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J. M. Bello Rivas, B. Ivorra, A. M. Ramos,
J. Harmand and A. Rapaport

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http://www.mat.ucm.es/deptos/ma
e-mail:matemática_aplicada@mat.ucm.es

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Juan M. Bello Rivas[1], Benjamin Ivorra[1], Angel M. Ramos[1], Jérôme Harmand[2], Alain Rapaport[2]

Universidad Complutense de Madrid,
Departamento de Matemática Aplicada
Facultad de Ciencias Matemáticas, 28040 Madrid, Spain
[2] LBE-INRA, Narbonne, France
[3] UMR MISTEA and INRA-INRIA MODEMIC
Montpellier, France

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Abstract

In this paper, we focus on the modeling, simulation and shape optimization of a dispersive bio-reactor in which a substrate is degraded by a microbial ecosystem in an non homogeneous environment. Two different modeling approaches are used in order to obtain a low computational model to quickly evaluate the behavior of our bio-reactor. The first one is based on coupled spatial and time dependent EDPs. The second one, obtained by optimization, is based on two interconnected systems of ODEs with coefficient calibrated using the first PDE model. Preliminary results assuming a Monod kinetics are presented.

Keywords: Dispersive bioreactors, Shape optimization, Optimal design, Global optimization, Genetic algorithms.

1 Introduction

The optimal design —the characterization of the main design parameters of a system under performance/economical/footprint constraints— of biosystems has attracted a lot of attention these last years. Indeed, the diversity of unitary systems and the large spectrum of optimization criteria has led to the search for the "best solution" with respect to a given optimization problem, in particular in the field of catalytic chemical

reactions. The problem under consideration in most studies can be stated as follows: given

1. the model of the process,
2. the input and required output reactant concentrations (that is to say, the conversion rate is specified), and
3. the flow rate to be processed, what are the volumes of N tanks in series such that the total volume of the whole process be minimal?

A rigorous solution to this problem for catalytic biosystems (i.e., a biological reaction in which the activity of the biocatalyst is assumed to be constant) exhibiting Michaelis-Menten kinetics was proposed by [LUY 82], while the solution for a fairly large class of autocatalytic systems (including, in particular, the well-known Monod and Haldane kinetics) was proposed by [HIL 89]. Recently, these results were revisited and extended by [HAR 03], [HAR 05] and [NEL 06].

However, these studies suffer of two important drawbacks:

- While the proposed results are valid for small and medium sized systems, the diffusion phenomena that occur in larger tanks were not studied;
- The dimensioning parameters were not considered —only the total volume of the systems were optimized. However, with respect to a real case, design parameters such as the diameter or the height of any biological or chemical system will influence its performance.

In the present paper we propose to couple hydrodynamics with biological phenomena occurring in a diffusive bio-reactor which the main design parameters (reactor shape and total volume) are optimized with respect to the output concentration. To do so, we present a particular spatial modeling based on coupled PDEs. We also define a second model, computationally cheaper, based on two systems of ODEs with coefficient calibrated using the outputs given by the PDE model. The objective of this second model is to quickly provide the behavior of the considered bioreactor.

The paper is organized as follows. First, the PDE and ODE models of the system and the way they are compared are presented. Then, the optimization problem and the optimization method used to sole it are give. Finally, some preliminary results are given.

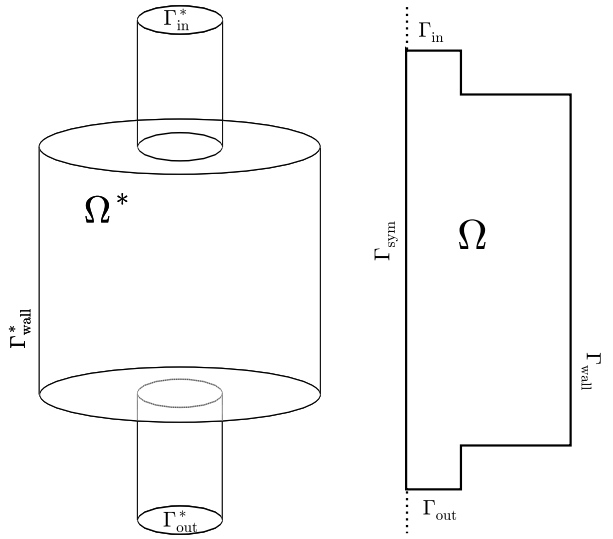
2 Mathematical model

In this Section we present the two models used to describe the behavior of the considered bio-reactors.

2.1 Device description

The bioreactor under consideration is depicted in Figure 1(a). It contains a certain amount of biomass that resides in Ω^* and reacts with a diluted substrate entering through an inlet Γ^*_{in} that is located at the top. At the bottom there is an outlet Γ^*_{out} allowing the uncontaminated liquid to leave the container.

The device's geometry is that of a solid of revolution and, consequently, it can be characterized by a 2D model. The symmetry axis Γ_{sym} is shown as a dotted line in Figure 1(b), the container region is denoted by Ω, the wall is Γ_{wall}, and the inlet and outlet are (respectively) Γ_{in} and Γ_{out}. Note that $\partial\Omega = \Gamma_{\text{in}} \cup \Gamma_{\text{wall}} \cup \Gamma_{\text{out}} \cup \Gamma_{\text{sym}}$.



(a) 3D representation of the bioreactor

(b) 2D symmetric representation of the bioreactor

In the numerical experiments that we performed the length of Γ_{wall} was set to 5 m. and the radius of the inlet and outlet were fixed at $\Gamma_{\text{in}} = \Gamma_{\text{out}} = 0.5\text{m}$.

2.2 PDEs based modeling

Background material on a similar device can be found in [GRI 01].

The fluid is modelled using the Incompressible Navier-Stokes equations

$$\begin{cases} \rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + \eta\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}\right)\right] + \mathbf{F}, & \text{in } \Omega \\ \nabla\cdot\mathbf{u} = \mathbf{0} & \text{in } \Omega \end{cases}, \quad (1)$$

where $\mathbf{u} = (u, v)$ is the velocity field [m/s], p is the pressure [Pa], ρ is the density [kg/m^3], η is the dynamic viscosity [Pa $\cdot$ s], and $\mathbf{F} = (0, -g_0 \cdot \eta)$ is the volume force [N/m^3], with $g_0 \simeq 9.8$ [m/s^2] being the standard gravity constant.

The boundary conditions are:
$\mathbf{u}\cdot\mathbf{n} = 0$, in Γ_{sym}, $\mathbf{t}\cdot\left[-p\mathbf{I} + \eta\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}\right)\right]\mathbf{n} = 0$, in Γ_{sym}, $\mathbf{u} = \mathbf{u}_0$, in Γ_{in}, $\eta\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}\right)\mathbf{n} = 0$, in Γ_{out}, $p = 0$, in Γ_{out}, $\mathbf{u} = \mathbf{0}$, in Γ_{wall}, where $\mathbf{u}_0 = (0, v_0)$ gives a parabolic velocity condition $v_0 = Q(x - \frac{1}{2})(x + \frac{1}{2})$ at the inlet with $Q = 0.2$ m/s.

The process of convection and diffusion of the substrate inside Ω is modelled by:

$$\frac{\partial s}{\partial t} + \nabla \cdot (-D_1 \nabla s) = -\mu(s)\, x - \mathbf{u} \cdot \nabla s, \text{ in } \Omega, \tag{2}$$

where s stands for the concentration of the substrate [mol/m^3], and $D_1 = 2 \cdot 10^{-8}$ [m^2/s] is the diffusion coefficient. The reaction rate μ is a Monod (Michaelis-Menten) kinetic function of the form $\mu(c) = \mu_{\max} \frac{c}{1+c}$, with $\mu_{\max} = 0.05$ [s^{-1}].

The boundary conditions are given by $-\mathbf{n} \cdot \mathbf{N} = N_0$, in Γ_{in} $\mathbf{n} \cdot \mathbf{N} = 0$, in $\Gamma_{\text{sym}} \cup \Gamma_{\text{wall}}$, $\mathbf{n} \cdot (-D_1 \nabla s) = 0$, in Γ_{out}, where $\mathbf{N} = -D_1 \nabla s + s\,\mathbf{u}$, and the inward flux is given by $N_0 = S_{\text{in}}\, v$ [mol/(m^2 $\cdot$ s)] taking $S_{\text{in}} = 1$ in this case. The tank starts with a homogeneous value of x set to 0.5 [mol/m^3].

For the biomass, the convection and diffusion are governed by equations similar to (2) (changing the sign of $\mu(s)x$) with a diffusion coefficient $D_2 = 3 \cdot 10^{-8}$ [m^2/s], $N_0 = 0$ [mol/(m^2 $\cdot$ s)] and an uniform initial bioreactor concentration of 0.5[mol/(m^2 s)].

This system of PDEs is solved by using a Finite Element Method approach described in [IVO 06-b].

2.3 ODE based modeling and comparison with PDE based model

We have performed a comparison between the PDE model and other model based on ODEs systems which model two bio-reactors, obtained by dividing the main bio-reactor in two interconnected sub-volumes: one volume is $\alpha \cdot V$, which receive and reject the contaminated flow, and the other one $(1-\alpha) \cdot V$, which is connected with the previous tank.

This model is defined by the following dynamical system

$$\begin{cases} \dot{x}_1 = \mu(s_1)\, x_1 - \dfrac{\bar{Q}}{\alpha V} x_1 + \dfrac{d}{\alpha V}(x_2 - x_1), \\ \dot{s}_1 = -\mu(s_1)\, x_1 + \dfrac{\bar{Q}}{\alpha V}(S_{\text{in}} - s_1) + \dfrac{d}{\alpha V}(s_2 - s_1), \\ \dot{x}_2 = \mu(s_2)\, x_2 + \dfrac{d}{(1-\alpha)V}(x_1 - x_2), \\ \dot{s}_2 = -\mu(s_2)\, x_2 + \dfrac{d}{(1-\alpha)V}(s_1 - s_2), \\ \quad x_1(0) = x_2(0) = S_{\text{in}}, \\ \quad s_1(0) = s_2(0) = 0, \end{cases} \tag{3}$$

where x_1 and x_2 correspond to the evolution of the biomass and s_1 and s_2 correspond to the evolution of the substrate in the two sub-volumes, $\alpha \in (0,1)$, $d > 0$, and $\bar{Q} = 4/3\pi r^3 Q$ with $r = 0.5$ being the radius of the inlet and Q having the same value as in Section 2.2.

If we denote by $S_{\text{out}}^{\text{ODE}}$ the value of s_1 when [3] reaches its steady state then we can construct a mapping

$$S_{\text{in}} \mapsto S_{\text{out}}^{\text{ODE}}(S_{\text{in}}; \alpha, d).$$

The equivalent of the previous mapping for **PDE** can be defined as a correspondence between S_{in} and the concentration of substrate at the outlet after enough time has passed:

$$S_{\text{in}} \mapsto S_{\text{out}}^{\text{PDE}}(S_{\text{in}}) = \frac{\int_{\Gamma_{\text{out}}} c \, \mathrm{d}\Gamma}{\int_{\Gamma_{\text{out}}} \mathrm{d}\Gamma} \tag{4}$$

These two functions $S_{\text{out}}^{\text{ODE}}$ and $S_{\text{out}}^{\text{PDE}}$ provide us with the basis for comparison of the two models. We performed the following two numerical experiments for the cylindrical shape described in Section 2.4 for S_{in} ranging from 0.25 to 10 mol/m^3:

ODE1 For each value of S_{in} we computed the values of α and d that minimized $(S_{\text{out}}^{\text{ODE}}(S_{\text{in}}; \alpha, d) - S_{\text{out}}^{\text{PDE}}(S_{\text{in}}))^2$. The resulting values are shown in Figure 3.2.

ODE2 For the set $\{S_{\text{in}}^i \,|\, i = 1, \ldots, 5\}$, we computed the pair α, d that minimized $\sum_{i=1}^{5} (S_{\text{out}}^{\text{ODE}}(S_{\text{in}}^i; \alpha, d) - S_{\text{out}}^{\text{PDE}}(S_{\text{in}}^i))^2$. The resulting values are $\alpha = 0.304$, $d = 0.072$

2.4 Optimization problem

Once we know how the model behaves, we would like to find a shape that results in the most efficient bioreactor. This problem amounts to finding

$$\arg\min_{s \in \Theta} J(s), \tag{5}$$

where Θ is the set of all admissible shapes, and J is our fitness function to be defined in the next section. The set of admissible shapes is characterized by the tanks that can be obtained by varying the degrees of freedom labeled with a, b_1, b_2, and c in Figure 1. The contour of Γ_{wall} results from interpolation using a shape-preserving piecewise cubic hermite polynomial.

Each tank is simulated for approximately half an hour ($t_{\max} = 2000$s.) and at the end of this period, we compute the flux of the substrate through the outlet using the formula

$$Z = -\int_{\Gamma_{out}} s \, v \, \mathrm{d}\Gamma.$$

We denote by Z^{cyl} the result of evaluating Z for the cylindrical bioreactor whose shape is characterized by the parameters $a = c = 1.5$, $b_1 = 2.5$, $b_2 = 2$ (its volume is approximately 66 m^3).

The fitness of a given shape is determined according to the expression

$$J = P \max\left\{0, Z - Z^{\text{cyl}}\right\} + \text{Volume}, \tag{6}$$

where P is a penalty taken as 10^9 and Z is the result of evaluating (2) for the current shape. With this choice of fitness function, the optimization process favors shapes that yield a value of Z smaller than that of the purely cylindrical bioreactor and, among those, it chooses the ones that minimize the tank's volume.

The optimization problems presented in Section 2.4 have been solved using an hybrid genetic algorithm described in the next section.

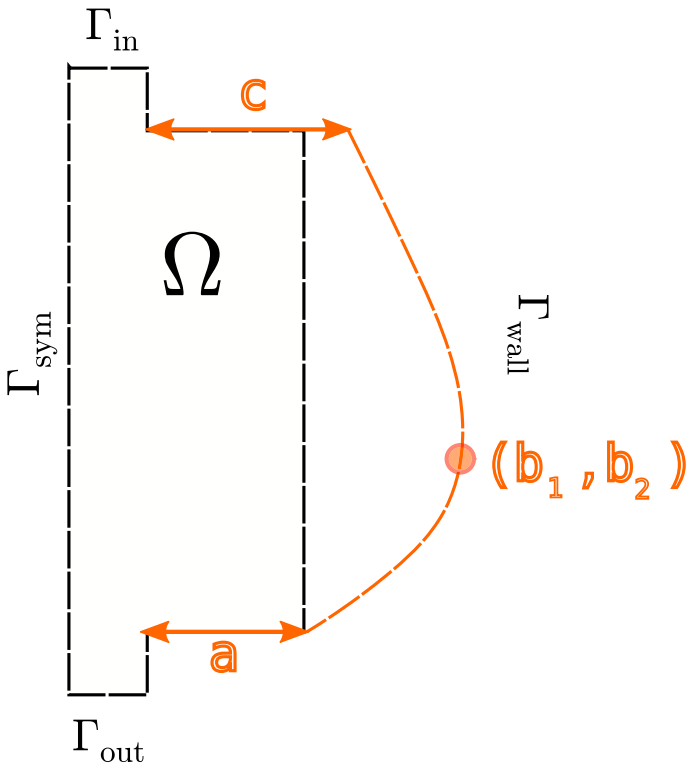


Figure 1: Shape parameterization.

2.5 Optimization algorithm

From a general point of view, the formulation of a global optimization problem, in its minimization form, is given by:

$$\min_{x \in \Theta} h(x) \tag{7}$$

where $h : \Theta \to \mathbb{R}$ is the cost function and x is the optimization parameter belonging to an admissible space $\Theta \subset \mathbb{R}^N$, with $N \in \mathbb{N}$.

In next sub-sections, we describe in detail the optimization method. First, in Section 2.5.1, we briefly introduce the considered genetic algorithm (GA). Then, we introduce in Section 2.5.2 a method based in the optimization of the initial population of the GA to improve its performances.

2.5.1 Genetic algorithm

Genectic Algorithms (GAs) approximate the solution of the minimization problem (7). They are based on principles related to Darwinian evolution [GOL 89]. GAs are applied in biogenetics, computer science, engineering, economics, chemistry, manufacturing, mathematics, physics

and other fields. A genetic algorithm works by repeatedly modifying a population of artificial structures through the application of genetic operators. They use techniques such as inheritance, mutation, selection, and crossover. GAs are typically black-box methods that use fitness information exclusively; they do not require gradient information or other internal knowledge of the problem.

A first family, called *population*, $X^0 = \{x_l^0 \in \Theta, j = 1, ..., N_p\}$ of $N_p \in \mathbb{N}$ possible solutions of the optimization problem, called *individuals*, is randomly generated in the search space Θ. Starting from this population, we build recursively $N_g \in \mathbb{N}$ new populations, called *generations*, $X^i = \{x_l^i \in \Theta, j = 1, ..., N_p\}$ with $i = 1, .., N_g$ through three stochastic operators, called selection, crossover and mutation. More precisely we present here a matrix-form approach for GAs:

Initially, a new *population*, $X^0 = \{x_j^0 \in \Theta, j = 1, ..., N_p\}$ of $N_p \in \mathbb{N}$ candidate solutions is created. Each candidate solution, also called *individual*, is randomly generated in the search space Θ. From the initial population, a new offspring $X^i = \{x_j^i \in \Theta, j = 1, ..., N_p\}$ with $i = 1, .., N_g$ and $N_g \in \mathbb{N}$ is obtained by recursively applying three stochastic steps, *i.e.,* selection, crossover and mutation. Note that X^i can be rewritten using the following $N_p \times N$-real valued matrix form:

$$X^i = \begin{bmatrix} x_1^i(1) & \dots & x_1^i(N) \\ \vdots & \ddots & \vdots \\ x_{N_p}^i(1) & \dots & x_{N_p}^i(N) \end{bmatrix} \tag{8}$$

In the following, the components of the GA generation (or iteration) are briefly described.

Selection: Individuals are selected through a fitness-based process, where fitter solutions (as measured by a fitness function) are typically more likely to be selected. To this aim, each individual, x_j^i is ranked with respect to its cost function value $h(x_j^i)$, i.e. the lower its $h(x_j^i)$ value, the higher is the ranking and therefore, the higher is its chances to be selected. Then, N_p individuals are randomly selected from X^i to become *parents*.

Introducing a binary $N_p \times N_p$ matrix $\mathcal{S}^i$, generated according to previous ranking and selection processes, with $\mathcal{S}_{j,k}^i = 1$ if the k-th individual of X^i is the selected *parent* number j and $\mathcal{S}_{j,k}^i = 0$ otherwise, we define:

$$X^{i+1,1} = \mathcal{S}^i X^i. \tag{9}$$

Crossover: Crossover is a genetic operator that combines (mates) two parents to produce two new individuals called *children*. The idea behind crossover is that the new individuals may be better than both parents if they take the best characteristics from each of the parents. Crossover occurs during evolution according to a user-definable *crossover probability*. More precisely, we determine, with a probability $p_c \in [0, 1]$, if two consecutive parents in $X^{i+1,1}$ exchange data or if they are directly copied into the intermediate population $X^{i+1,2}$.

Let us introduce a real-valued $N_p \times N_p$ matrix $\mathcal{C}^i$, where for each couple of consecutive lines $(2j-1, 2j)$ with $1 \leq j \leq \lfloor \frac{N_p}{2} \rfloor$. The coefficients of the $(2j-1)$-th and $2j$-th rows are given by:

$$\mathcal{C}^i_{2j-1,2j-1} = \lambda_1, \quad \mathcal{C}^i_{2j-1,2j} = 1 - \lambda_1, \quad \mathcal{C}^i_{2j,2j-1} = \lambda_2, \quad \mathcal{C}^i_{2j,2j} = 1 - \lambda_2$$

In this expression:

- $\lambda_1 = \lambda_2 = 1$ if parents are directly copied (with a probability $1-p_c$).
- λ_1 and λ_2 are randomly chosen in $]0, 1[$ if a data exchange occurs between the two parents (with probability p_c).

Other coefficients of $\mathcal{C}^i$ are set to 0. If N_p is odd, the N_pth parent is directly copied, i.e $\mathcal{C}^i_{N_p,N_p} = 1$.

This step can be summarized as:

$$X^{i+1,2} = \mathcal{C}^i X^{i+1,1}. \tag{10}$$

Mutation: Mutation is a genetic operator that alters one or more new parameter values for some individuals of the population. With these new parameter values, the genetic algorithm may be able to increase the population diversity and then the probability to escape from local minima. Mutation occurs during evolution according to a user-definable mutation probability, i.e. each child is modified (or mutated) with a fixed probability $p_m \in [0, 1]$.

Let us consider, for instance, a random perturbation matrix $\mathcal{E}^i$ with an j-th line equal to:

- a random vector $\epsilon_j \in \mathbb{R}^N$, according to the admissible space Θ, if a mutation is applied to the ith child (with probability p_m).
- 0 if no mutation is applied to the j-th child (with probability 1-p_m).

Therefore, the new population can be written as:

$$X^{i+1} = X^{i+1,2} + \mathcal{E}^i. \tag{11}$$

which can be rewritten as:

$$X^{i+1} = \mathcal{C}^i \mathcal{S}^i X^i + \mathcal{E}^i. \tag{12}$$

The algorithm stops when a maximum number of iterations N_g is reached, although other termination criteria could be defined based, for example, on a tolerance ϵ. When the termination criterion is satisfied, the GA returns an output denoted by $\text{GAO}(X^0; N_p, N_g, p_m, p_c, \epsilon) = \text{argmin}\ \{h(x^i_j)/x^i_j \in X^i, i = 1, ..., N_p,\ j = 1, ..., N_g)$.

As Goldberg stated in [GOL 89], with these three basic evolution processes, it is generally observed that the best obtained individual is getting closer after each generation to the optimal solution of the problem.

Genetic algorithms do not require sensitivity computation, perform global and multi-objective optimization and are easy to parallelize. However, their drawbacks remain their weak mathematical background, their computational complexity, their slow convergence and their lack of accuracy. So, it is recommended, when it is possible, to complete the GA iterations by a descent method. This is especially useful when the functional is flat around the minimum [DUM 89].

2.5.2 Hybrid genetic algorithm

In this subsection, we describe a method to improve the performance of the genetic algorithm based on the optimization of the GA initial population.

From a general point of view, we consider an optimization algorithm $\mathrm{CA} : V \to \Theta$, called *core optimization algorithm*, to solve (7). Here V is the search space where we can choose the initial condition for CA. The other optimization parameters of CA (such as the stopping criterion, number of iteration, etc.) are fixed by the user.

We assume the existence of a suitable initial condition $v \in V$ such that, for a given precision $\epsilon > 0$, $|\,\mathrm{CA}(v) - \min_{x\in\Theta} h(x)| < \epsilon$. Thus, solving numerically (7) with the considered core optimization algorithm means to solve

$$\begin{cases} \text{Find } v \in V \text{ such that} \\ \mathrm{CA}(v) \in \mathrm{argmin}_{x\in\Theta}\, h(x). \end{cases} \tag{13}$$

In the case where the core optimization algorithm is the GA presented in Section 2.5.1, problem (13) can be rewritten as:

$$\begin{cases} \text{Find } X^0 \in V = \Theta^{N_p} \text{ such that} \\ \mathrm{GAO}(X^0; N_p, N_g, p_m, p_c, \epsilon) \in \mathrm{argmin}_{w\in\Theta}\, h(w) \end{cases} \tag{14}$$

where N_p, N_g, p_m, p_c and ϵ are the parameters considered to be fixed.

The solution of (14) may be determined, for instance, by using the following hybrid algorithm based on the secant method and denoted by HGA (Hybrid Genetic Algorithm):

Algorithm 1 $\mathrm{HGA}(t_\ell, N_p, N_g, p_m, p_c, \epsilon)$

Input: $t_\ell \in \mathbb{N}, N_p, N_g, p_m, p_c$, and ϵ.

Randomly generate $X_1^0 = \{x_{1,j}^0 \in \Theta, j = 1, ..., N_p\}$

for ℓ from 1 to t_ℓ **do**

Set $o_l \in \mathrm{argmin}\{h(x) : x \in \mathrm{GAO}(X_l^0; N_p, N_g, p_m, p_c, \epsilon)\}$.

for j from 1 to N_p **do**

$$x_{l+1,j}^0 = \begin{cases} x_{l,j}^0 & \text{if } h(o_l) = h(x_{l,j}^0), \\ \mathrm{proj}_\Theta(x_{l,j}^0 - h(o_l)\frac{o_l - x_{l,j}^0}{h(o_l) - h(x_{l,j}^0)}) & \text{otherwise,} \end{cases}$$

where $\mathrm{proj}_\Theta : \mathbb{R} \to \Theta$ is a projection algorithm over Θ defined by the user.

end for

Construct $X_{l+1}^0 = \{x_{l+1,j}^0 \in \Theta, j = 1, ..., N_p\}$.

end for

Output: $\mathrm{argmin}\{\mathrm{GAO}(X_m^0; N_p, N_g\ , p_m, p_c, \epsilon),\ m = 1, ..., t_\ell\}$.

HGA intends to optimize, individual by individual, the initial population of GAO. For each individual in the initial population X_l^0, with $l = 1, 2, ..., t_{\ell-1}$:

- If there is a significant evolution of the cost function value between this individual and the best element found by GAO($X_l^0; N_p, N_g, p_m, p_c, \epsilon$), the secant method used in Step 1.2 generates, in the optimized initial population X_{l+1}^0, a new individual close to this best element.
- Otherwise, the secant method allows to create a new individual in X_{l+1}^0 far from the current solution given by GAO($X_l^0; N_p, N_g, p_m, p_c, \epsilon$).

The numerical experiments in [IVO 06-a] seem to indicate that considering algorithm GAO reduces the computational complexity of GAs. In particular, this allows to consider smaller values for N_p and N_g than those required for GAO alone. A complete validation of this algorithm on various industrial problems can be found in [IVO 06-c, IVO 09, IVO 06-b, IVO 07, DEB 06].

3 Results

3.1 Optimal shape

In order to solve the optimization problem 5, we have use the particular MATLAB implementation of the algorithm HGA, described in Section 2.5, included in the *Global Optimization Platform* software (freely available at `http://www.mat.ucm.es/momat/software.html`). The algorithm parameters are set to:

- $t_{\ell_1} = 20$, $N_g = 20$, $N_p = 20$ and $\epsilon = 0$ (i.e., HGA runs until the given computational complexity).
- The selection is a roulette wheel type [GOL 89] proportional to the rank of the individuals in the population.
- The crossover is barycentric in each coordinate with a probability of $p_c = 0.55$.
- The mutation process is non-uniform with a probability of $p_m = 0.5$.
- A one-elitism principle, that consists in keeping the current best individual in the next generation, has also been imposed.
- 10 iterations of the steepest descent method are performed at the end of the HGA starting from the obtained solution.

The number of cost function evaluation is about 6000. Each evaluation of the cost function (6) (implemented using Matlab and COMSOL Multiphysics 3.5a toolboxes [INF 09]), in both 2D and 3D cases, requires about 40s on a Intel Quad-core 2.8Ghz 64bits computer with 12GB of RAM. Thus, the optimization process takes approximatively 67 hours.

After running the optimization procedure described in the preceding section, we obtain the optimal shape displayed in Figure 2. The total volume has been reduced by 20% which is a significative improvement of the bioreactor's characteristics.

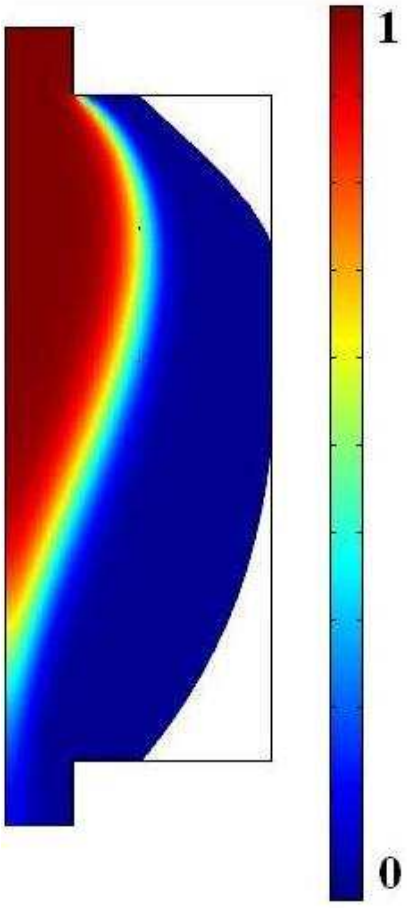


Figure 2: Bioreactor shape obtained after the optimization process. The normalized substrate concentration distribution and old shape are also presented.

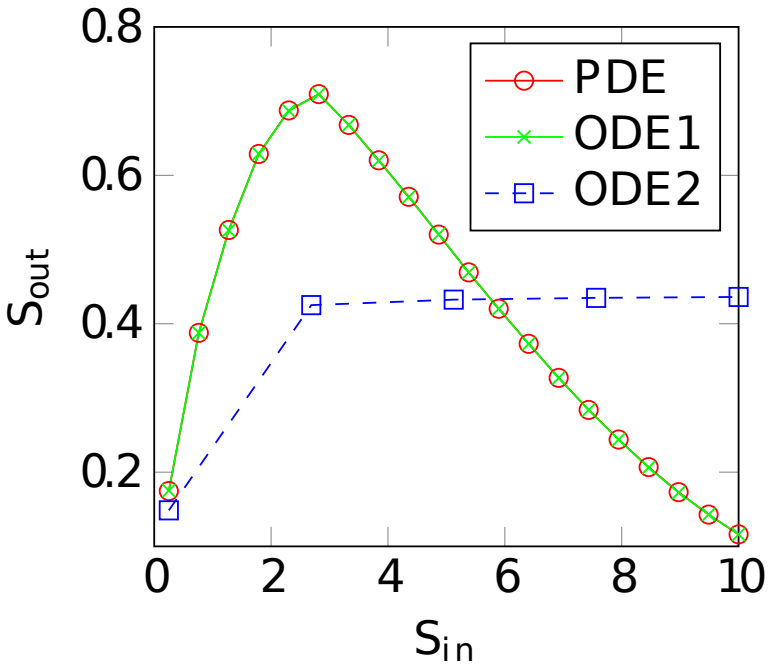


Figure 3: Dependence of S_{out} on S_{in} for the three different models: **PDE**, **ODE1** and **ODE2**.

3.2 Comparison between different models

Results are presented in Figure 4. As we can observe on this Figure, for each S_{in} there exists a pair (α, d) which fits the PDE and ODE1 models, whose values increase as S_{in} increases. However, the values of d present important oscillations when S_{in} is high. Those oscillations are due to numerical instabilities which can be mitigated by decreasing the time steps used in the ODE model. When solving the multi-objective problem ODE2, we have found values of (α, d) which produce substrate concentrations with tendencies similar to the PDE model (increasing then constant). A more in-depth analysis should be conducted in order to better match the ODE2 and PDE models. For instance, this could be achieved by increasing the number of ODEs and variables considered.

4 Conclusions

In this work, we have presented two models, based respectively on PDEs and ODEs, for describing the behavior of a particular bio-reactor. The PDE model has been used to reduce the bio-reactor volume keeping its cleaning efficiency. The second model, based on ODE, is computationally low and has been calibrated to reproduce similar results to the PDE one. Those first results are encouraging and further studies should contemplate

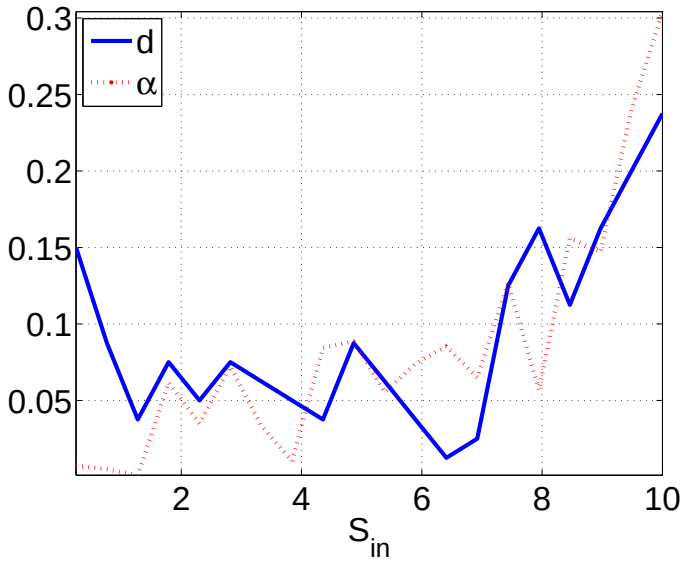


Figure 4: Optimal values of α (continuous line) and d (dotted line) for each value of S_{in} in **ODE1**.

a more complex shape optimization (for instance, considering the bioreactor height) and a more comple ODE model (involving more ODEs and coefficients). Among possible extensions, we should consider cases where the bioreactor is equipped with a system of retention of biomass (either moving or fixed bed bioreactor).

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