon}(u^\varepsilon))$ . Nonetheless, the proof, in essence, requires that we consider  $\text{tr}_{S_\varepsilon}(g(u^\varepsilon))$ . We believe that a proof of the general case might need an extension of the results in [6] or a completely new approach. A different proof, applying the periodic unfolding method, of the convergence in the case  $\alpha = 1$  and  $g = 0$  (with a source boundary term) can be found in [5].

For the cases  $\alpha > 1$  it is known that the convergence results can be extended to broader families of nonlinearities by applying the same techniques. In particular, by using the techniques of [16] we think possible to get a similar result to Theorem 1 for some cases  $\alpha > 1$  under assumption (1.4) for any  $p \in [0, 1]$  but this would be a very technical task that we shall not consider here.

For the homogenized problem, we have the following optimality result:

**Theorem 2.** *Let  $1 \leq \alpha < \frac{N}{N-2}$ ,  $0 < \theta < |Y|$ ,  $C, D$  be fixed proper subsets of  $Y$  and  $\tilde{\varepsilon} > 0$ . Let us assume that*

$$(2.2) \quad T \text{ satisfies the uniform } \tilde{\varepsilon}\text{-cone property.}$$

*We define*

$$\begin{aligned} U_{adm} &= \{\bar{C} \subset T \subset \bar{D} : T \text{ satisfies (2.2) and } |T| = \theta\}, \\ C_\theta(D) &= \{T \subset D : T \text{ is open, convex and } |T| = \theta\}. \end{aligned}$$

*Then, at fixed volume  $\theta \in (0, |Y|)$ , there exists a domain of maximal (and minimal) effectiveness for the homogenized problem in the class of  $T \in U_{adm} \cap C_\theta(D)$ .*

For small (non-critical) holes, we can characterize the optimizer's shape.

**Theorem 3.** *For the case  $1 < \alpha < \frac{N}{N-2}$ , the ball is the domain  $T$  of maximal effectiveness for a set volume in the class of star-shaped  $C^2$  domains with fixed volume.*

**Remark 2.** This is opposed to the homogenization with respect to the exterior domain  $\Omega$ . In this context, when  $\Omega$  is a ball has least effectivity, as can be shown by rearrangement techniques (see [13]). In the context of product domains,  $\Omega = B \times \Omega''$  is the least effective on the class  $\Omega = \Omega' \times \Omega''$  for set volume, at least for convex or concave kinetics (see [14, 15, 22]).

Through standard procedures in weak solution theory, one easily gets the following result (see, e.g., [3]).

**Proposition 1** (Well-posedness). *Under the assumptions (1.2) and (1.3), there exists a unique solution  $u^\varepsilon \in H^2(\Omega^\varepsilon)$  of (1.1).*

**Proposition 2** (Strong maximum principle). *Under the assumptions (1.2) and (1.3),  $u_\varepsilon > 0$  in  $\Omega_\varepsilon$ .*

*Proof.* By the weak maximum principle, we have that  $u_\varepsilon \geq 0$ . Now, we can apply the comparison principle with  $\underline{u}_\varepsilon$ , the non-negative solution of

$$\begin{cases} -\Delta \underline{u}_\varepsilon = f & \text{in } \Omega^\varepsilon, \\ \underline{u}_\varepsilon = 0 & \text{on } \partial\Omega^\varepsilon, \end{cases}$$

to obtain  $u_\varepsilon \geq \underline{u}_\varepsilon$  in  $\Omega^\varepsilon$ . For  $\underline{u}_\varepsilon$ , we can apply the estimate in [18]

$$\underline{u}_\varepsilon(x) \geq c \left( \int_\Omega f(y) \, d(y, \partial\Omega^\varepsilon) \, dy \right) d(x, \partial\Omega^\varepsilon), \quad x \in \Omega^\varepsilon,$$

which proves the result.  $\square$

**Remark 3.** We can illustrate a couple of the steps of the homogenization process by means of the following COMSOL simulation.

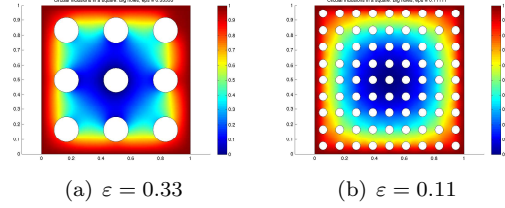


FIGURE 1. Fixed bed reactors with big pellets ( $r_\varepsilon = \varepsilon$ ) and the level set of the solution of problem (1.1) for  $f = 0$ , and kinetic (1.4) where  $p = \frac{1}{2}$ ,  $\mu(\varepsilon) = \varepsilon$ .

### 3. EFFECTIVENESS HOMOGENIZATION

Since the cases  $\alpha = 1$  and  $\alpha > 1$  require different techniques and provide different results, we will divide the proof of Theorem 1 in two parts.

#### 3.1. Big holes ( $\alpha = 1$ ).

*Proof of Theorem 1 in the case  $\alpha = 1$ .* From [6] (see also [27, 28, 9]), it holds that

$$\varepsilon \int_{S_\varepsilon} g(u^\varepsilon(x)) d\sigma \rightarrow \frac{|\partial T|}{|Y|} \int_{\Omega} g(u(x)) dx, \quad \text{as } \varepsilon \rightarrow 0.$$

Since, by explicit computation,  $|S_\varepsilon| = n(\varepsilon)|\partial(\varepsilon T)| = n(\varepsilon)\varepsilon^{N-1}|\partial T|$ , when the cells tend to cover the total volume,

$$n(\varepsilon)|Y|\varepsilon^N = n(\varepsilon)|\varepsilon Y| \rightarrow |\Omega|, \quad \text{as } \varepsilon \rightarrow 0,$$

and we have that  $|S_\varepsilon|\varepsilon \rightarrow |\Omega||\partial T|$ , as  $\varepsilon \rightarrow 0$ . Hence, as  $\varepsilon \rightarrow 0$ ,

$$\eta_\varepsilon(T) = \frac{1}{|S_\varepsilon|} \int_{S_\varepsilon} g(u^\varepsilon(x)) d\sigma \rightarrow \frac{1}{|\Omega|} \int_{\Omega} g(u) dx = \eta(T),$$

which proves the result.  $\square$

**Remark 4.** The above convergence remains true for the kinetic (1.4) in the case of domains in which there exists  $\delta > 0$  such that  $u^\varepsilon \geq \delta$  uniformly on  $\varepsilon$ , that is, no dead core exists. For the solution  $u$ , the region where  $u = 0$  (which might have positive measure) is known in the literature as a *dead core*. Conditions for the existence and location of a dead core in this and other kinds of equations can be found in [13], [2] and in the references therein. In the case when a dead core exists, even though the limit theorem does not apply, the strong maximum principle (Proposition 2) suggests that the effectiveness is higher prior to the homogenization process.

**3.2. Small non critical holes** ( $1 < \alpha < \frac{N}{N-2}$ ). In [28], the authors show that for  $\varphi \in H^1(\Omega^\varepsilon, \partial\Omega) = \{\varphi \in H^1(\Omega^\varepsilon) : \varphi = 0 \text{ on } \partial\Omega\}$  and for  $r_\varepsilon = C\varepsilon^\alpha$ , one has the estimate:

$$(3.1) \quad \left| \frac{\varepsilon^{-\gamma}}{C^{N-1}|\partial T|} \int_{S_\varepsilon} \varphi ds - \int_{\Omega^\varepsilon} \varphi dx \right| \leq K\varepsilon^{\frac{N-\alpha(N-2)}{2}}.$$

Taking into account the explicit computation of  $|S_\varepsilon|$ , we have that

$$(3.2) \quad \left| \frac{1}{|S_\varepsilon|} \int_{S_\varepsilon} \varphi ds - \frac{1}{|\Omega|} \int_{\Omega^\varepsilon} \varphi dx \right| \rightarrow 0.$$

Since we are concerned with fixed volumes, we can set  $C = 1$ .

We are now in the position to prove Theorem 1 for  $\alpha > 1$ .

*Proof of Theorem 1 in the case  $\alpha > 1$ .* Let us consider the change  $w^\varepsilon = 1 - u^\varepsilon$ . So,  $w^\varepsilon = 0$  on  $\partial\Omega$ . We can apply the homogenization results in [27] and [28] for  $w^\varepsilon$  and deduce directly the corresponding ones for  $u^\varepsilon$ . Thus, we have that

$$(3.3) \quad \begin{aligned} & \left| \frac{1}{|S_\varepsilon|} \int_{S_\varepsilon} g(u^\varepsilon) ds - \frac{1}{|\Omega|} \int_{\Omega} g(u_0) dx \right| \leq \left| \frac{1}{|S_\varepsilon|} \int_{S_\varepsilon} g(u^\varepsilon) ds - \frac{1}{|S_\varepsilon|} \int_{S_\varepsilon} g(u_0) ds \right| \\ & + \left| \frac{1}{|S_\varepsilon|} \int_{S_\varepsilon} g(u_0) ds - \frac{1}{|\Omega|} \int_{\Omega} g(u_0) dx \right| \leq C\varepsilon^{-\gamma} \|u_\varepsilon - u_0\|_{L^2(S_\varepsilon)} \\ & + \left| \frac{1}{|S_\varepsilon|} \int_{S_\varepsilon} g(u_0) ds - \frac{1}{|\Omega|} \int_{\Omega} g(u_0) dx \right| \rightarrow 0, \end{aligned}$$

which concludes the proof.  $\square$

#### 4. EXISTENCE OF OPTIMAL PELLET SHAPES

Once we know the effect that a general obstacle  $T$  causes, it seems reasonable to perform domain optimization. First, we show an abstract result of existence of optimal particle shape. We will focus on the homogenized models (1.10) and (1.14). We can prove Theorem 3 directly by applying the isoperimetric inequality.

*Proof of Theorem 3.* Applying the comparison principle, we can see that  $u$  is a decreasing function of  $|\partial T|$  and, since  $g$  is increasing, we have that  $\eta$  is an increasing function of  $u$ . Therefore,  $\eta$  is a decreasing function of  $|\partial T|$ . For fixed volume  $|Y \setminus T|$ , the volume of  $T$  is fixed. The isoperimetric inequality (see, e.g. [13]) guaranties that a ball is the domain of minimum  $|\partial T|$ , hence the domain of optimal effectiveness.  $\square$

**Remark 5.** Optimization of the effectiveness considering the homogenized domain  $\Omega$  (the chemical reactor) has also been studied (see [13, 14, 15] and the references therein). In this situation, the existence of a *dead core* affects the effectiveness negatively.

**Remark 6.** Dealing with the optimization of the domain  $\Omega$ , **there exist no optimal shapes** considering a general framework (see [2], [15]). We conjecture that new results may be also obtained by applying methods analogous to the ones that follow.

**Remark 7.** As in [9], the problem in which we consider reactions inside the pellets can also be addressed for  $\alpha = 1$ . Let us consider the system of equations

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

with  $D_f, D_p > 0$  and  $f \in L^2(\Omega)$ . If we introduce the matrix  $A = D_f \chi_{Y \setminus T} + D_p \chi_T$ , where  $I$  is the identity matrix in  $\mathcal{M}_N(\mathbb{R})$ , then the homogenized problem for big pellets is (see [9])

$$\begin{cases} -\operatorname{div}(A^0 \nabla u) + a \frac{|T|}{|Y \setminus T|} g(u) = f & \text{in } \Omega, \\ u = 1 & \text{on } \partial\Omega, \end{cases}$$

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

$$a_{ij}^0 = \int_Y \left( a_{ij} + a_{ik} \frac{\partial \chi_j}{\partial y_k} \right) dy,$$

in terms of the functions  $\chi_j$ ,  $i = 1, \dots, N$ ,  $Y$ -periodic solutions of the cell problems

$$-\operatorname{div}(A \nabla (y_j + \chi_j)) = 0.$$

In this context, the results would be analogous and the proofs perhaps even simpler. The problem has been recently studied without continuity conditions (see [19]).

Coming back to the proof of Theorem 2, we see in (1.10) that, for  $\alpha = 1$ , the effect of  $T$  is present in three terms:  $|\partial T|$ ,  $|Y \setminus T|$  and  $a_0(T)$ . Therefore, any sensible choice of topology for the set of admissible domains  $T$  in a search for optimal shape obstacles must make this expressions continuous.

A logical choice of topology in the “space of shapes” is the one given by the Hausdorff distance

$$d_H(\Omega_1, \Omega_2) = \sup \left\{ \sup_{x \in \Omega_1} d(x, \Omega_2), \sup_{x \in \Omega_2} d(x, \Omega_1) \right\}.$$

For the optimization, we will restrict ourselves to a general enough family of domains, but in which we can define a topology which makes the family compact. It is well known (see, for example, [25]) that the following result holds true.

**Theorem 4** ([25]). *The class of closed subsets of a compact set  $D$  is compact for the Hausdorff convergence.*

A proof for the continuity of the effective diffusion under the Hausdorff distance in  $U_{adm}$  can be found in [21].

**Lemma 1** ([21]). *If  $U_{adm}$  is compact with respect to the Hausdorff metric and if  $(T_n) \subset U_{adm}$ ,  $T_n \rightarrow T$  as  $n \rightarrow \infty$ ,  $T \in U_{adm}$ , then  $a_0(T_n) \rightarrow a_0(T)$  in  $\mathcal{M}_N(\mathbb{R})$ .*

The behaviour of the measure  $|Y \setminus T|$  is slightly more delicate (we include a commentary even though, in our case, this will be constant). For this, a distance with a definition similar to Hausdorff metric, the Hausdorff complementary distance

$$d_{H^c}(\Omega_1, \Omega_2) = \sup_{x \in \mathbb{R}^n} |d(x, \Omega_1^c) - d(x, \Omega_2^c)|,$$



has the following property: for open domains  $(\Omega_n)_n, \Omega$ ,  $d_{H^c}(\Omega_n, \Omega) \rightarrow 0$  as  $n \rightarrow \infty$  implies  $\liminf_n |\Omega_n| \geq |\Omega|$ . However, lower semicontinuity of the measure of the boundary ( $|\partial T|$ ) is, in general, false (see [21] for some counterexamples). Nevertheless, the set of **convex** domains has a number of very interesting properties (see [26]).

**Lemma 2** ([26]). *The topological spaces  $(C_\theta(D), d_H)$  and  $(C_\theta(D), d_{H^c})$  are equivalent.*

The continuity of the boundary measure is provided by the following result, proved in [4].

**Lemma 3** ([4]). *Let  $(\Omega_n), \Omega \in C_\theta(D)$ . If  $\Omega_1 \subset \Omega_2$ , then  $|\partial\Omega_1| \leq |\partial\Omega_2|$ . Moreover, if  $\Omega_n \xrightarrow{d_H} \Omega$ , then  $|\Omega_n| \rightarrow |\Omega|$  and  $|\partial\Omega_n| \rightarrow |\partial\Omega|$ , as  $n \rightarrow \infty$ .*

For the continuity of solutions with respect to  $T$ , we need the following theorem on the continuity of the associated Nemitskij operators (see, for example, [12] and [23]).

**Lemma 4** ([23]). *Let  $G : \Omega \rightarrow \mathbb{R} \rightarrow \mathbb{R}$  be a Carathéodory function such that (1.9) holds true for  $q = \frac{r}{t}$  with  $r \geq 1$  and  $t < \infty$ . Then, the map*

$$L^r(\Omega) \rightarrow L^t(\Omega) \quad v \mapsto G(x, v(x))$$

*is continuous in the strong topologies.*

**Lemma 5.** *Let  $\mathcal{A}$  be the set of elliptic matrices and let  $g$  satisfy (1.9). Let  $u(A, \lambda)$  be the unique solution of*

$$\begin{cases} -\operatorname{div}(A\nabla u) + \lambda g(u) = f, & \text{in } \Omega, \\ u = 1, & \text{on } \partial\Omega, \end{cases}$$

*Then, the application*

$$\mathcal{A} \times \mathbb{R}_+ \rightarrow H^1(\Omega) \quad (A, \lambda) \mapsto u(A, \lambda),$$

*is continuous in the weak topology.*

*Proof.* Let  $G(u) = \int_0^u g(s)ds$  and

$$J_{A,\lambda}(v) = \frac{1}{2} \int_{\Omega} (A\nabla v) \cdot \nabla v + \int_{\Omega} \lambda G(v) - \int_{\Omega} f v.$$

We know that  $u(A, \lambda)$  is the unique minimizer of this functional. Let  $A_n \rightarrow A$  and  $\lambda_n \rightarrow \lambda$  be two converging sequences. It is easy to prove that  $u_n = u(A_n, \lambda_n)$  is bounded in  $H^1(\Omega)$  and, up to a subsequence,  $u_n \rightharpoonup u$  in  $H^1$  as  $n \rightarrow \infty$ . Therefore,  $\int_{\Omega} (A\nabla u) \cdot \nabla u \leq \liminf_n \int_{\Omega} (A_n \nabla u_n) \cdot \nabla u_n$ . We can apply Theorem 4 to show that  $G(u_n) \rightarrow G(u)$  in  $L^1$  as  $n \rightarrow \infty$  (see details for a similar proof, for example, in [9]) and we have that  $u = u(A, \lambda)$ .  $\square$

**Corollary 1.** *The map  $(I, \lambda) \mapsto u$ , where  $I$  is the identity matrix, is continuous in the weak topology of  $H^1$ .*

**Corollary 2.** *In the hypotheses of Lemma 5, the maps  $(A, \lambda) \mapsto \int_{\Omega} g(u(A, \lambda))$  and  $(I, \lambda) \mapsto \int_{\Omega} g(u(I, \lambda))$  are continuous.*

With these tools, we can prove now our main result.

*Proof of Theorem 2.* First, we have that Lemmas 1 and 3 imply that the application  $T \mapsto (a_0(T), \lambda(T))$  is continuous. Then, Corollary 2 implies that  $T \mapsto \eta(T)$  is continuous (with either  $a_0(T)$  or  $I$ ). Therefore, since  $C_\theta(D)$  is closed and  $U_{adm}$  is compact, by Lemma 1 we have the compactness of  $U_{adm} \cap C_\theta(D)$  and then the existence of maximizers.  $\square$

**Remark 8.** Some numerical experiences comparing the effectiveness for different shapes where presented in [17].

## REFERENCES

- [1] R. ARIS AND W. STRIEDER, *Variational Methods Applied to Problems of Diffusion and Reaction*, vol. 24 of Springer Tracts in Natural Philosophy, Springer-Verlag, New York, 1973.
- [2] C. BANDLE, *A note on Optimal Domains in a Reaction-Diffusion Problem*, Zeitschrift für Analysis und ihre Anwendungen, 4 (3) (1985), pp. 207–213.
- [3] H. BRÉZIS, *Monotonicity Methods in Hilbert Spaces and Some Applications to Nonlinear Partial Differential Equations*, in Contributions to Nonlinear Functional Analysis, E. Zarantonello, ed., Academic Press, Inc., New York, 1971, pp. 101–156.
- [4] G. BUTTAZZO AND P. GUASONI, *Shape Optimization problems over classes of convex domains*, Journal of Convex Analysis, 4,2 (1997), pp. 343–352.
- [5] I. CHOURABI AND P. DONATO, *Homogenization and correctors of a class of elliptic problems in perforated domains*, Asymptotic Analysis, 92 (2015), pp. 1–43.
- [6] D. CIORANESCU AND P. DONATO, *Homogénéisation du problème de Neumann non homogène dans des ouverts perforés*, Asymptotic Analysis, 1 (1988), pp. 115–138.
- [7] D. CIORANESCU, P. DONATO, AND R. ZAKI, *Asymptotic behavior of elliptic problems in perforated domains with nonlinear boundary conditions*, Asymptotic Analysis, 53 (2007), pp. 209–235.
- [8] D. CIORANESCU AND J. S. J. PAULIN, *Homogenization in open sets with holes*, Journal of Mathematical Analysis and Applications, 71 (1979), pp. 590–607.
- [9] C. CONCA, J. I. DÍAZ, A. LIÑÁN, AND C. TIMOFTE, *Homogenization in Chemical Reactive Flows*, Electronic Journal of Differential Equations, 40 (2004), pp. 1–22.
- [10] C. CONCA, J. I. DÍAZ, AND C. TIMOFTE, *Effective Chemical Process in Porous Media*, Mathematical Models and Methods in Applied Sciences, 13 (2003), pp. 1437–1462.
- [11] C. CONCA AND P. DONATO, *Non-homogeneous Neumann problems in domains with small holes*, Modélisation Mathématique et Analyse Numérique, 22 (1988), pp. 561–607.
- [12] G. DAL MASO, *An Introduction to  $\Gamma$ -Convergence*, Progress in Nonlinear Differential Equations, Birkhäuser Boston, Boston, MA, 1993.
- [13] J. I. DÍAZ, *Nonlinear Partial Differential Equations and Free Boundaries, Vol.I.: Elliptic equations*, Research Notes in Mathematics, Pitman, London, 1985.
- [14] J. I. DÍAZ AND D. GÓMEZ-CASTRO, *Steiner symmetrization for concave semilinear elliptic and parabolic equations and the obstacle problem*, in Dynamical Systems and Differential Equations, AIMS Proceedings 2015 Proceedings of the 10th AIMS International Conference (Madrid, Spain), American Institute of Mathematical Sciences, nov 2015, pp. 379–386.
- [15] ———, *On the Effectiveness of Wastewater Cylindrical Reactors: an Analysis Through Steiner Symmetrization*, Pure and Applied Geophysics, 173 (2016), pp. 923–935.
- [16] J. I. DÍAZ, D. GÓMEZ-CASTRO, A. V. PODOL'SKII, AND T. A. SHAPOSHNIKOVA, *Homogenization of the  $p$ -Laplace operator with nonlinear boundary condition on critical size particles: identifying the strange terms for some non smooth and multivalued operators*, Doklady Mathematics, 94 (2016), pp. 387–392.
- [17] J. I. DÍAZ, D. GÓMEZ-CASTRO, AND C. TIMOFTE, *On the influence of pellet shape on the effectiveness factor of homogenized chemical reactions*, in Proceedings Of The XXIV Congress On Differential Equations And Applications XIV Congress On Applied Mathematics, 2015, pp. 571–576.
- [18] J. I. DÍAZ, J.-M. MOREL, AND L. OSWALD, *An elliptic equation with singular nonlinearity*, Communications in Partial Differential Equations, 12 (1987), pp. 1333–1345.
- [19] M. GAHN, M. NEUSS-RADU, AND P. KNABNER, *Homogenization of Reaction-Diffusion Processes in a Two-Component Porous Medium with Nonlinear Flux Conditions at the Interface*, SIAM Journal on Applied Mathematics, 76 (2016), pp. 1819–1843.
- [20] M. V. GONCHARENKO, *Asymptotic behavior of the third boundary-value problem in domains with fine-grained boundaries*, Proceedings of the Conference “Homogenization and Applications to Material Sciences” (Nice, 1995), GAKUTO (1997), pp. 203–213.
- [21] J. HASLINGER AND J. DVORAK, *Optimum Composite Material Design*, ESAIM Mathematical Modelling and Numerical Analysis, 1 (1995), pp. 657–686.
- [22] D. KINDERLEHRER AND G. STAMPACCHIA, *An introduction to variational inequalities and their applications*, vol. 31, Academic Press, New York, 1980.
- [23] J. L. LIONS, *Quelques Méthodes de Résolution pour les Problèmes aux Limites non Linéaires*, Dunod, Paris, 1969.
- [24] O. A. OLEINIK AND T. A. SHAPOSHNIKOVA, *On the homogenization of the Poisson equation in partially perforated domains with arbitrary density of cavities and mixed type conditions on their boundary*, Atti

- della Accademia Nazionale dei Lincei. Classe di Scienze Fisiche, Matematiche e Naturali. Rendiconti Lincei. Matematica e Applicazioni, 7 (1996), pp. 129–146.
- [25] O. PIRONNEAU, *Optimal Shape Design for Elliptic Equations*, Springer Series in Computational Physics, Springer-Verlag, Berlin, 1984.
- [26] N. VAN GOETHEM, *Variational problems on classes of convex domains*, Communications in Applied Analysis, 8 (2004), pp. 353–371.
- [27] M. N. ZUBOVA AND T. A. SHAPOSHNIKOVA, *Homogenization of boundary value problems in perforated domains with the third boundary condition and the resulting change in the character of the nonlinearity in the problem*, Differential Equations, 47 (2011), pp. 78–90.
- [28] ———, *Averaging of boundary-value problems for the Laplace operator in perforated domains with a nonlinear boundary condition of the third type on the boundary of cavities*, Journal of Mathematical Sciences, 190 (2013), pp. 181–193.

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