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AN APPLICATION OF SHAPE DIFFERENTIATION TO THE EFFECTIVENESS OF A STEADY STATE REACTION-DIFFUSION PROBLEM ARISING IN CHEMICAL ENGINEERING

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Dedicated to our colleague and good friend Alfonso Casal on his 70th birthday

Abstract. In applications it is common to arrive at a problem where the choice of an optimal domain is considered. One such problem is the one associated with the steady state reaction diffusion equation given by a semilinear elliptic equation with a monotone nonlinearity g. In some contexts, in particular in chemical engineering, it is common to consider the functional given by the integral of this nonlinear term of the solution dived by the measure of the domain Ω in which the pde takes place. This is often related with the effectiveness of the reaction. In this paper our aim is to study the differentiability of such functional as study connected to the optimality of the best chemical reactor.

1. Introduction and statement of results

The main goal of this article is to analyze the differentiability, with respect to the domain Ω, of the *effectiveness factor*

$$\mathcal{E}(\Omega) = \frac{1}{|\Omega|} \int_\Omega \beta(w_\Omega) dx$$

where w_Ω is the solution of the problem arising in chemical catalysis [2, 3]

$$\begin{aligned} -\Delta w + \beta(w) &= \hat{f}, \quad \text{in } \Omega, \\ w &= 1, \quad \text{on } \partial\Omega. \end{aligned} \tag{1.1}$$

The model can be obtained in different ways, including homogenization techniques: see, e.g. [6] and [5]. By introducing the change in variable $u = 1 - w$ the problem can be reformulated as

$$\begin{aligned} -\Delta u + g(u) &= f, \quad \text{in } \Omega, \\ u &= 0, \quad \text{on } \partial\Omega. \end{aligned} \tag{1.2}$$

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where $g(u) = \beta(1) - \beta(1-u)$ and $f = \beta(1) - \hat{f}$. In this case instead of the effectiveness factor we can study $\eta(\Omega) = 1 - \mathcal{E}(\Omega)$

$$\eta(\Omega) = \frac{1}{|\Omega|} \int_\Omega g(u_\Omega) dx \,, \tag{1.3}$$

where u_Ω is the solution of (1.2). In the chemical context this factor represents the amount of reaction taking place.

This kind of problems fall with the family of problems studied by several authors in the literature (see, e.g. [18, 19, 20] and the references therein). In the most general case this family of problems may be described by:

$$\begin{aligned} A(u(D)) &= f, \quad \text{in } D, \\ B(u(D)) &= g, \quad \text{on } \partial D \end{aligned} \tag{1.4}$$

and the functional can by given generally as

$$J(D) = \int_D C(u_D) dx,$$

where A, B, C may contain also some derivatives of u_D. In this paper we shall concentrate our attention in problem (1.2) and we shall provide elementary and direct proofs of results which could be obtained from the general theory but under stronger assumptions (see, for instance, the statement taken from [20] which is reproduced here in Section 2).

As mentioned before, our aim is to study the differentiability of functional (1.3). We consider a fixed domain open bounded regular set of $\mathbb{R}^n$, Ω_0, and study its deformations given by a function $\theta : \mathbb{R}^n \to \mathbb{R}^n$, so that the new domain is $\Omega = (Id + \theta)\Omega_0$. We consider, as it is the case in chemistry catalysis, g and f such that $0 \le u \le 1$. We also mention that this kind of differentiation result also appears in many other contexts. Besides the above mentioned references we recall here the articles [7] for a linear problem with a Dirichlet constant boundary condition and [17] were a semilinear equation arising in combustion was considered (corresponding, in our formulation to take $g(u) = -e^u$).

To obtain this properties in the sense of derivatives, we consider two approaches, mimicking the approach in differential geometry. We first consider the global differentiability of solutions (as it was done in the linear cases in [15, 1] and the most general case in [20]), which unfortunately requires derivatives in spaces of too regular functions, and then we take advantage of the differentiation along curves (the approach followed in [21]).

Let us call, for simplicity, u_Ω the solution of (1.2). This corresponds to the Lagrangian understanding of the problem in the sense that the functional under study is study in terms of the direct domain Ω. However, we can consider the Eulerian understanding of the problem by recalling that in this family of domains, $\Omega = (Id + \theta)\Omega_0$, we can introduce a new function $v_\theta : \Omega_0 \to \mathbb{R}$ defined by

$$v_\theta = (I+\theta)^* u_{(I+\theta)\Omega_0} = u_{(I+\theta)\Omega_0} \circ (I + \theta), \tag{1.5}$$

simplifying the study of the differentiability of u_Ω and the functional $\eta(\Omega)$ with respect to Ω.

Our proof relies heavily on the Implicit Function Theorem. The application of this theorem requires an uniform choice of functional space, which would require some additional information on u. This kind of problems in the functional setting is well portrayed in [4].

For the nonlinearity g we shall consider the following assumptions:

Hypothesis 1.1. g is nondecreasing

Hypothesis 1.2. The Nemitskij operator for g (which we will denote again by g in some circumstances, as a widely accepted abuse of notation) $G : H^1(\Omega) \to L^2(\Omega)$ defined by

$$G(u) = g \circ u \tag{1.6}$$

is of class C^m for some $m \geq 1$.

We recall that Hypothesis 1.2 immediately implies that $[DG](v)\varphi = g'(v)\varphi$ for $\varphi, v \in H^1(\Omega)$ and that if G is of class $\mathcal{C}^k$ with $k > 1$ then necessarily $g(s) = as + b$ for some $a, b \in \mathbb{R}$.

Our first result collects some general results on the differentiability of the solution u_Ω with respect to Ω:

Theorem 1.3. *Let g satisfy Hypothesis 1.1 and 1.2. Then, the map $W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \to H_0^1(\Omega_0)$,*

$$\theta \mapsto v_\theta$$

(where v_θ is defined by (1.5)) is of class $\mathcal{C}^l$ in a neighbourhood of 0 if $f \in H^k(\mathbb{R}^n)$ where $l = \min\{k, l\}$. Furthermore, the application $u : W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \to L^2(\mathbb{R}^n)$,

$$\theta \mapsto u_{(I+\theta(\Omega_0))}$$

(where u_θ is extended by zero outside $(I + \theta)(\Omega_0)$) is differentiable at 0. In fact $u' : W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \to H^1(\Omega)$ and

$$u'(0)\theta + \nabla u_{\Omega_0} \cdot \theta \in H_0^1(\Omega).$$

As in differential geometry, to compute a derivative we can take two routes. The first one is to show the existence of a global derivative, and this allows to compute some properties of our functions. The other one, is to compute the derivative along curves.

Definition 1.4. We say that Φ is a curve of deformations if $\Phi : [0, T) \to W^{1,\infty}(\Omega_0)$ with $\det \Phi(\tau) > 0$.

Hypothesis 1.5. We will say that θ is a curve of small perturbations of the identity (with direction V) if $\Phi(\tau) = I + \theta(\tau)$ is a curve of deformations and

(1) $\theta : [0, T) \to W^{1,\infty}(\mathbb{R}^n)$ is differentiable at 0,
(2) $\theta(0) = 0$,
(3) $\theta'(0) = V$.

Sometimes we consider higher order derivatives too. We will refer to θ or Φ indistinctively, since they relate by $\Phi(\tau) = I + \theta(\tau)$. Thus, the above theorem leads to:

Corollary 1.6. *Let Φ be a a curve of deformations of class $\mathcal{C}^k$. Then $\tau \mapsto v_{\theta(\tau)}$ is of class $\mathcal{C}^l$ with $l = \min\{m, k\}$.*

Our second result concerns the characterization of u'.

Theorem 1.7. *Let g satisfy Hypothesis 1.1 and 1.2. Let θ be a curve satisfying assumptions 1.5. Then u is differentiable along Φ at least at 0. That is, the directional derivative $\frac{d}{d\tau}(u \circ \Phi)$ exists, and it is the solution u' of*

$$\begin{aligned} -\Delta u' + \lambda g'(u_{\Omega_0})u' = 0 \quad &\text{in } \Omega_0, \\ u' = -\nabla u_{\Omega_0} \cdot V, \quad &\text{on } \partial\Omega_0. \end{aligned} \tag{1.7}$$

We point out that the above result shows, in other terms, that $u'(0)\theta$ is the unique weak solution of

$$\begin{aligned} -\Delta u' + \lambda g'(u_{\Omega_0})u' = 0, \quad &\text{in } \Omega_0, \\ u' = -\nabla u_{\Omega_0} \cdot \theta, \quad &\text{on } \partial\Omega_0. \end{aligned} \tag{1.8}$$

As consequence we have the following result.

Corollary 1.8. *The function $u' : W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \to H^1(\Omega)$ is continuous. In fact, since the solution u of (1.2) $u \in W^{2,p}(\Omega)$ for any $p \in [1, +\infty)$ then for any $q \in [1, p]$,*

$$\begin{aligned} |u'(0)(\theta)|_q &\le c|\nabla u \cdot \theta|_{L^p(\partial\Omega_0)} \\ &\le c|\theta|_\infty |\nabla u_{\Omega_0}|_{L^p(\partial\Omega_0)} \\ &\le c(p)|\theta|_\infty |u_{\Omega_0}|_{W^{2,p}(\Omega_0)}. \end{aligned}$$

Concerning the differentiability of the effectiveness factor functional we have the following theorem.

Theorem 1.9. *Under the assumptions of Theorem 1.3, let*

$$\hat{\eta}(\theta) = \int_{(I+\theta)\Omega_0} g(u_{(I+\theta)\Omega_0}) dx. \tag{1.9}$$

Then η is of class $\mathcal{C}^m$ in a neighbourhood of 0. It holds that

$$\hat{\eta}^{(m)}(0)(\theta_1, \cdots, \theta_m) = \int_{\Omega_0} \frac{d^n}{d\theta_n \cdots d\theta_1} (g(v_\theta) J_\theta) \, dx. \tag{1.10}$$

Its first derivative can be expressed in terms of u,

$$\hat{\eta}'(0)(\theta) = \int_{\Omega_0} (g'(u_{\Omega_0})u' \ + \operatorname{div}(g(u_{\Omega_0})\theta)) \, dx, \tag{1.11}$$

and if ∂G is Lipschitz

$$\hat{\eta}'(0)(\theta) = \int_{\Omega_0} g'(u_{\Omega_0})u' \, dx + g(0) \int_{\partial\Omega_0} \theta \cdot n \, dS, \tag{1.12}$$

where $u' = u'(0)(\theta)$.

Corollary 1.10. *Under the assumptions of Theorem 1.3 it holds that*

$$\eta'(\theta) = \frac{1}{|\Omega_0|} \Big(\int_{\Omega_0} g'(u_{\Omega_0})u' \, dx - \eta(0) \int_{\partial\Omega_0} \theta \cdot n \, dS \Big).$$

Corollary 1.11. *Under the assumptions of Theorem 1.3 if Φ is a volume preserving curve then*

$$\eta'(\theta) = \frac{1}{|\Omega_0|} \int_{\Omega_0} g'(u_{\Omega_0})u' \, dx \, .$$

We point out that if g is Lipschitz (i.e. $g \in W^{1,\infty}(\mathbb{R})$) then we obtain

$$|\eta(\theta) - \eta(0)| = |\eta'(0)(\lambda\theta)| \le c|g'|_\infty |u|_{W^{2,p}} |\theta|_\infty .$$

This allows to get some generalizations of the last result in cases in which the absorption term g is not so regular, as for instance when $\beta(w) = w^q$ and $q \in (0,1)$. Nevertheless, if there is a non-empty dead core (in the literature the dead core is defined as $\{x \in \Omega : w_\Omega(x) = 0\}$ where w_Ω is the solution of (1.1)) some additional arguments must be developed, in the line of [14], where some unbounded potentials are considered. This will the subject of a separated paper by the authors [12].

We end this paper by presenting, in Section 5, some applications of the above results in terms of the Schwarz and Steiner symmetrization as well as by illustrating them for some special families of domains by means of some numerical experiences.

2. Functional setting: Nemitskij operators and the implicit function theorem

Let us formalize what we mean by a shape functional. At the most fundamental level it should be a function defined over a set of domain, that is defined over $\mathfrak{C} \subset \mathcal{P}(\mathbb{R}^n)$. Since we want to differentiate we, at the very least, need to define proximity, that is a way to define *neighbourhood of a set*. As it is usual in the literature of shape optimization we work over the set of weakly differentiable bounded deformations with bounded derivative, the Sobolev space $W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$.

Definition 2.1. We say that J is defined on a neighbourhood of $\Omega_0 \subset \mathbb{R}^n$ if there exists U a neighbourhood of 0 on $W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$ such that J is defined over $\{(Id + \theta)(\Omega_0) : \theta \in U\}$. We say that J is differentiable at Ω_0 if the application $W^{1,\infty}(\mathbb{R}^n; \mathbb{R}^n) \to \mathbb{R}$,

$$\theta \mapsto J((Id + \theta)(\Omega_0))$$

is differentiable at 0.

We present a sufficient condition so that Hypothesis 1.2 holds. This is widely used in the context of partial differential equations, but as far as we know no reference is known besides it being an exercise in [16]. That being the case we provide the usual proof. Other conditions, mainly on the growth of g can be considered so that assumptions 1.1.1.2 holds.

Lemma 2.2. *Let $g \in W^{2,\infty}(\mathbb{R})$. Then the Nemitskij operator* (1.6) *in the sense $L^p(\Omega) \to L^2(\Omega)$ is of class $\mathcal{C}^1$ for all $p > 2$. In particular, Hypothesis 1.2 holds.*

Proof. Let us define G the Nemitskij operator defined in (1.6). Consider it $G : L^p(\Omega) \to L^2(\Omega)$ for $p \ge 2$. We first have that, for $L = \max\{\|g\|_\infty, \|g'\|_\infty, \|g''\|_\infty\}$

$$\|G(u) - G(v)\|_{L^2}^2 = \int_\Omega |g(u) - g(v)|^2 dx \le L \int_\Omega |u - v|^2 dx2$$

so that F is continuous. For $p > 2$ let $\varphi \in \mathcal{C}^\infty(\Omega)$ we compute

$$\|g(u + \varphi) - g(u) - g'(u)\varphi\|_{L^2}^2 = \int_\Omega |g'(\xi(x)) - g'(u(x))|^2 |\varphi(x)|^2 dx$$

for some function ξ by the intermediate value theorem. We, of course, have that

$$|g'(\xi(x)) - g'(u((x))| \le L|\xi(x) - u(x)| \le L|\varphi(x)|$$
$$|g'(\xi(x)) - g'(u(x))| \le 2L$$

$$|g'(\xi(x)) - g'(u(x))| \le L 2^{1-\alpha} |\varphi(x)|^\alpha, \quad \forall \alpha \in (0,1)\,.$$

Therefore,

$$\|g(u+\varphi) - g(u) - g'(u)\varphi\|_{L^2}^2 \le L^2 2^{2-2\alpha} \int_\Omega |\varphi(x)|^{2+2\alpha} dx\,.$$

Let $2 < p < 4$ then we have that $p = 2 + 2\alpha$ with $0 < \alpha < 1$. We then have that

$$\|g(u+\varphi) - g(u) - g'(u)\varphi\|_{L^2} \le L 2^{1-\alpha} \|\varphi(x)\|_{L^p}^{1+\alpha}$$

which proves the Frechet differentiability. Of course for $p > 4$ we have that $L^p(\Omega) \hookrightarrow L^3(\Omega)$. Furthermore, for any given dimension n we have Sobolev inclusions $H^1(\Omega) \hookrightarrow L^p(\Omega)$ with $p > 2$, proving the differentiability. □

Some other well-known results are quoted now.

Theorem 2.3. *Let $g \in W^{1,p}(\mathbb{R}^n)$. Then the map $\mathfrak{G} : W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \to L^p(\mathbb{R}^n)$ given by $\theta \mapsto g \circ (I + \theta)$ is differentiable in a neighbourhood of 0 and*

$$\mathfrak{G}'(0) = (\nabla g) \circ (I + \theta)\,.$$

Theorem 2.4 ([15, Lemme 5.3.3.])**.** *Let $g \in W^{1,p}(\mathbb{R}^n)$,*

$$\Psi : W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \to W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$$

continuous at 0 with $\Psi(0) = I$, $W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \to L^p(\mathbb{R}^n) \times L^\infty(\Omega)$,

$$\theta \mapsto (g(\theta), \Psi(\theta))$$

differentiable at 0, with $g(0) \in W^{1,p}(\mathbb{R}^n)$ and

$$g'(0) : W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \to W^{1,p}(\mathbb{R}^n)$$

continuous. Then the application $\mathfrak{G} : W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \to L^p(\mathbb{R}^n)$,

$$\mathfrak{G}(\theta) = g(\theta) \circ \Psi(\theta)$$

is differentiable at 0 and

$$\mathfrak{G}'(0) = g'(0) + \nabla g(0) \cdot \Psi'(0).$$

To conclude this section we state a classical result.

Theorem 2.5 (Implicit Function Theorem)**.** *Let X, Y and Z be Banach spaces and let U, V be neighbourhoods on X and Y, respectively. Let $F : U \times V \to Z$ be continuous and differentiable, and assume that $D_y F(0,0) \in \mathcal{L}(Y, Z)$ is bijective. Let assume, further, that $F(0,0) = 0$. Then there exists W neighbourhood of 0 on X and a differentiable map $f : W \to Y$ such that $F(x, f(x)) = 0$. Furthermore, for x and y small, $f(x)$ is the only solution y of the equation $F(x,y) = 0$. If F is of class $\mathcal{C}^m$ then so is f.*

3. Differentiation of solutions. Proof of Theorems 1.3 and 1.7

For the reader convenience we repeat here the general result in [20]:

Theorem 3.1. *Let D be a bounded domain such that ∂D be a piecewise $\mathcal{C}^1$ and assume that D is locally on one side of ∂D. Let u_0 be the solution of (1.4). Let us use the notation $\mathcal{C}^k = \mathcal{C}^k(\mathbb{R}^n, \mathbb{R}^n)$ and $k \ge 1$. Assume that*

$$u(\theta) \in W^{m,p}((I + \theta)D) \tag{3.1}$$

and that for every open set D' close to D (for example $D' = (I+\theta)D$ for small θ' in the norm of $\mathcal{C}^k$),

$$\begin{gathered}
A : W^{m,p}(D') \to \mathcal{D}'(D') \\
B : W^{m,p}(D'^{1,1}(D') \\
C : W^{m,p}(D'^{1}(D') \\
A, B, C : W^{m-1,p}(D') \to \mathcal{D}'(D) \text{ differentiable}
\end{gathered} \tag{3.2}$$

and $\mathcal{C}^k \to W^{m,p}$: $\theta \mapsto u(\theta) \circ (I+\theta)$ is differentiable at 0. Then:

(1) *The solution is differentiable in the sense that $u : \mathcal{C}^k \to W^{m-1,p}_{\rm loc}(D)$ is differentiable and the derivative the local derivative u' in the direction of τ satisfies*
$$\frac{\partial A}{\partial u}(u_0)u' = 0, \quad \text{in } D. \tag{3.3}$$
(2) *If $\theta \mapsto B(u(\theta)) \circ (I+\theta)$ is differentiable at 0, into $W^{1,1}(D)$, $B(u_0) \in W^{2,1}(D)$ and $g \in W^{2,1}(\mathbb{R}^n)$, then u' satisfies*
$$\frac{\partial B}{\partial u}(u_0)u' = -\tau \cdot n \frac{\partial}{\partial n}(B(u_0) - g). \tag{3.4}$$
(3) *If $\theta \mapsto C(u(\theta)) \circ (I+\theta)$ is differentiable at 0 into $L^1(D)$, and $C(u_0) \in W^{1,1}(D)$, then $\theta \mapsto J(\theta)$ is differentiable and its directional derivative in the direction of τ is:*
$$\frac{\partial J}{\partial \theta}(0)\tau = \int_D \frac{\partial C}{\partial u} u' \, dx + \int_{\partial D} \tau \cdot n C(u_0) \, dS. \tag{3.5}$$

Let us prove now our first contribution.

Proof of Theorem 1.3. We take several steps. For simplicity, allow the notation
$$\Omega_\theta = (I+\theta)(\Omega_0).$$
We first check that v_θ satisfies
$$-\operatorname{div}(A(\theta)\nabla v) + \lambda J_\theta g(v_\theta) = (f \circ (I+\theta))J_\theta$$
in $H^{-1}(\Omega)$, where
$$A(\theta) = J_\theta (I + D\theta)^{-1}(I +^t D\theta)^{-1}, \quad J_\theta = \det J(I+\theta)\,.$$
For that, consider for a given $\varphi \in H^1_0(\Omega_0)$ the auxiliar function $\varphi_\theta = \varphi \circ (I+\theta)^{-1} \in H^1_0(\Omega_\theta)$ by definition of u_θ we have
$$\int_{\Omega_\theta} (\nabla u_\theta \nabla \varphi_\theta + \lambda g(u_\theta)\varphi_\theta) \, dx = \int_{\Omega_\theta} f \varphi_\theta \, dS \quad \forall \varphi \in H^1_0(\Omega_0).$$
Then by a change of variable, the result follows.

Let us define the operator $F : W^{1,\infty} \times H^1_0(\Omega_0) \to H^{-1}(\Omega_0)$, by
$$F(\theta, v) = \operatorname{div}(A(\theta)\nabla v) + \lambda J_\theta g(v) - (f \circ (I+\theta))J_\theta$$
of class $\mathcal{C}^1$ (or $\mathcal{C}^m$) in a neighbourhood of $\theta = 0$. On that direction we check

- $\theta \in W^{1,\infty} \mapsto J_\theta = \det(I + D\theta) \in L^\infty$ of class $\mathcal{C}^\infty$ since $\theta \in W^{1,\infty} \to I + D\theta \in L^\infty(\mathbb{R}^n, \mathcal{M}_n)$ and det is a polynomic operator.
- $\theta \in W^{1,\infty} \mapsto (I + D\theta)^{-1} = \sum_{q \geq 0} (-1)^q D\theta^q \in L^\infty(\mathbb{R}^n, \mathcal{M}_n)$ is $\mathcal{C}^\infty$,
- $(A, v) \in L^\infty(\mathbb{R}^n, \mathcal{M}_n) \times H^1_0(G) \mapsto -\operatorname{div}(A\nabla v) \in H^{-1}(G)$ is $\mathcal{C}^\infty$ since it is bilinear and continuous.

- Through the lemma $\theta \mapsto k(\theta) = (f \circ (I + \theta))J_\theta \in L^2(\mathbb{R}^n) \subset H^{-1}(\Omega_0)$ is $\mathcal{C}^1$ so $F \in \mathcal{C}^1$. Note that, if $f = 0$ then $F \in \mathcal{C}^m$.

It holds that

$$D_v F(0,0)\varphi = -\Delta\varphi + \lambda g'(u(\cdot : 0))\varphi$$

and, since $g' \geq 0$, we have that $D_v(0,v) : H_0^1(G) \to H^{-1}(G)$ is a isomorphism by Lax-Milgram's theorem. Through the implicit function theorem (theorem 2.5) there exists a map $\theta \in W^{1,\infty} \to v(\theta) \in H_0^1(\Omega_0)$ of class $\mathcal{C}^1$ is $f \in H^1(\mathbb{R}^n)$ and $\mathcal{C}^m$ if $f = 0$ such that

$$F(\theta, v(\theta)) = 0\,.$$

If we we consider uniqueness for the elliptic problem we find that

$$v(\theta) = v_\theta.$$

Simple substitution returns u_θ. By Theorem 2.4 we have the differentiability of u. □

Once this is done we can make explicit calculations for the directional derivative.

Proof of Theorem 1.7. Let us now characterize the directional derivative. Let $\theta \in W^{1,\infty}$ be fixed, let us call $u' = u'(0)(\theta)$ and let Φ a curve of perturbations of the identity with $V = \theta$. We differenciate on the variational formulation

$$\int_{\mathbb{R}^n} f\varphi \,\mathrm{d}x = \int_{\mathbb{R}^n} (-u_\tau \Delta\varphi + \lambda g(u_\tau)\varphi)\, dx \quad \varphi \in \mathcal{C}_c^\infty(\Omega)$$

to obtain

$$0 = \int_{\Omega_0} (-u'\Delta\varphi + \lambda g'(u_0)u'\varphi)\, dx, \quad \varphi \in \mathcal{C}_c^\infty(\Omega) \tag{3.6}$$

(observe that $h(x) = \lambda g'(u_0(x))$ is a known function). This means that u' is a very weak solution of the aforementioned equation (1.8). Since we know that $u' \in L^2(\mathbb{R}^n)$ we can apply regularity theory for this equation.

For the boundary condition $v_\theta = 0$ on $\partial\Omega_0$, for all θ and therefore $v' = 0, \partial\Omega_0$. Since $v_\tau = u_\tau \circ \Phi(\tau)$ we have

$$u' + \nabla u_{\Omega_0} \cdot \theta = v' \in H_0^1(\Omega_0)$$

which provides the boundary condition. Therefore, we have

$$\int_{\Omega_0} (-u'\Delta\varphi + \lambda g'(u_0)u'\varphi)\, dx = \int_{\partial\Omega_0} ((\nabla u_{\Omega_0} \cdot \theta)\partial_{\mathbf{n}}\varphi)\, dS, \quad \varphi \in \mathcal{C}_0^2(\Omega) \tag{3.7}$$

we can obtain a Kato type inequality to shows uniqueness of very weak solutions (see [13]). For the regularity we apply the following classical trick. Since u' is know we can take $\tilde{f} = -\lambda g'(u_0)u' \in L^2(\Omega)$ and $\tilde{\eta} = -\nabla u \cdot \theta \in L^2(\partial\Omega)$ and find z the unique solution in $H^1(\Omega_0)$ of

$$\begin{aligned} -\Delta z &= \tilde{f}, \quad \text{in } \Omega \\ z &= \tilde{\eta}, \quad \text{on } \partial\Omega \end{aligned}$$

classical theory. Then z is a very weak solution of (3.7) and, by uniqueness, $u'(0) = z \in H^1(\Omega)$. □

Remark 3.2. In the case that further regularity is necessary $v \in H_0^1 \cap H^m$ then deformation must taken in $W^{m,\infty}$. A theory analogous to that on [15] for higher differentiability can be obtained for the non-linear case.

4. Differentiation the functional. Proof of Theorem 1.9 and its corollaries

We shall follow a reasoning similar to the one presented in [15]. Let us define $G_t = \Phi(t, G)$ and consider a function f such that $f(\tau) \in L^1(G_t)$. We take interest on the map $I : \mathbb{R} \to \mathbb{R}$,

$$I(\tau) = \int_{G_\tau} f(\tau, x)\, dx = \int_G f(\tau, \Phi(\tau, y)) J(\tau, y)\, dy \tag{4.1}$$

where $f(\tau, x) = f(\tau)(x)$,

$$J(\tau, y) = \det(D_y \Phi(\tau, y)).$$

Theorem 4.1. *Let Φ very assumptions 1.5, f such that $f : [0, T) \to L^1(\mathbb{R}^n)$ is differentiable at 0 and*

$$f(0) \in W^{1,1}(\mathbb{R}^N)\,.$$

Then, $\tau \mapsto I(\tau) = \int_{G_\tau} f(\tau)$ is differentiable at 0 and

$$I'(0) = \int_G f'(0) + \operatorname{div}(f(0)V)\,.$$

If G is an open set with Lipschitz boundary then

$$I'(0) = \int_G f'(0) + \int_{\partial G} f(0) n \cdot V.$$

In simpler terms, under regularity it holds that

$$\frac{\partial}{\partial \tau}\Big|_{\tau=0} \Big(\int_{G_\tau} f(\tau, x) dx \Big) = \int_{\Omega_0} \Big\{ \frac{\partial f}{\partial \tau}(0, x) + \operatorname{div}\Big(f(0, x) \frac{\partial \Phi}{\partial \tau}(0, x) \Big) \Big\} dx. \tag{4.2}$$

We have some immediate consequences of Theorem 4.1

Lemma 4.2. *Let $g \in W^{1,1}(\mathbb{R}^N)$ and $\Psi : [0, T) \to W^{1,\infty}$ be continuous at 0 such that $\Psi : [0, T) \to L^\infty$ is differentiable at 0, and let Z be its derivative. Then the mapping $[0, T) \to L^1(\mathbb{R}^n)$,*

$$\tau \mapsto g \circ \Psi(\tau)$$

is differentiable at 0 and $G'(0) = \nabla g \cdot Z$.

Lemma 4.3 (Differentiation under the integral sign)**.** *Let E be a Banach space and $f : E \times \Omega \to \mathbb{R}$ be such that $\tilde{f} : E \to L^1(\Omega)$*

$$\tilde{f}(x) = f(x, \cdot)$$

is differentiable at x_0. Let $F : E \to \mathbb{R}$,

$$F(x) = \int_\Omega f(x, y) dy\,.$$

Then F is differentiable at x_0 and

$$DF(x) = \int_\Omega (D_x \tilde{f})(x)(y).$$

Now we can prove the third of our main results.

Proof of Theorem 1.9. It is classical that we can differentiate under the integral sign

$$\int_\Omega f(t,x)dx$$

with respect to t as many times as f is differentiable, and that the integral commutates with the derivative. This shows the derivability with vJ_θ under the integral sign. For the remaining equations we have to be a little more subtle and apply the previous theorem. Let $f(\tau) = g \circ u_\tau$. From the know formulas we must compute

$$f'(\tau) = (g' \circ u_0)u'$$

Thus

$$\frac{\partial}{\partial \tau}\Big|_{\tau=0}\Big(\int_{G_\tau} g(u_\tau)\,dx\Big) = \int_{\Omega_0} \{g'(u_0)u' + \operatorname{div}(g(u_0)\Phi'(0))\}\,dx.$$

If Ω_0 is Lipschitz then

$$\frac{\partial}{\partial \tau}\Big|_{\tau=0}\Big(\int_{G_\tau} g(u_\tau)\,dx\Big) = \int_{\Omega_0} g'(u_0)u'x + g(0)\int_{\partial\Omega_0} \Phi'(0)\cdot n\,dS. \tag{4.3}$$

Equation (1.10) is guaranteed since $g(v) : W^{1,\infty} \to H_0^1(\Omega) \to L^1(\Omega)$ is $\mathcal{C}^1$, and so we can differentiate under the integral sign. □

To show equation (1.10) we need a formula of differentiation under the integral sign

Proof of Corollary 1.10. Given the functional

$$I(\Omega) = \frac{1}{|\Omega|}\int_\Omega g \circ u_\Omega dx$$

If we do not impose constant volume we have also to differentiate the volume measure

$$I(\Phi) = \frac{\int_{\Phi(G)} g \circ u_{\Phi(\Omega_0)}dx}{\int_{\Phi(G)} dx}$$

over a curve of deformations $\Phi(\tau)$ we have, applying the formula of differentiation of fractions

$$\begin{aligned}\frac{\mathrm{d}I}{\mathrm{d}\tau}\Big|_{\tau=0} = \frac{1}{|\Omega_0|^2}\Big(&|\Omega_0|\frac{d}{d\tau}\Big(\int_{\Phi(G)} g \circ u_{\Phi(\Omega_0)}dx\Big)\\ &- \Big(\int_{\Omega_0} \operatorname{div}\Phi'(0)\cdot n\,dx\Big)\Big(\int_{\Phi(G)} g\circ u_{\Phi(\Omega_0)}dx\Big)\Big),\end{aligned}$$

which, once simplified, gives the result. □

The proof of Corollary 1.11 relies on the following Proposition.

Proposition 4.4. *Let $\Phi(\tau)$ be a volume preserving family of deformations of Ω_0 in the sense of Hypothesis 1.5. Then*

$$\int_{\Omega_0} \operatorname{div}\Phi'(0)\,dx = 0.$$

If G is Lipschitz then

$$\int_{\partial\Omega_0} \Phi'(0)\cdot n\,dS = 0.$$

Proof. Define $G_\tau = \Phi(\Omega_0, \tau)$; then

$$c = \int_{G_\tau} 1 \, \mathrm{d}x \,.$$

From this and theorem 4.1 we obtain

$$0 = \int_{\Omega_0} \frac{\partial 1}{\partial \tau} + \operatorname{div}\left(1\Phi'(0)\right) \, \mathrm{d}x,$$

which proves the first part of the result. The second is an immediate consequence of the divergence theorem. □

Remark 4.5. Note that the condition $\Phi(0) = I$ is paramount. For example consider the family of deformations

$$\Phi(\tau)(x, y) = \Big((1+\tau)x, \frac{1}{1+\tau}y\Big) \,.$$

These are isovolumetric deformations of any circle centered at 0, and of course $\Phi(0) = 0$. We can compute

$$\operatorname{div} \Phi'(\tau) = 1 - \frac{1}{(1+\tau)^2} \,.$$

This is only zero at $\tau = 0$ (that is where $\Phi(\tau) = I$) even though the transformations are isovolumetric at any given τ.

Remark 4.6. *For generalizing to the case $g = g(x, u)$, we need to assume that the Nemitskij operator $G : W^{1,\infty}(\Omega) \times H^1(\Omega) \to L^2(\Omega)$,*

$$G(\Phi, v) = g(\Phi(x), v(x))$$

is C^m and that

$$\frac{\partial g}{\partial v}(x, v) \geq 0.$$

In this case the operator on the implicit function theorem will be

$$F(\theta, v) = -\operatorname{div}(A(\theta)v) + g((I+\theta)^{-1}, v)J_\theta = fJ_\theta$$

with derivative

$$D_v F(0, v)\varphi = -(\Delta\varphi)(x) + \frac{\partial g}{\partial v}(x, v(x))\varphi(x).$$

5. Applications

Rearrangement techniques: Schwarz and Steiner symmetrization. From Schwarz symmetrization we know (see e.g. [8], [9]) that, if g is either concave or convex and θ is volume preserving then $\eta(\theta) \leq \eta(0)$ (that is: the sphere is the least effective reactor). Therefore

$$\int_G g'(u_0)u' = \tilde{\eta}'(0) = 0.$$

For the Steiner symmetrization we know that, as we have proven in [10], for concave g, and in [11], for convex g (note that this is equivalent to concave β), the following holds:

Theorem 5.1. *Let g be a concave or convex continuous nondecreasing function such that $g(0) = 0$. Let $f \in L^2(\Omega)$ be nonnegative, i.e. $f \geq 0$, and $|B| = |\Omega''|$ with B a ball. Then*

$$\eta(\Omega' \times \Omega'') \leq \eta(\Omega' \times B). \tag{5.1}$$

So, for $G = B \times G_2 \ni (x, y)$, we have for all deformations $\theta = (\theta_1, 0)$ with θ_1 volume preserving and g convex or concave,

$$\begin{aligned}
\int_G g'(u_0)u' &= \int_{G_2} \int_B (g'(u_0)u' + \operatorname{div}(g(u_0)\theta) \\
&= \int_{G_2} \int_B (g'(u_0)u' + \operatorname{div}_x(g(u_0)\theta_1) \\
&= \int_{G_2} \Big\{ \int_B g'(u_0)u' + g(0) \int_{\partial B} \theta_1 \cdot n \Big\} \\
&= \int_{G_2} \int_B g'(u_0)u' \\
&= \int_G g'(u_0)u' \,.
\end{aligned}$$

Whenever the Nemitskij operator for g is of class $\mathcal{C}^2$ we get

$$\eta'(0)(\theta) = 0, \quad \eta''(0)(\theta, \theta) \leq 0\,.$$

Applying the bounds for $\eta'(0)$ we have as consequence an a priori estimate of the effectiveness factor in terms of the value of the functional for a circular cylinder:

Proposition 5.2. *If B is a ball such that $|B| = |\Omega'|$ then*

$$\eta(B \times \Omega'') - c(p)|g'|_\infty |u|_{W^{2,p}} |\theta|_\infty \leq \eta(\Omega' \times \Omega'') \leq \eta(B \times \Omega'').$$

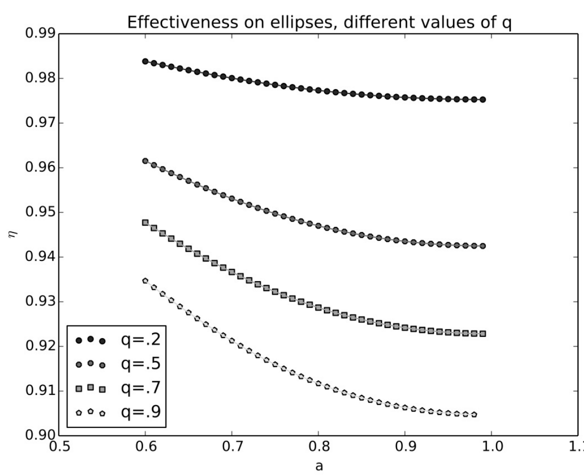
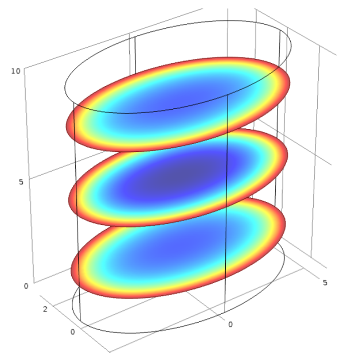
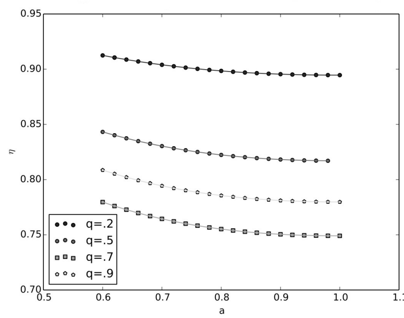


Figure 1. Effectiveness on isovolumetric ellipses with smaller semiaxes a, for the kinetic $g(u) = 1 - (1 - u)^{1/q}$.

Numerical experiments. The following numerical experiments were performed with COMSOL Multiphysics.

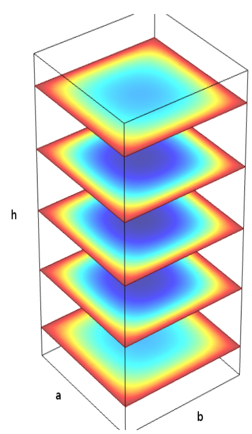


Solution in elliptic cylinder

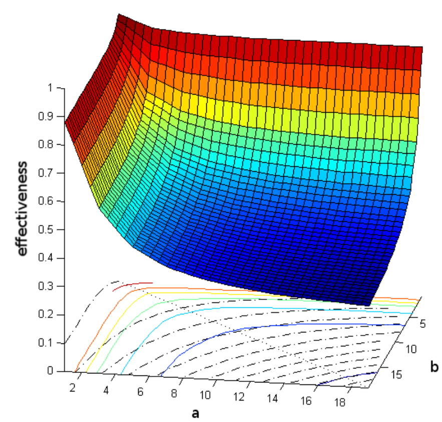


Curve of the effectiveness

FIGURE 2. Effectiveness on elliptic cylinders with smaller semiaxes a, for the kinetic $g(u) = 1 - (1-u)^{1/q}$, $0 < q < 1$ (this kinetic corresponds to $\beta(w) = w^q$, which is known in chemistry as the Freundlich isotherm).



Solution in rectangular cylinder



Surface of the effectiveness for $h = 10$ and a, b as parameters. Dotted lines represent curves of equal area

FIGURE 3. Effectiveness on rectangular cylinders $[0,a] \times [0,b] \times [0,h]$, for the kinetic $g(u) = 1 - (1-u)^2$ and $h = 10$.

Example 5.3 (Schwarz symmetrization)**.** Let $g = g_1 + g_2$ where g_1 is convex and g_2 is concave. It is well known, see [8] and [9], that a sphere is the least effective reactor for our problem in each isoperimetric family (to be more precise, isovolumetric families). We can see this in terms of derivatives through a family of ellipses

$$\Phi(x, y, \tau) = (a(\tau)x, a(-\tau)y)$$

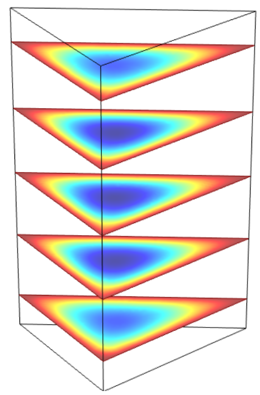


FIGURE 4. A triangular cylinder.

for a regular such that $a(0) = 1$, even when we have no volume conservation. It turns out that since this is a symmetric curve of linear transformations we have that

$$I(\tau) = I(-\tau)\,.$$

Since we have differentiability it must hold that $I'(0) = 0$. Since we have that this is a minimum and we are able to differentiate twice $I''(0) = 0$.

Example 5.4 (Steiner symmetrization)**.** The same computations hold for transformations

$$\Phi(x, y, z, \tau) = (a(\tau)x, a(-\tau)y, z)$$

This is a particular case of the results in [10] and [11]. If we consider a (uniparametric) family of elliptic cylinders of fixed height then we have the analogous result .

We can even do this analysis on two parametric families, for example in square or triangular cylinder were we consider both dimensions on the basis.

This analysis can be repeated over other families, like triangular cylinders with results of the same exact nature.

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