

On the effectiveness of wastewater cylindrical reactors: an analysis through Steiner symmetrization

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Abstract

The mathematical analysis of the shape of chemical reactors is studied in this paper through the research of the optimization of its effectiveness η such as introduced by R. Aris around 1960. Although our main motivation is the consideration of reactors specially designed for the treatment of wastewaters our results are relevant also in more general frameworks. We simplify the modelling by assuming a single chemical reaction with a monotone kinetics leading to a parabolic equation with a non necessarily differentiable function. In fact we consider here the case of a single, nonreversible catalysis reaction of chemical order q , $0 < q < 1$ (i.e. the kinetics is given by $\beta(w) = \lambda w^q$ for some $\lambda > 0$). We assume the chemical reactor of cylindrical shape $\Omega = G \times (0, H)$ with G an open regular set of \mathbb{R}^2 not necessarily symmetric. We show that among all the sections G with prescribed area the ball is the set of lowest effectiveness $\eta(t, G)$. The proof uses the notions of Steiner rearrangement. Finally, we show that if the height H is small enough then the effectiveness can be made as close to 1 as desired.

Keywords: wastewater treatment, chemical reactor tanks, effectiveness, Steiner symmetrization

1 Introduction

One of the more important problems on environment in Geosciences is the treatment of wastewater flows. Most industrial wastewater treatments are carried out in a series of cylindrical type tanks. In some of them a diffusion-reaction process takes place specially in the trickling filter phase in which wastewater flows downward through a bed of rocks, gravel, slag, peat moss, or plastic media reacting on a layer (or film) of microbial slime covering the bed media. The process (see, e.g., [RoSaRomVi12], [ViRosSaRo11], [RosViSagSaRo14] and its references) involves adsorption of organic compounds in the wastewater by the microbial slime layer, diffusion of air into the slime layer to provide the oxygen required for the biochemical oxidation of the organic compounds. In this paper we shall assume that an ideal homogenization process was applied (by passing to the limit $\varepsilon \rightarrow 0$ on the porosity of the solid bed) so that the chemical reaction can be assumed as distributed over all the reactor cylinder (see, e.g. [CoDTi03], [CoDLiTi04] and their references). Simplifying the modeling process we arrive to the consideration of a single, nonreversible catalysis reaction of q -order on a chemical reactor Ω of cylindrical shape

$$\Omega = G \times (0, H),$$

with G an open regular set of \mathbb{R}^2 (or more in general \mathbb{R}^N) not necessarily symmetric. We point out that, in spite of the above mentioned motivation, our mathematical results can be applied to a larger framework (for instance the own structure of the set Ω can be taken much more in general (see Section 3). It

is useful to separate the boundary of Ω in its lateral parts $\partial_l \Omega$ and its horizontal parts $\partial_h \Omega$, so that $\partial_l \Omega = \partial G \times (0, H)$ and $\partial_h \Omega$ consists in the union of the top and bottom boundaries: $\partial_h \Omega = (\partial_h \Omega)^H \cup (\partial_h \Omega)_0$ with $(\partial_h \Omega)^H = \Omega \times \{H\}$ and $(\partial_h \Omega)_0 = G \times \{0\}$. We shall use also the notation $\mathbf{x} = (x, y)$ with $x = (x_1, x_2) \in G$ and $y \in (0, H)$. A similar notation can be introduced if \mathbb{R}^2 is replaced by \mathbb{R}^N and $(0, H)$ by a set in \mathbb{R}^m .

In order to fix ideas we shall consider here the following parabolic model

$$\begin{cases} \frac{\partial w}{\partial t} - \Delta w + \lambda \beta(w) = 0 & \text{in } (0, +\infty) \times \Omega, \\ w = 1 & \text{on } (0, +\infty) \times \partial_l \Omega, \\ \frac{\partial w}{\partial n} = \mu(1 - w) & \text{on } (0, +\infty) \times \partial_h \Omega, \\ w(0, \mathbf{x}) = w_0(\mathbf{x}) & \text{on } \Omega, \end{cases} \quad (1)$$

where

$$\beta(w) = w^q, \quad 0 < q \leq 1$$

(q is called reaction order), $\lambda > 0$,

$$w_0 \in L^\infty(\Omega), \quad 0 \leq w_0 \leq 1, \quad (2)$$

\mathbf{n} denotes the unit normal exterior vector to $\partial_h \Omega$ and the Robin coefficient μ is taken in a generalized way as $\mu \in [0, +\infty]$. In fact we assume that the value of μ can be different for the top or the bottom surfaces, i.e.

$$\mu = \begin{cases} \mu_H & \text{on } (\partial_h \Omega)^H = G \times \{H\}, \\ \mu_0 & \text{on } (\partial_h \Omega)_0 = G \times \{0\}. \end{cases}$$

So, very often $\mu_H = 0$ (which corresponds to the case of an open tank) and/or $\mu_0 = +\infty$ (which must be understood as a Dirichlet type boundary condition $w = 1$ on $(0, +\infty) \times (\partial_h \Omega)_0$ and that corresponds to a tank alimented also from the bottom).

The limit case, the case of 0-order reactions, $q = 0$, can also be considered (see Remark 5) with the help of some special multivalued maximal monotone graph of \mathbb{R}^2 . We also mention that some larger generality can be considered also concerning the differential operator (see Remark 5).

As mentioned before, as proved in [CoDLiTi04], this is the limit as $\varepsilon \rightarrow 0$ of the following models

$$\begin{cases} -\Delta w^\varepsilon = f & \text{in } \Omega^\varepsilon, \\ \frac{\partial w^\varepsilon}{\partial \nu} + \mu(\varepsilon)\beta(w^\varepsilon) = 0 & \text{on } S^\varepsilon, \\ w^\varepsilon = 1 & \text{on } \partial \Omega, \end{cases} \quad (3)$$

where Ω^ε is a domain with fixed obstacles (which due to the chemical implications we will call pellets), where $\varepsilon > 0$ has to do with the size of each obstacle and S^ε represents the boundary of the pellets and $\partial \Omega$ the boundary of the reactor. This kind of problem is an intuitive model of fixed bed reactors. In this sense problem (1) can be seen as a homogenized problem for fixed bed reactors. This can model a large of process in Geosciences.

Due to one of those "gifts" of interdisciplinarity, problem (1) also models the heat energy stored by the Earth. The so called Sellers model considers the averaged surface atmospheric climate proposing the equation :

$$\frac{\partial w}{\partial t} - \Delta w + \beta(u) = QH(u).$$

In the above model the functions H and β are assumed Lipschitz continuous. There is a different model proposed by Budyko in which the function H is assumed to be discontinuous but we shall not pay attention here to this case (see [D96]). The techniques presented in this paper (mainly the application of the Trotter-Kato formula and its consequences) are extensible to the Sellers model, since the operator is omega-accretive (see [BeCrPa]).

We shall also consider, as by-product of our results concerning the parabolic problem, the associate stationary problem (formally obtained when making $t \rightarrow +\infty$)

$$\begin{cases} -\Delta w + \lambda\beta(w) = 0 & \text{in } \Omega, \\ w = 1 & \text{on } \partial_t\Omega, \\ \frac{\partial w}{\partial n} = \mu(1 - w) & \text{on } \partial_h\Omega. \end{cases} \quad (4)$$

The main optimality element in the study of the shape of such chemical reactors is given in terms of a notion introduced in 1957 by R. Aris (see references in [StAr73]): the so called *effectiveness* factor which is defined as:

$$\eta(t : G, H) := \frac{1}{H|G|} \int_{\Omega} \beta(w(t, \mathbf{x})) d\mathbf{x}.$$

In a pioneering work, R. Aris presented, in his book [StAr73], in collaboration with W. Strieder, the study of a linear model ($q = 1$) for a finite number of catalyst particles, which they always consider spherical. Here we will consider cylinders of arbitrary basis and reactions of order less or equal than one, which are much more frequent in practice, but which result in non linear models requiring delicate mathematical tools. We recall that when $0 < q < 1$ the solutions may give rise to a *dead core*, an interior region where no reaction is taking place. This dead core, which can be defined, for a given $t \geq 0$, as

$$N_w(t) = \{\mathbf{x} \in \Omega : w(t, \mathbf{x}) = 0\}.$$

We shall not give here estimates on the size and location of the dead core regions (see Section 4, Remark 4). Obviously, the presence of dead cores affects negatively the global effectiveness, and is to be avoided in the shape optimization process. Intuitively, it represents volume where no catalyst is present, and thus no reaction is taking place.

Although more realistic models may incorporate more complex and sophisticated aspects what the ones here presented, our main goal is to give a conceptual justification of why these reactors are wide and low. In fact, we shall prove here that among all the sections G , with prescribed area, the ball is the set of lowest effectiveness $\eta(t : G, H)$ (Theorem 2.1). Our proof uses the notions of Steiner rearrangement. In contrast to that, we shall also show that if the height of the tank H is small enough then the effectiveness can be made as close to 1 as desired (Theorem 2.2).

The organization of this paper is the following: the above main results are stated in Section 2 where some numerical experiences are commented. Section 3 is devoted to the proof of Theorem 2.1. The notion of Steiner rearrangement of a function is introduced and several properties showing the comparison in mass of the Steiner rearrangement of the solution of problem (1) and the solution of the "symmetrized problem" are given. In particular we show how the so called Trotter-Kato formula can be applied even under non-autonomous formulation. Finally, Section 4 contains the proof of Theorem 2.2 as well as a series of remarks on more general frameworks in which our main results remain valid.

2 Main results and some numerical experiences

Thanks to the maximum principle, it is clear that the solution w of (1) must satisfy that $0 \leq w(t, \mathbf{x}) \leq 1$ for a.e. $\mathbf{x} \in \Omega$ and for any $t \geq 0$. Then, in which follows, it will be useful to introduce the change of unknown $u = 1 - w$ for which the problem may be rewritten as

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u + \lambda g(u) = \lambda\beta(1) & \text{in } (0, +\infty) \times \Omega, \\ u = 0 & \text{on } (0, +\infty) \times \partial_t\Omega, \\ -\frac{\partial u}{\partial n} = \mu u & \text{on } (0, +\infty) \times \partial_h\Omega, \\ u(0, x) = u_0(x) & \text{on } \Omega, \end{cases} \quad (5)$$

where

$$g(u) = \beta(1) - \beta(1 - u). \quad (6)$$

Thus, we can assume that g is a continuous increasing function with $g(0) = 0$. We recall that the existence and uniqueness of a weak solution $u \in C([0, +\infty) : L^1(\Omega)) \cap L^\infty((0, +\infty) \times \Omega)$ is today a well-known

result. Moreover, it is also known that when $t \rightarrow +\infty$ then $u(t, \cdot) \rightarrow u_\infty(\cdot)$ in $L^2(\Omega)$ (see e.g. [DTh94] and its references).

We shall start by giving a rigorous proof of the well known principle (from an experimental point of view) that among all cylindrical reactors with prescribed volume the one with a circular section is the least effective:

Theorem 2.1. *For fixed basis volume $|G|$ effectiveness is least on a circle. That is, let $A > 0$ and let B the ball centered at the origin and let G be any other n -dimensional open regular set such that $|G| = |B| = A$. Then*

$$\eta(t : B, H) \leq \eta(t : G, H).$$

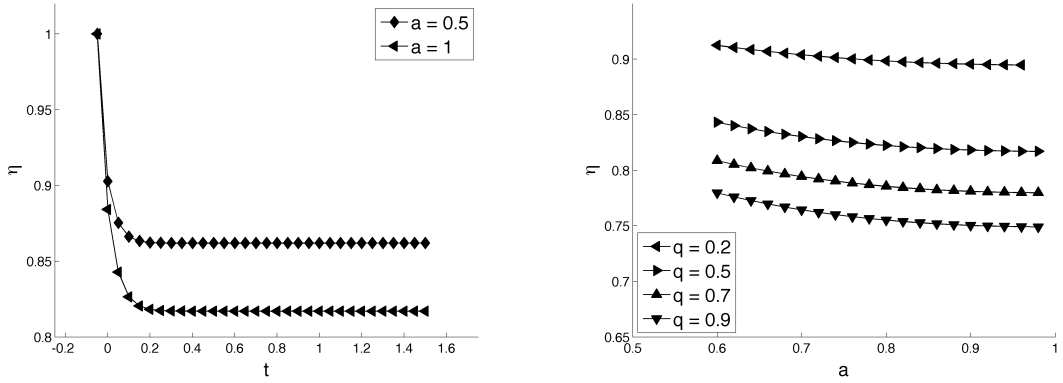
Moreover, the same inequality holds for the associated stationary problems.

Remark 1. In contrast to the case in which the effectiveness is compared with the one on a ball of \mathbb{R}^3 having the same volume than Ω , the proof of the above theorem for the stationary case seems quite complicated without proving first the analogous result for the associated parabolic problem. That was one of our motivations not to simplify our formulation to the easier case of the stationary problem.

In order to illustrate the conclusion of Theorem 2.1 we produced a numerical experience concerning a particular (one-parametric) family of elliptic cylinders $G_a \times (0, H)$. The elliptic cylinders are assumed with a prescribed volume V . So, given the lower semiaxis a , the greater semiaxis b_a is given by the identity $\pi a b_a = \frac{V}{H}$. In other words, the ellipse family is defined by the parameter a trough the expression

$$G_a = \left\{ (x_1, x_2) \in \mathbb{R}^2 : \left(\frac{x_1}{a}\right)^2 + \left(\frac{x_2}{b_a}\right)^2 = 1 \right\}, \quad b_a = \frac{V}{H\pi a}. \quad (7)$$

The image below shows a minimum of the effectiveness over this one-parametric family of elliptic cylinders $\Omega_a = E_a \times (0, 1)$, in which if we choose $V = \pi H$ and so the value $a = 1$ corresponds to the case of a circular section.



(a) Time evolution of the effectiveness for two cylinders, one circular $a = 1$ and one elliptical $a = 0.5$ both of the same volume, with initial condition $w_0 = 1$ on Ω

(b) Effectiveness for the elliptic problem for different values of G_a and q

Figure 1: Effectiveness factor for a family of ellipses with the same area.

Our second main result deals with the pure Dirichlet problem ($\mu = +\infty$) and gives a detailed statement of the well known principle (from an experimental point of view) that among all cylindrical reactors with prescribed volume low reactors are very effective. We introduce the auxiliary function $\psi \in C^2(\Omega)$ given as the unique solution of

$$\begin{cases} -\Delta\psi = 1 & \text{in } \Omega, \\ \psi = 0 & \text{on } \partial\Omega. \end{cases} \quad (8)$$

Theorem 2.2. Assume $\mu = +\infty$. Let $V = |\Omega| = |G|H = AH > 0$ be a fixed volume and let B_H be the ball of \mathbb{R}^N centered at the origin such that $|B_H| = A$. Assume also

$$1 - w_0(\mathbf{x}) \leq \lambda\psi(\mathbf{x}) \quad \text{a.e. } \mathbf{x} \in \Omega.$$

Then

$$\eta(t : G, H) \rightarrow 1 \quad \text{as } H \rightarrow 0. \quad (9)$$

More precisely, for any $t > 0$ and a.e $\mathbf{x} \in \Omega$

$$1 \geq \beta(w(t, \mathbf{x})) \geq 1 - \left(\frac{V(4 + 2(N + 1))(2N + 1)^{-\frac{N+1}{2}} H^2}{\pi^2 \omega_{N+1}} \right)^{2/(N+3)}. \quad (10)$$

The above estimate holds also for the solution of the associate stationary problem (4).

In order to illustrate quantitatively conclusion 2 we produced a numerical experience concerning the family of symmetric cylinder reactors $B_r \times (0, H)$. Motivated by the special case considered in [Ar75] (see its Figure 4.5.1) when computing curves for this phenomenon for the linear case $q = 1$, we have taken $H = \gamma^{-2} \left(\frac{16}{3}\right)^{\frac{1}{3}}$ and $r = \gamma \left(\frac{2}{3}\right)^{\frac{1}{3}}$ with γ a variable parameter. In the next figure we can see how $H \rightarrow 0$ implies $\eta \rightarrow 1$. We can also see how, in this case, $\eta \rightarrow 1$ as $q \rightarrow 0$ (this is because, for this volume, no dead core exists even in the worst case scenario).

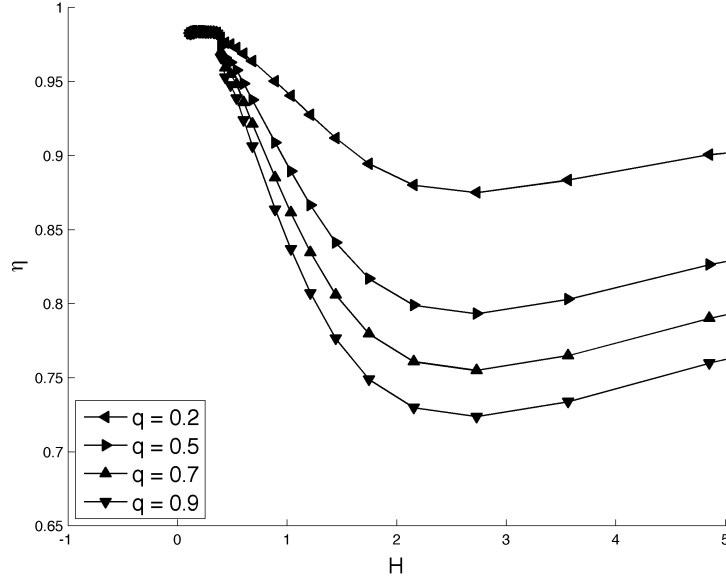


Figure 2: Effectiveness for the elliptic problem on cylinder with varying aspect ratio. Simulation.

Remark 2. The numerical experiences were produced by using a semi-implicit iterative algorithm (see [Sp95] for a proof of the convergence in an abstract framework which includes, as a special case, problem (1) under the conditions assumed in this paper). The chosen scheme applies finite differences in time and finite elements in space. The time discretization for time step h is

$$u_{n+1} - h\Delta u_{n+1} = u_n - hg(u_n).$$

The scheme is chosen implicit in time on the diffusion so that the operator in u_{n+1} is coercive, and thus the sequence is uniquely determined in $H_0^1(\Omega)$. However, the method is explicit in the nonlinearity, which makes the problem linear in u_{n+1} , thus allowing for faster simulations. The implementation of the finite element method was performed through the automated library FEniCS, which meshes simple domains in 2 and 3 dimensions, constructs the continuous Galerkin finite elements necessary and solves the linear systems.

3 The circular section is the least effective: Steiner symmetrization. Proof of Theorem 2.1

The proof of Theorem 2.1 will use some inequalities on Steiner symmetrization obtained in [AlTrDL96]. As a matter of fact, we shall improve also a previous result by the authors ([DG-C14a]) corresponding, essentially, to the case $q \geq 1$. It turns out that our result remains true under a more general setting by replacing the *vertical space* \mathbb{R} by \mathbb{R}^m . We start by recalling that given a general measurable function $h : \mathbb{R}^N \times \mathbb{R}^m \rightarrow \mathbb{R}$, with $N, m \geq 1$, for a fixed $y \in \mathbb{R}^m$ we can define the Steiner distribution function $\mu_h : \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}$ by means of

$$\mu_h(t, y) = |\{x \in \mathbb{R}^N : |h(x, y)| > t\}|.$$

The Hardy-Littlewood-Polya decreasing rearrangement $h^* : [0, +\infty) \times \mathbb{R}^m \rightarrow \mathbb{R}$ is given as

$$h^*(s, y) = \sup\{t > 0 : \mu_h(t, y) > s\} = \inf\{t > 0 : \mu_h(t, y) \leq s\}.$$

It is well known that if ω represents a generic measurable subset of $\mathbb{R}^N \times \mathbb{R}^m$ then

$$\int_0^s h^*(\sigma, y) d\sigma = \sup_{|\omega|=s} \int_{\omega} h(\mathbf{x}, y) d\mathbf{x}. \quad (11)$$

Finally, for $y \in \mathbb{R}^m$ prescribed, we define the Steiner symmetrization of h with respect to \mathbf{x} as

$$h^\#(\mathbf{x}, y) = h^*(\omega_N |\mathbf{x}|^N, y),$$

where ω_N is the measure of the N -dimensional ball. The basic idea underlying Steiner symmetrization is to consider the integral of the function over *slices*. Given $s > 0$ and $y \in \mathbb{R}^m$ we take very particular *slices* of the form

$$G(y) = \{\mathbf{x} \in \mathbb{R}^N : u(\mathbf{x}, y) > u^*(s, y)\}$$

where $|G(y)| = s$ (by construction of u^*). Variable s should formally be included in the definition but this will not lead to confusion.

Explicit calculations can be performed in simple cases. The following figure provides an example of the exact distribution function and Steiner rearrangement for the function

$$u(x, y) = \begin{cases} 0, & |(x, y)| > 1, \\ 2(1 - x^2 - y^2), & \frac{1}{2} \leq |(x, y)| \leq 1, \\ 1, & |(x, y)| < \frac{1}{2}. \end{cases}$$

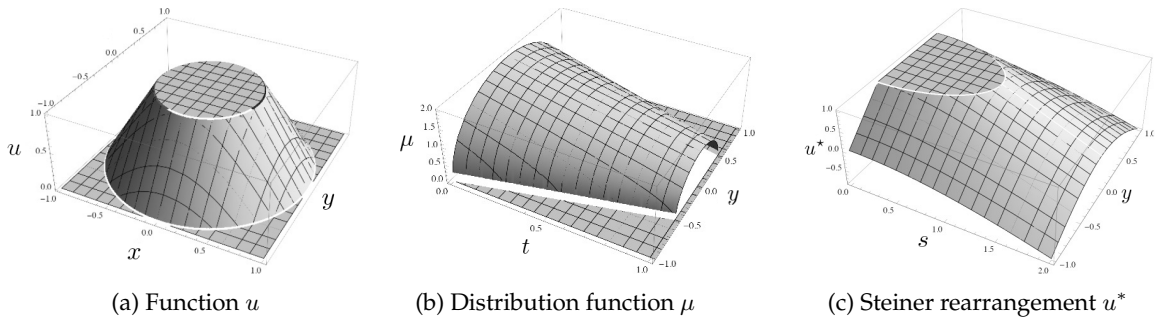


Figure 3: Computation of Steiner symmetrization

In this Section we shall use a more general framework. We introduce the following notations:

$$\Omega = \Omega' \times \Omega''$$

and $(x, y) \in \Omega' \times \Omega''$ for an arbitrary point (note that in our initial framework $\Omega' = G$ and $\Omega'' = (0, H)$). We shall denote by B a ball such that $|B| = |\Omega'|$ and then we introduce

$$\Omega^\# = B \times \Omega''.$$

Remark 3. In the case where we rearrange with respect to all variable, i.e. no y is presented (and, in an abuse of notation $m = 0$) the symmetrization is known as Schwarz symmetrization. Since it will be useful to use both symmetrizations, for Schwarz rearrangement we will use the notation \tilde{u} . We also introduce the truncation at level $y \in \Omega''$ as

$$u_y(x) = u(x, y), \quad (x, y) \in \Omega' \times \Omega''.$$

Is clear from the definition that,

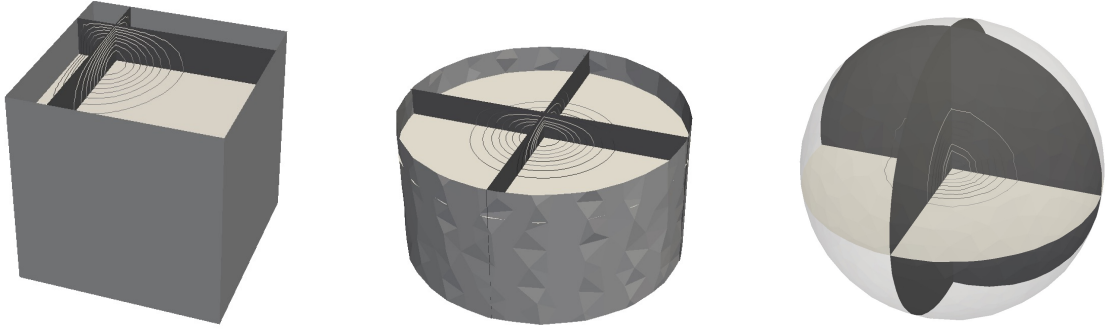
$$\widetilde{u_y}(s) = u^*(s, y).$$

For the case where time is introduced, even though the application is written $u(t, x, y)$ we will never rearrange with respect to t .

The image below (Figure 4) shows an artistic comparison between Steiner and Schwarz symmetrizations for the function

$$u(x, y, z) = e^{-10x^2 - 5y^2 - 10z^2} (1 - x)x(1 - y)y(1 - z)z, \quad (x, y, z) \in [0, 1]^3$$

This function has a single maximum point, and we show cross cuts of symmetrizations.



(a) A given measurable function on $\Omega = [0, 1]^3$, which we choose constant on the boundary. (b) Steiner symmetrization with respect to (x, y) . (c) Schwarz symmetrization.

Figure 4: Comparison of Steiner and Schwarz rearrangements of a given function.

Our main result leading to the conclusion of Theorem 2.1 is the following:

Theorem 3.1. Let β be a concave continuous nondecreasing function such that $\beta(0) = 0$. Give $T > 0$ arbitrary and let $f \in L^2(0, T : L^2(\Omega))$ with $f \geq 0$ in $(0, T)$ and let $w_0 \in L^2(\Omega)$ be such that $0 \leq w_0 \leq 1$. Let $\delta > 0$ be fixed and $w \in C([0, T] : L^2(\Omega)) \cap L^2(\delta, T : H_0^1(\Omega))$ and $z \in C([0, T] : L^2(\Omega^\#)) \cap L^2(\delta, T : H_0^1(\Omega^\#))$ be the unique solutions of

$$(P) \begin{cases} \frac{\partial w}{\partial t} - \Delta w + \lambda \beta(w) = f(t) & \text{in } \Omega \times (0, T), \\ w = 1 & \text{on } \partial\Omega \times (0, T), \\ w(0) = w_0 & \text{on } \Omega, \end{cases}$$

$$(P^\#) \begin{cases} \frac{\partial z}{\partial t} - \Delta z + \lambda \beta(z) = f^\#(t), & \text{in } \Omega^\# \times (0, T), \\ z = 1, & \text{on } \partial\Omega^\# \times (0, T), \\ z(0) = z_0, & \text{on } \Omega^\#, \end{cases}$$

where $z_0 \in L^2(\Omega^\#)$, $0 \leq z_0 \leq 1$ is such that

$$\int_s^{|\Omega'|} z_0^*(\sigma, y) d\sigma \leq \int_s^{|\Omega'|} w_0^*(\sigma, y) d\sigma, \quad \forall s \in [0, |\Omega'|] \text{ and a.e. } y \in \Omega''.$$

Then, for any $t \in [0, T]$, $s \in [0, |\Omega'|]$ and a.e. $y \in \Omega''$

$$\int_s^{|\Omega'|} z^*(t, \sigma, y) d\sigma \leq \int_s^{|\Omega'|} w^*(t, \sigma, y) d\sigma. \quad (12)$$

In terms of the comparison of the effectiveness we have the following consequence (which will be proved in Section 3) leading to the proof of Theorem 2.1:

Corollary 3.2. *In the assumptions of Theorem 3.1, for any $t \in [0, +\infty)$ we have*

$$\int_{\Omega^\#} \beta(z(t, \mathbf{x})) d\mathbf{x} \leq \int_{\Omega} \beta(w(t, \mathbf{x})) d\mathbf{x}. \quad (13)$$

The interest on the above two results is that the conclusions remains true for the associated stationary problems.

Corollary 3.3. *The mass and effectiveness comparison given by (12) and (13), respectively, remain valid for the solutions of the corresponding stationary problems.*

As mentioned before, Theorem 3.1 extends previous result by the authors ([DG-C14a]). For the proof of this result we apply, essentially, the same techniques as in the cited article, but with some refinements concerning the nature of the nonlinear term $\beta(w)$ (i.e. $g(u)$ in the equivalent formulation (5)). In contrast to our work [DG-C14a] we shall work with the increasing rearrangement. We start by recalling the following simple property : if $f : [0, |\Omega'|] \rightarrow \mathbb{R}$ is a real function such that $0 \leq f \leq L$ then $(L - f)^*(s) = L - f^*(|\Omega'| - s)$ and in particular

$$\int_0^s (L - f(t))^* dt = L - \int_{|\Omega'| - s}^{|\Omega'|} f^*(t) dt$$

(the proof can be found, for instance in [M84]).

As in [DG-C14a], we shall prove the above theorem by means of the Trotter-Kato formula. So we shall need to consider previously two auxiliary problems. The first problem corresponds to the associated linear diffusion problem:

Proposition 3.4. *Let $0 \leq w_0, z_0 \leq 1$*

$$(A) \begin{cases} \frac{\partial w}{\partial t} - \Delta w = 0, & (0, T) \times \Omega \\ w = 1, & (0, T) \times \partial\Omega \\ w = w_0, & \{0\} \times \Omega \end{cases} \quad (A^\#) \begin{cases} \frac{\partial z}{\partial t} - \Delta z = 0, & (0, T) \times \Omega^\# \\ z = 1, & (0, T) \times \partial\Omega^\# \\ z = z_0, & \{0\} \times \Omega^\# \end{cases}$$

and

$$\int_s^{|\Omega'|} z_0^*(\sigma, y) d\sigma \leq \int_s^{|\Omega'|} w_0^*(\sigma) d\sigma, \quad s \in [0, |\Omega|].$$

Then

$$\int_s^{|\Omega'|} z^*(t, \sigma, y) d\sigma \leq \int_s^{|\Omega'|} w^*(t, \sigma, y) d\sigma, \quad s \in [0, |\Omega|].$$

Proof. Let us consider $u = 1 - w$ and $v = 1 - z$. Then u and v are solutions of the problems

$$(B) \begin{cases} \frac{\partial u}{\partial t} - \Delta u = 0, & (0, T) \times \Omega \\ u = 0, & (0, T) \times \partial\Omega \\ u = u_0, & \{0\} \times \Omega \end{cases} \quad (B^\#) \begin{cases} \frac{\partial v}{\partial t} - \Delta v = 0, & (0, T) \times \Omega^\# \\ v = 0, & (0, T) \times \partial\Omega^\# \\ v = v_0, & \{0\} \times \Omega^\# \end{cases}$$

where now $u_0, v_0 \geq 0$ are given as $u_0 = 1 - w_0$ and $v_0 = 1 - z_0$. Since, for any $\tau \in [0, |\Omega'|]$, we have that

$$\int_0^\tau u_0^*(\sigma) d\sigma = L - \int_{|\Omega'| - \tau}^{|\Omega'|} w_0^*(\sigma) d\sigma \leq L - \int_{|\Omega'| - \tau}^{|\Omega'|} z_0^*(\sigma) d\sigma \leq \int_0^\tau v_0^*(\sigma) d\sigma$$

then

$$\int_0^\tau u_0^*(\sigma, y) d\sigma \leq \int_0^\tau v_0^*(\sigma, y) d\sigma.$$

Under this conditions, it is proven in [Ch04] that, for any $t \geq 0$ and for any $\tau \in [0, |\Omega'|]$, we have the comparison

$$\int_0^\tau u^*(t, \sigma, y) d\sigma \leq \int_0^\tau v^*(t, \sigma, y) d\sigma. \quad (14)$$

The key idea the proof of the result in [Ch04] is to integrate each term of the equation of problem (B) over the sets $\Omega_y(s) = \{x \in \mathbb{R}^N : (x, y) \in \Omega \text{ and } u(t, x, y) > u^*(t, s, y)\}$ for each $t > 0$ and to use the differentiation formula

$$\left(\frac{\partial^2 F}{\partial y_i \partial y_j} \right)_{i,j} \geq \int_{\Omega_y(s)} \left(\frac{\partial^2 u}{\partial y_i \partial y_j} \right)_{i,j}, \quad (15)$$

where

$$F(t, s, y) = \int_0^s u^*(t, \sigma, y) d\sigma.$$

Inequality (15) was proved for the first time in the literature in the paper [AlTrDL96] (see also an alternative proof in [FeMe98]). In [Ch04] we find the application of this formula to the parabolic problem (with the additional proof of the comparison with respect the formula obtained for the case of radially symmetric sections).

Applying (14), finally we arrive to the conclusion since

$$\int_{|\Omega'|-\tau}^{|\Omega'|} z^* = L - \int_0^\tau v^* \leq L - \int_0^\tau u^* = \int_{|\Omega'|-\tau}^{|\Omega'|} w^*.$$

which concludes the proof. \square

The second auxiliary problem corresponds to a distributed nonlinear ordinary differential equation.

Proposition 3.5. *Let β be a concave continuous nondecreasing function such that $\beta(0) = 0$. Let u, v satisfy*

$$(B) \quad \begin{cases} w_t + \lambda\beta(w) = 0, & \Omega \times (0, T), \\ w = w_0, & \Omega \times \{0\}, \end{cases} \quad (B^\#) \quad \begin{cases} z_t + \lambda\beta(z) = 0, & \Omega^\# \times (0, T), \\ z = z_0, & \Omega^\# \times \{0\}. \end{cases}$$

Assume

$$\int_s^{|\Omega'|} z_0^*(\sigma, y) d\sigma \leq \int_s^{|\Omega'|} w_0^*(\sigma, y) d\sigma, \quad \forall s \in [0, |\Omega'|], \text{ a.e. } y \in \Omega''.$$

Then we have

$$\int_s^{|\Omega'|} z^*(t, \sigma, y) d\sigma \leq \int_s^{|\Omega'|} w^*(t, \sigma, y) d\sigma \quad \forall t > 0, s \in [0, |\Omega'|], \text{ a.e. } y \in \Omega''.$$

Proof. For any $\varepsilon > 0$ and $y \in \Omega''$ prescribed, let $w_{\varepsilon, y}(t, x)$, $z_{\varepsilon, y}(t, x)$ be the solutions of the (ε, y) -parametric family of semilinear parabolic problems

$$(P(\varepsilon, y)) \quad \begin{cases} \frac{\partial w}{\partial t} - \varepsilon \Delta_x w + \lambda\beta(w) = f_y(t) & \text{in } \Omega \times (0, T), \\ w = 1 & \text{on } \partial\Omega' \times (0, T), \\ w(0) = (w_0)_y & \text{on } G, \end{cases}$$

$$(P^\#(\varepsilon, y)) \quad \begin{cases} \frac{\partial z}{\partial t} - \varepsilon \Delta z + \lambda\beta(z) = f_y^\#(t) & \text{in } B \times (0, T), \\ z = 1 & \text{on } \partial B \times (0, T), \\ z(0) = (z_0)_y & \text{on } B. \end{cases}$$

Notice that the diffusion operator is only dependent of the x -variables. Then, by Theorem 1 of [D91] we know that, for any $\varepsilon > 0$ and $y \in \Omega''$ prescribed,

$$\int_s^{|\Omega'|} \widetilde{z_{\varepsilon, y}}(t, \sigma) d\sigma \leq \int_s^{|\Omega'|} \widetilde{w_{\varepsilon, y}}(t, \sigma) d\sigma \quad \forall t > 0, s \in [0, |\Omega'|]. \quad (16)$$

Moreover, we can know apply Theorem 3.16 on [Br73]

$$\begin{aligned} z_{\varepsilon,y} &\rightarrow z_y & \text{as } \varepsilon \rightarrow 0 & \text{ in } C([0,T] : L^2(B)), \\ w_{\varepsilon,y} &\rightarrow w_y & \text{as } \varepsilon \rightarrow 0 & \text{ in } C([0,T] : L^2(G)). \end{aligned}$$

Then, passing to the limit in (16) we get

$$\int_s^{|\Omega'|} \widetilde{z}_y(t, \sigma) d\sigma \leq \int_s^{|\Omega'|} \widetilde{w}_y(t, \sigma) d\sigma \quad \forall t > 0, s \in [0, |\Omega'|].$$

Finally, it is enough to observe that since $y \in \Omega''$ is prescribed then the Schwarz rearrangement $\widetilde{w}_y(t, \sigma)$ coincides with the Steiner rearrangement $w^*(t, \sigma, y)$ (see Remark 3) and the result holds. \square

3.1 Proof of Theorem 3.1.

Proof of Theorem 3.1. The special case $f = 0$ is easier. Since we know

$$\int_{\tau}^{|\Omega'|} z_0^*(\sigma, y) d\sigma \leq \int_{\tau}^{|\Omega'|} w_0^*(\sigma, y) d\sigma, \quad \forall s, \forall y$$

applying Proposition 3.4 and 3.5 inductively we get

$$\begin{aligned} &\int_{\tau}^{|\Omega'|} \left[\left(S_A \left(\frac{t}{n} \right) S_B \left(\frac{t}{n} \right) \right)^n z_0 \right]^* (\sigma, y) d\sigma \\ &\leq \int_{\tau}^{|\Omega'|} \left[\left(S_{A^\#} \left(\frac{t}{n} \right) S_{B^\#} \left(\frac{t}{n} \right) \right)^n w_0 \right]^* (\sigma, y) d\sigma \end{aligned}$$

where S_A is the semigroup associated to problem (A) and analogously for $S_B, S_P, S_{A^\#}, S_{B^\#}$ and $S_{P^\#}$. Taking limits, applying the Trotter-Kato formula (see Proposition 4.3 [Br73]) and applying convergence under the integral sign we get

$$\int_0^s [S_P(t)z_0]^*(\sigma, y) d\sigma \leq \int_0^s [S_{P^\#}(t)w_0]^*(\sigma, y) d\sigma$$

for any $t \in [0, T]$, for any $s \in [0, |\Omega'|]$ and a.e. $y \in \Omega''$.

For the case $f \neq 0$ and time dependent the Trotter-Kato formula can be also applied (see, e.g. [VWZ08]). In fact, to deal with the affine case $f(t) \neq 0$ we shall use a "reduction of order technique" argument which can be found on [BeCrPa]. We point out that by an approximation argument and then passing to the limit process we can assume, without loss of generality, that in fact $f \in H^1(0, T; L^2(\Omega))$. We shall argue by using the formulation of the problem with homogeneous Dirichlet condition, that is $u = 1 - w$ as unknown, for the case of the general set Ω and with $v = 1 - z$ as unknown for the ball $\Omega^\#$. We also introduce the following notations:

$$\hat{f}(t) = \lambda\beta(1) - f(t).$$

and given any function $\theta \in H^1(0, T; L^2(\Omega))$, for a.e. $t \in (0, T)$ we define the function $\theta(t + \cdot) \in H^1(0, T; L^2(\Omega))$ by the application $s \mapsto \theta(t + s)$. We also introduce the vectorial function $U(t) = (u(t), f(t + \cdot)) \in L^2(\Omega) \times H^1(0, T; L^2(\Omega))$. We proceed in a similar way for the case of the domain $\Omega^\#$: we define $V(t) = (v(t), f^\#(t + \cdot)) \in L^2(\Omega^\#) \times H^1(0, T; L^2(\Omega^\#))$. Then, it is easy to see that U, V are the respective unique solutions of the "autonomous vectorial problems"

$$\begin{cases} \frac{\partial U}{\partial t} + \hat{L}U = 0, & t \in (0, T) \\ U(0) = (u_0, \hat{f}) \end{cases} \quad \begin{cases} \frac{\partial V}{\partial t} + \hat{L}V = 0, & t \in (0, T) \\ V(0) = (v_0, \hat{f}^\#) \end{cases}$$

where

$$\hat{L}(u, \xi) = (-\Delta u + g(u) - \xi(0 + \cdot), \xi').$$

Here ξ' represents simply the derivative of ξ . We can use a decomposition $\hat{L} = \hat{L}_1 + \hat{L}_2$ in the following way:

$$\hat{L}_1(u, \xi) = (-\Delta u + h(t)g(u), 0), \quad \hat{L}_2(u, \xi) = (-\xi(0 + \cdot), \xi').$$

Let us define the problems

$$\begin{aligned} (C) \left\{ \begin{array}{l} \frac{\partial U}{\partial t} + \hat{L}_1 U = 0, \\ U(0) = (u_0, \hat{f}), \end{array} \right. , \quad (C^\#) \left\{ \begin{array}{l} \frac{\partial V}{\partial t} + \hat{L}_1 V = 0, \\ V(0) = (v_0, \hat{f}^\#), \end{array} \right. \\ (D) \left\{ \begin{array}{l} \frac{\partial U}{\partial t} + \hat{L}_2 U = 0, \\ U(0) = (u_0, \hat{f}), \end{array} \right. , \quad (D^\#) \left\{ \begin{array}{l} \frac{\partial V}{\partial t} + \hat{L}_2 V = 0, \\ V(0) = (v_0, \hat{f}^\#), \end{array} \right. \end{aligned}$$

and the correspondent solution operators

$$\begin{aligned} S_C(t)(u_0, \hat{f}) &= (S_P(t)u_0, \hat{f}), \quad S_{C^\#}(t)(v_0, \hat{f}^\#) = (S_P(t)v_0, \hat{f}^\#), \\ S_D(t)(u_0, \hat{f}) &= \left(u_0 + \int_0^t \hat{f}(s) ds, \hat{f} \right), \quad S_{D^\#}(t)(v_0, \hat{f}^\#) = \left(v_0 + \int_0^t \hat{f}^\#(s) ds, \hat{f}^\# \right). \end{aligned}$$

Let Q be the projection operator such that $u(t) = QU(t)$. Let us study QS_C and QS_D . Since, for any $t \in [0, T]$, for any $s \in [0, |\Omega'|]$ and a.e. $y \in \Omega''$,

$$\int_0^s u_0^*(\sigma, y) d\sigma \leq \int_0^s v_0^*(\sigma, y) d\sigma,$$

we have, by the above explicit formulas (for the first component we apply the similar proof as in the case $f = 0$)

$$\begin{aligned} \int_0^s [Q S_C(t)(u_0, f)]^*(\sigma, y) d\sigma &\leq \int_0^s [Q S_{C^\#}(t)(v_0, f^\#)]^*(\sigma, y) d\sigma, \\ \int_0^s [Q S_D(t)(u_0, f)]^*(\sigma, y) d\sigma &\leq \int_0^s [Q S_{D^\#}(t)(v_0, f^\#)]^*(\sigma, y) d\sigma. \end{aligned}$$

By applying an induction argument again we get

$$\begin{aligned} \int_0^s \left[Q \left(S_C \left(\frac{t}{n} \right) S_D \left(\frac{t}{n} \right) \right)^n (u_0, f) \right]^*(\sigma, y) d\sigma \\ \leq \int_0^s \left[Q \left(S_{C^\#} \left(\frac{t}{n} \right) S_{D^\#} \left(\frac{t}{n} \right) \right)^n (v_0, f^\#) \right]^*(\sigma, y) d\sigma. \end{aligned}$$

Finally, since all the operators are maximal monotone operators on their respective Hilbert spaces, we can take limits by applying the Trotter-Kato formula (which justify the convergence of the limits) and the result holds. \square

3.2 Proof of Corollary 3.2: end of the proof of Theorem 2.1.

For the proof we shall need a classical result.

Lemma 3.6 ([HLitP29]). *Let $\tilde{y}, \tilde{z} \in L^1(0, M)$, $\tilde{y}, \tilde{z} \geq 0$ a.e.. Suppose y is non-increasing and*

$$\int_0^s \tilde{y}(\sigma) d\sigma \leq \int_0^s \tilde{z}(\sigma) d\sigma, \quad \forall s \in [0, M].$$

Then, for every continuous non-decreasing convex function Φ we have

$$\int_0^s \Phi(\tilde{y}(\sigma)) d\sigma \leq \int_0^s \Phi(\tilde{z}(\sigma)) d\sigma \quad \forall s \in [0, M].$$

Proof of Corollary 3.2. Applying the theorem and lemma 3.6 to

$$\Phi(s) = \beta(1) - \beta(1-s), \quad \tilde{y}(\sigma) = 1 - z^*(|\Omega'| - \sigma, y), \quad \tilde{z}(\sigma) = 1 - w^*(|\Omega'| - \sigma, y)$$

we get that

$$\int_s^{|\Omega'|} \beta(z^*(t, \sigma, y)) d\sigma \leq \int_s^{|\Omega'|} \beta(w^*(t, \sigma, y)) d\sigma.$$

It is a classical result (see [M84]) that for F Borel and u measurable it holds that

$$\int_{\Omega'} F(u) = \int_0^{|\Omega'|} F(u^*)$$

In particular the comparison holds between w and z . All that remains is to integrate on Ω'' , apply Fubini's theorem and the result follows. \square

3.3 The elliptic case

Proof of Corollary 3.3. Since there is uniqueness of solutions for the stationary problem (4) then, by applying Corollary 3 of [DTh94] we get that $w(t) \rightarrow w$ in $H^1(\Omega)$, as $t \rightarrow +\infty$ (with w the unique solution of problem (4) with $\mu = +\infty$, i.e. the Dirichlet problem $w = 1$ on $\partial\Omega$). Moreover, since the application $u \mapsto u^*$ is continuous with respect to the convergence in L^1 (see e.g. [M84]) we get that the mass comparison is stable by passing to the limit as $t \rightarrow +\infty$ and the result holds. \square

4 Proof of Theorem 2.2 and further remarks.

We shall use the function $\bar{u} = \lambda\psi$ is a supersolution (we recall that ψ is given by (8)). We shall apply the following previous result in the literature due to C. Bandle [Ba85]:

Theorem 4.1. *Let $\Omega \subset \mathbb{R}^n$ be an open bounded set of measure $V = |\Omega|$ such that Ω is contained between two parallel $(n-1)$ -dimensional hyperplanes at distance 2ρ and let ψ be the solution of problem (8). Then*

$$\|\psi\|_{\infty}^{1+\frac{n}{2}} \leq CV\rho^2$$

with

$$C = \frac{(4+2n)(2n)^{-\frac{n}{2}}}{\pi^2\omega_n}. \quad (17)$$

Proof of Theorem 2.2. Thanks to the assumption on the initial datum, since we are dealing with the Dirichlet problem ($\mu = +\infty$ in (5)) and $0 \leq u = 1 - w \leq 1$, $0 \leq g(u) \leq 1$, we get that $\bar{u} = \lambda\psi$ is a supersolution of problem (5). Then, applying Theorem 4.1 to $\Omega = G \times (0, H)$, i.e. with $n = N+1$ and $2\rho = H$, we get that

$$\|u\|_{L^\infty(0,T;L^\infty(\Omega))} \rightarrow 0, \text{ as } H \rightarrow 0,$$

and, in particular

$$\operatorname{ess\,inf}_{(0,T) \times \Omega} \beta(w) \rightarrow 1, \text{ as } H \rightarrow 0.$$

More precisely, for any $t \geq 0$ and a.e $\mathbf{x} \in \Omega$

$$1 \geq \beta(w(\mathbf{x}, t)) \geq 1 - \left(\frac{V(2N+6)(2N+1)^{-\frac{N+1}{2}}}{\pi^2\omega_{N+1}} H^2 \right)^{2/(N+3)}, \quad (18)$$

which proves the assertion for the case of the parabolic problem (even if $V = |\Omega| = |G|H$ is prescribed). In the case of the associate stationary problem, since we know that $w(t) \rightarrow w$ in $H^1(\Omega)$, as $t \rightarrow +\infty$ (see the proof of Corollary 3.3) then, by the dominated Lebesgue theorem we know that $\beta(w(t)) \rightarrow \beta(w)$ in $L^\infty(\Omega)$, as $t \rightarrow +\infty$ and thus the estimate (18) remains valid replacing $\beta(w(t))$ by $\beta(w)$ (since the bounds are independent of t). \square

Remark 4. We shall not enter in this paper in the study of the free boundary (the boundary of the dead core) associated to the solutions $w(t)$ and w of the parabolic and elliptic problems (1) and (4) respectively. We recall that the key assumption for the formation of such free boundary is the condition $0 < q < 1$. We send the reader to the monographs [D85] and [AnDSh01] for an extensive treatment with numerous references.

Remark 5. All the results of this paper can be generalized to more general frameworks according different point of views. For instance, with respect to the diffusion operator it is possible to replace the Laplacian operator $-\Delta w$ by a general second order elliptic operator of the type

$$\begin{aligned} Lu = & - \sum_{i,j=1}^N \frac{\partial}{\partial x_j} \left(a_{ij}(x, y) \frac{\partial u}{\partial x_j} \right) - \sum_{h,k=1}^m \frac{\partial}{\partial y_k} \left(b_{hk}(y) \frac{\partial u}{\partial y_h} \right) \\ & - \sum_{i=1}^N \sum_{h=1}^m \frac{\partial}{\partial y_h} \left(c_{ih}(y) \frac{\partial u}{\partial x_i} \right) - \sum_{i=1}^N \sum_{h=1}^m \frac{\partial}{\partial x_i} \left(d_{hi}(y) \frac{\partial u}{\partial y_h} \right) \end{aligned} \quad (19)$$

with bounded coefficients (here we followed the notation of Section 3). In that case, the comparison via Steiner symmetrization is made with respect the solution (on a cylinder of symmetric section) associated to the operator

$$L^\# v = -\Delta_x v - \sum_{h,k=1}^m \frac{\partial}{\partial y_k} \left(b_{hk}(y) \frac{\partial v}{\partial y_h} \right).$$

No special change in the statements arises if the operator Lu involves transport first order terms of the type

$$\sum_{k=1}^m b_k(y) \frac{\partial u}{\partial y_k}.$$

Quasilinear terms with respect to the x -variable (that is, those in which Steiner symmetrization is performed) can be allowed, too. The presence of transport terms in the x -variable can also be considered, but then the expression of the rearranged operator $L^\# v$ must be modified (see, e.g., [ChMo01] and its references). On the other hand, it is still an open problem how to deal with quasilinear terms in the y -variables. We point out that Theorem 4.1 (which play a fundamental role in the proof of Theorem 2.2) was obtained in [Ba85] for the case of a general second order elliptic operator of the type (19). Concerning the reaction term $\beta(w) = w^q$, the results of this paper can be extended also to the case $q = 0$ by means of the consideration of the maximal monotone graph of \mathbb{R}^2 given by

$$\beta(w) = 0 \text{ if } w < 0, \beta(w) = 1 \text{ if } w > 0 \text{ and } \beta(0) = [0, 1]. \quad (20)$$

(see, e.g., [D85], Chapter 2). As a matter of fact, the proof of Proposition 3.5 (and thus Theorem 3.1) remains valid under the same assumptions on β that Theorem 1 on [D91], i.e. β nondecreasing function with $\beta(0) = 0$ and such that

$$\beta = \beta_1 + \beta_2 \quad (21)$$

where β_1 is concave and β_2 is convex. The results can be extended also to the "enthalpy formulation" of some porous media type equations (associated to a linear operator Lu) in the spirit of the framework presented in [D91], [D92] and [D01]. It is also possible to extend the results to the more realistic case of suitable coupled systems of the type

$$\begin{cases} \frac{\partial w}{\partial t} - d_w \Delta w + R_1(w, u) = 0 & \text{in } (0, +\infty) \times \Omega, \\ \frac{\partial u}{\partial t} - d_u \Delta u + R_2(w, u) = 0 & \text{in } (0, +\infty) \times \Omega, \end{cases}$$

under suitable structural assumptions on the coupling reaction terms $R_1(w, u)$ and $R_2(w, u)$ (see Theorem 3 of [D91] for $d_w, d_u > 0$ and [DSt94] for $d_w > 0$ and $d_u = 0$). Some results on the Steiner rearrangement for the case of Neumann boundary conditions can be found in [FeMe05] and [Ch04].

Remark 6. It can be shown (see [BaVe03]) that, in spite of Theorem 2.2, domains Ω of optimal effectiveness do not exist for reactions $\beta(w) = w^q$ with $0 < q < 1$. Nevertheless, for the limit case of zero order reactions (with $\beta(w)$ given by (20)) any result proving that there is no dead core for a concrete Ω shows that the effectiveness attains its maximum value for this domain Ω (several criteria for the nonformation of the dead core were given in Chapter 2 of [D85]).

Remark 7. The study of the optimality of the effectiveness factor in terms of shape differentiation on Ω is the main object of the paper [DG-C14b].

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