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On the influence of pellet shape on the effectiveness factor of homogenized chemical reactions

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Abstract— One of the most popular principles of Nanotechnology, especially in the context of composite media, says, roughly speaking, that one of the reasons for the optimality of certain composite media comes from the fact that when the size of the small particles decreases (maintaining a prescribed total volume) then their total surface increases and this leads to peculiar properties which cannot be observed when the particles are big. What is really relevant in this context is a suitable balance between the total surface and the homogenized diffusion. In order to fix ideas, we consider the case of adsorption chemical reactions on the surface of a set of particles in a periodic composite structure (medium). We know that the solution of our problem converges to the solution of a related homogenized semilinear elliptic problem. Our main goal is to study the behaviour of the so-called *effectiveness factor* η_ε for the chemical reactions, defined at the microscale, and to establish the relation between this factor and the corresponding one η defined for the homogenized problem. Moreover, we shall study the effect of the shape of the pellets (in particular, their total surface $|\partial T|$ and the homogenized diffusion coefficient $a_0(T)$) in the homogenized effectiveness factor. We prove the existence of an optimal convex shape of the particles for the effectiveness functional.

Introduction

Let Ω be an open bounded connected set in $\mathbb{R}^N$ and let us insert in it a set of identical periodically distributed obstacles T^ε. Let us denote the resulting domain by Ω^ε ε being a small parameter related to the characteristic size of the obstacles. We assume that the size of the obstacles is of the order of $r(\varepsilon)$. In such a domain, we shall study a semilinear problem involving diffusion and suitable chemical reactions taking place on the boundary of the inclusions. There exists a critical size of the inclusions that separates different asymptotic behaviours of the solution of such a problem. We shall discuss here only the case of the so-called *big particles*. The case of *small particles* and, in particular, the interesting case of *critical particles* will be addressed in a forthcoming paper. Under suitable hypotheses, it is well-known that the solution of our problem converges, as ε goes to zero, to the solution of a new elliptic PDE, containing an extra-term generated by the chemical reactions taking place on the surface of the particles.

Our main goal is to study the behaviour of the so-called *effectiveness factor* η_ε and to establish the relation between this factor and the corresponding one defined for the homogenized problem. We shall be also interested in analyzing the effect of the shape of the particles (in particular, their total surface $|\partial T|$ and the homogenized diffusion coefficient $a_0(T)$) in both functionals. We shall prove the existence of convex shapes which maximize the effectiveness.

One of the most popular principles of Nanotechnology, especially in the context of composite media, says, roughly speaking, that one of the reasons for the optimality of certain composite media comes from the fact that when the size of the small particles decreases (maintaining a prescribed total volume) then their total surface increases and this leads to peculiar properties which cannot be observed when the particles are big (see e.g. [22], [18] and [5]).

We show some numerical experiments in which this ratio is not the only relevant parameter, but rather the one given by a balance between the measure of the surface of the pellets and their shape.

1 Problem setting

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 ε be a real parameter taking values in a sequence of positive numbers converging to zero. ε represents a small parameter related to the characteristic size of the particles. Let T be another open bounded subset of $\mathbb{R}^N$, with the boundary ∂T of class C^2. T will be called *the elementary particle* and

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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 $\overline{T} \subset Y$. Let $r : \mathbb{R}_+ \to \mathbb{R}_+$ be a continuous map, related to the size of the pellet. We shall assume that $r(\varepsilon) \sim \varepsilon$. These are known as *big particles*. The case of *small particles*, when $\lim_{\varepsilon\to 0} r(\varepsilon)/\varepsilon = 0$ and $r(\varepsilon) < \varepsilon/2$, will be treated in a forthcoming paper.

REMARK 1 Even though the usual term in homogenization theory for the 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 reactors and towers. Therefore, we will refer to these *holes* as *pellets*, *particles* or even *inclusions* and *obstacles*.

For each ε and for any vector $\mathbf{i} \in \mathbb{Z}^N$, we shall denote by $T^\varepsilon_{\mathbf{i}}$ the translated image of $r(\varepsilon)T$ by the vector $\varepsilon\mathbf{i}$, $\mathbf{i} \in \mathbb{Z}^N$: $T^\varepsilon_{\mathbf{i}} = \varepsilon\mathbf{i} + r(\varepsilon)T$. Also, let us denote by T^ε the set of all the pellets contained in Ω, i.e.

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

and let the number of pellets be $n(\varepsilon) = \#\left\{\mathbf{i} \in \mathbb{Z}^N : \overline{T^\varepsilon_{\mathbf{i}}} \subset \Omega\right\}$. Set $\Omega^\varepsilon = \Omega \setminus \overline{T^\varepsilon}$. Therefore, Ω^ε 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 $S^\varepsilon = \cup\{\partial T^\varepsilon_{\mathbf{i}} \mid \overline{T^\varepsilon_{\mathbf{i}}} \subset \Omega, \mathbf{i} \in \mathbb{Z}^N\}$. So, $\partial\Omega^\varepsilon = \partial\Omega \cup S^\varepsilon$. We shall consider the homogenization of problems in the form

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

where ν is the exterior unit normal to S^ε,

(2) g is a maximal monotone graph such that $g(0) = 0$,

(single-valued or even multivalued) and

$$(3) \qquad f \in L^2(\Omega), \quad f \geq 0.$$

A particular case we shall discuss is the Freundlich isotherm:

$$(4) \qquad g(u) = |u|^{p-1}u, \qquad p \in (0, 1].$$

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

$$(5) \qquad g(u) = \begin{cases} 0 & u < 0, \\ [0, 1] & u = 0, \\ 1 & u > 0. \end{cases}$$

We address here the interesting cases in which $\mu(\varepsilon)|S^\varepsilon| = O(1)$. In fact, we can consider that if $r(\varepsilon) = \varepsilon^\alpha$, then $\mu(\varepsilon) = \varepsilon^{-\gamma}$, $\gamma = \alpha(N-1) - N$. In our case, i.e. for big particles, $\alpha = 1$, and so $\gamma = -1$.

Through standard procedures in weak solution theory, one easily gets the following result (see, e.g., [6]).

PROPOSITION 2 (WELL-POSSEDNESS) *Under the assumptions* (2) *and* (3), *there exists a unique solution* $u \in H^2(\Omega)$ *of* (1).

PROPOSITION 3 (STRONG MAXIMUM PRINCIPLE) *Under the assumptions* (2) *and* (3), $u_\varepsilon > 0$ *in* Ω_ε.

Proof. . By the 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

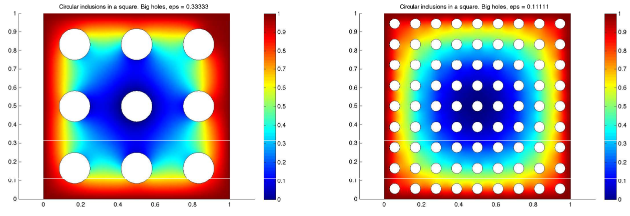
$$\begin{cases} -\Delta \underline{u}_\varepsilon = f & \text{in } \Omega^\varepsilon, \\ \underline{u}_\varepsilon = 0 & \text{on } \partial\Omega \cup S^\varepsilon, \end{cases}$$

to obtain $u_\varepsilon \geq \underline{u}_\varepsilon$ in Ω^ε. For $\underline{u}_\varepsilon$, we can apply the bound found in [15]

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

which proves the result. □

We can see a couples of the steps of the homogenization process in the following COMSOL simulation.



(a) $\varepsilon = 0.33$ (b) $\varepsilon = 0.11$

Figure 1: Fixed bed reactors with big pellets ($r_\varepsilon = \varepsilon$) and the level set of the solution of problem (1) for $f = 0$, (4) where $p = \frac{1}{2}$, $\mu(\varepsilon) = \varepsilon$.

2 Homogenization of the state equation

Assume that $r(\varepsilon) = \varepsilon$ and either a smooth kinetic

$$(6) \qquad |g'(v)| \leq C(1 + |v|^q), \qquad 0 \leq q < \frac{N}{N-2}$$

or not necessarily a smooth one with bounded growth

$$(7) \qquad |g(v)| \leq C(1 + |v|^q), \qquad 0 \leq q < \frac{N}{N-2}.$$

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

$$(8) \qquad \begin{cases} -\operatorname{div}(a_0(T)\nabla u) + \frac{|\partial T|}{|Y \setminus T|} g(u) = f & \text{in } \Omega, \\ u = 1 & \text{on } \partial\Omega. \end{cases}$$

The proof of existence and uniqueness of a weak solution for this problem can be found, e.g., in [12]. Here, $a_0(T) \in \mathcal{M}_N(\mathbb{R})$ 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 χ_i are the solutions of the so-called *cell problems*:

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

For the corresponding result in the case of small particles, we refer to [16]. Let us mention that in the critical case, i.e. the case in which $r(\varepsilon) = \varepsilon^{N/(N-2)}$, the extra-term arising in the homogenized equation is defined in terms of the solution of a functional equation involving the nonlinear function g.

2.1 Effectiveness and homogenization

For the case of smooth kinetics, we shall assume that $g(0) = 0$ and we shall impose growth condition (6) on the nonlinearity g. Inspired by the definition given in the linear case $p = 1$ by the chemical engineer R. Aris (see [1] and [2]), we define the notion of **effectiveness** of the pellet in this more general setting as follows:

$$\eta_\varepsilon(T) = \frac{1}{|S_\varepsilon|} \int_{S_\varepsilon} g(u_\varepsilon) d\sigma. \tag{10}$$

This is well defined since $g(u^\varepsilon) \in W_0^{1,\bar{q}}(\Omega)$, $\bar{q} = \frac{2N}{q(N-2)+N}$.

Definition (10) can be naturally extended to the homogenized case, as follows

$$\eta(T) = \frac{1}{|\Omega|} \int_\Omega g(u) dx. \tag{11}$$

PROPOSITION 4 *For $\varepsilon \to 0$, it follows that $\eta_\varepsilon(T) \to \eta(T)$.*

Proof. From [8] (see also [9]), it holds that

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

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,

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

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

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

which proves the result. □

REMARK 5 It is an open problem whether or not this convergence remains true under more general nonlinearities g. Our proof of the convergence relies on [8], in which one requires differentiability of $g(u^\varepsilon)$. We can define the effectiveness η_ε by means of $g(\mathrm{tr}_{S_\varepsilon}(u^\varepsilon))$. However, the proof, in essence, requires that we consider $\mathrm{tr}_{S_\varepsilon}(g(u^\varepsilon))$. It is our belief that a proof of the general case might need an extension of the results in [8] or a completely new approach.

REMARK 6 The convergence remains true for the kinetic (4) in the case of domains in which there exists $\delta > 0$ such that $u^\varepsilon \geq \delta$ uniformly on ε, 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 [12], [4] and the references therein. In the case when a dead core exists, even though the limit theorem does not apply, the strong maximum principle (Proposition 3) suggests that the effectiveness is higher prior to the homogenization process.

3 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 hole shape. We will focus on the homogenized model (8). Our main result is the following one:

THEOREM 7 *Let $0 < \theta < |Y|$, C, D be fixed proper subsets of Y and $\tilde{\varepsilon} > 0$. Let us consider the hypothesis*

(12) *T satisfies the uniform $\tilde{\varepsilon}$-cone property.*

We define

$$U_{adm} = \{\overline{C} \subset T \subset \overline{D} : T \text{ satisfies }, (12) \text{ and } |T| = \theta\},$$
$$C_\theta(D) = \{T \subset D : T \text{ is open, convex and } |T| = \theta\}.$$

At fixed volume $\theta \in (0, |Y|)$, there exists a domain of maximal effectiveness in the class of $T \in U_{adm} \cap C_\theta(D)$.

REMARK 8 Optimization of the effectiveness considering the homogenized domain Ω (the chemical reactor) has also been studied (see [13], [14] and the references therein). In this situation, the existence of a *dead core* affects the effectiveness negatively.

REMARK 9 Dealing with the optimization of the domain Ω, **there exist no optimal shapes** considering a general framework (see [4], [14]). We conjecture that new results may be also obtained by applying methods analogous to the ones that follow.

REMARK 10 As in [9], the problem in which we consider reactions inside the pellets can also be addressed. 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 $a, D_f, D_p > 0$ 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 $A^0 = (a^0_{ij})$ is the homogenized matrix, whose entries are defined as follows: $a^0_{ij} = \int_Y (a_{ij} + a_{ik} \frac{\partial \chi_j}{\partial y_k}) dy$, in terms of the functions χ_j, $i = 1, ..., N$, 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.

We see in (8) that the effect of T is present in three terms: $a_0(T), |\partial T|$ and $|Y \setminus T|$. Therefore, any sensible choice of topology for the set of admissible domains T in a search for optimal obstacles must make this expressions continuous.

A logical choice of topology in the space of shape is the one given by the Hausdorff distance

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

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, [23]) that the following result holds true.

THEOREM 11 ([23]) *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 [17].

LEMMA 12 ([17]) *If U_{adm} is compact with respect to the Hausdorff metric and if $T_n \to T$, $(T_n) \subset U_a$ as $n \to \infty$, $T \in U_{adm}$, then $a_0(T_n) \to a_0(T)$ in $\mathcal{M}_N(\mathbb{R})$.*

The behaviour of the measure $|Y - T|$ is slightly more delicate (we include a commentary even though, in our family, 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, $d_{H^c}(\Omega_n, \Omega) \to 0$ as $n \to \infty$ implies $\liminf_n |\Omega_n| \geq |\Omega|$. However, lower semicontinuity of the measure of the boundary ($|\partial T|$) is, in general, false (see [17] for some counterexamples). Nevertheless, the set of **convex** domains has a number of very interesting properties (see [24]).

LEMMA 13 ([24]) *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 theorem, proved in [7].

LEMMA 14 ([7]) *Let $(\Omega_n), \Omega \in C_\theta(D)$. If $\Omega_1 \subset \Omega_2$, then $|\partial\Omega_1| \leq |\partial\Omega_2|$. Moreover, if $\Omega_n \overset{d_H}{\to} \Omega$, then $|\Omega_n| \to |\Omega|$ and $|\partial\Omega_n| \to |\partial\Omega|$, as $n \to \infty$.*

For the continuity of solutions with respect to T, we need the following theorem of continuity of Nemitskij operators (see, for example, [19], [11] and [21]).

LEMMA 15 ([21]) *Let $G : \Omega \to \mathbb{R} \to \mathbb{R}$ be a Carathéodory function such that (7) with $q = \frac{r}{t}$ with $r \geq 1$ and $t < \infty$. Then, the map*

$$L^r(\Omega) \to L^t(\Omega) \qquad v \mapsto G(x, v(x))$$

is continuous in the strong topologies.

LEMMA 16 *Let $\mathcal{A}$ be the set of elliptic matrices and let g satisfy (7). Then, the application*

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

where u is the unique solution of

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

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 $A_n \to A$ and $\lambda_n \to \lambda$ be two converging sequences. It is easy to prove that $u_n = u(A_n, \lambda)$ is bounded in $H^1(\Omega)$ and, up to a subsequence, $u_n \rightharpoonup u$ in H^1 as $n \to \infty$. Therefore, $\int_\Omega (A \nabla u) \nabla u \leq \liminf_n \int_\Omega (A_n \nabla u_n) \nabla u_n$. We can apply Theorem 15 to show that $G(u_n) \to G(u)$ in L^1 as $n \to \infty$ (see details for a similar proof, for example, in [9]) and we have that $u = u(A, \lambda)$. □

COROLLARY 17 *In the hypotheses of the previous lemma, the map $(A, \lambda) \mapsto \int_\Omega g(u(A, \lambda))$ is continuous.*

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

Proof. of Theorem 7 First, we have that Lemmas 12 and 14 imply that the application $T \mapsto (a_0(T), \lambda(T))$ is continuous. Then, Corollary 17 implies that $T \mapsto \eta(T)$ is continuous. Therefore, since $C_\theta(D)$ is closed and U_{adm} is compact, by Lemma 12 we have the compactness of $U_{adm} \cap C_\theta(D)$ and the existence of maximizers. $\square$

4 Effectiveness for obstacles with some symmetries. Numerical experiments

There exists a large literature on the computation and behaviour of the homogenized coefficient $a_0(T)$, both from the mathematics and the engineering part (see, e.g., [3], [17], [20]). In these papers, one can find power series techniques and numerical analysis, generally for spherical obstacles. As it is common in the literature (e.g. [3]), we use the commercial software COMSOL. As said on the introduction, in nanotechnology, however, it is a common misconception that the measure of the surface alone, $|\partial T|$, is a good indicator of the effectiveness of the obstacle.

Considering obstacles with some symmetries (for $N = 2$ it is sufficient that they are invariant under a 90^0 rotation) in general, it is well known that $a_0(T) = \alpha(T)I$, where $\alpha(T)$ is a scalar (see, for example, [3], [20]) and I is the identity matrix in $\mathcal{M}_N(\mathbb{R})$. In this case, it can be easily proved that the effectiveness is an decreasing function of $\lambda(T) = |\partial T|/(\alpha(T)|Y \setminus T|)$ (it is a direct consequence of the comparison principle, see [12]). In fact, this is the only relevant parameter (once $g(u)$ is fixed) of the equation (8). The behaviour of the effectiveness with respect to the coefficient λ can also be numerically computed:

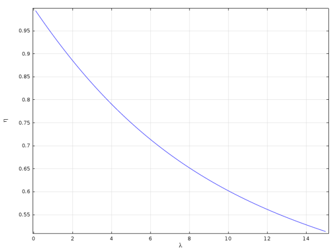
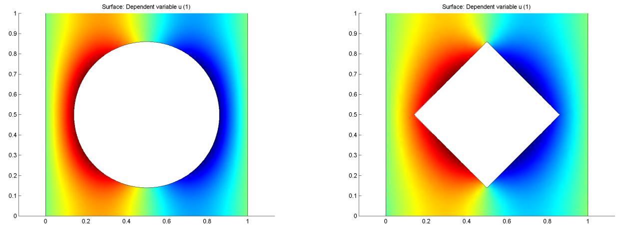


Figure 2: Plot of η as a function of λ when Ω is a 2D circle.

Let us consider, in two dimensions for simplicity, the following obstacles:



(a) Circular inclusions (b) Square inclusions

Figure 3: Two obstacles T, and the level sets of the solution of the cell problem (9)

We can numerically compute the homogenized diffusion coefficient $a_0(T)$ via a parametric sweep on the size of the obstacle.

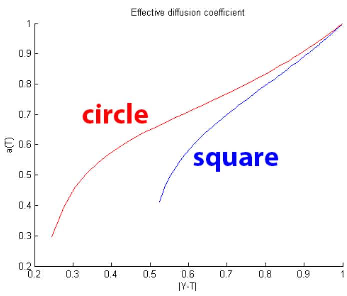
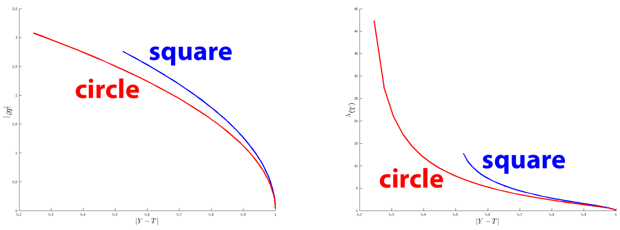


Figure 4: The effective diffusion coefficient $\alpha(T)$. Circular particles in red and square particles in blue

Now, we can couple this with direct computations of $|\partial T|$ and compare the behaviour of both indicators.



(a) Classical coefficient $|\partial T|$. (b) New coefficient $\lambda(T)$ as a function of the concentration $|Y \setminus T|$

Figure 5: Coefficients $|\partial T|$ and $\lambda(T)$. Circular particles in red and square particles in blue

Since $|Y \setminus T| = 1 - \theta$ and since η is monotone decreasing with respect to λ, what Figure 5 represents is a comparison between the effectiveness of circular and square pellets for different θ. We can conclude that, in the computed cases, circular pellets are more efficient. This could have also been deduced solely from the consideration of $|\partial T|$. However, even though the relative order is not affected, what we see in Figure 5 is that the behaviour close to minimum and maximum admissible θ (which correspond with $\theta = 0$ and the pellet touching the boundary of the cell) on each is radically different (notice the steepness). The fact that the circle appears to be more effective contrast with the fact that in the homogenized reactor Ω a sphere is worst (see [4], [13], [14]).

Acknowledgments

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