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OPTIMAL SOLUTION OF A DIFFUSIVE-REACTIVE SYSTEM WITH A CONTROL DISCRETE SOURCE TERM

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ABSTRACT: In this paper we study the numerical behavior of a diffusive-reactive system with a control source point. The idea was to first consider the problem with a fixed source point and then, according to the numerical results obtained, estimate the objective function adjusting a special class of functions using least squares. With this procedure, we study the behavior of a nonlinear system in a easy way.

KEYWORDS: diffusive-reactive system, finite differences, optimization problem.
AMS SUBJECT CLASSIFICATION (2000): 65M06, 90C20.

1. Introduction

In [1] the authors studied the behavior of an optimal solution of a diffusive equation with a discrete source term. Here, the goal is to obtain the optimal solution in a more general framework. Now the problem is a system of diffusive-reactive nonlinear partial differential equations with a discrete source term, which the position we want to control. In other words, our aim is to localize the source in order to maximize a certain objective function. In Section 2 we start by considering the differential problem that describes the physical phenomena with the assumption that the source term has a fixed position. We discretize the problem using a full discrete finite difference scheme and establish sufficient conditions for the convergence of the numerical solution to the exact one. In Section 3 a procedure to obtain the optimal position of the source term is presented. The procedure may be divided in two phases. Based on numerical experiments made for a fixed source point, we first introduce a family of curves, depending on a small set of parameters, that approximate the solution of the differential system. The parameters that identify the curves are obtained by least squares. We must note that the position of the source point is fixed but that position has influence on the value of the adjusted parameters. In the second phase the parameters are obtained in function of the position of the source. The optimal solution is obtained by injecting the parameters in the objective function.

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2. Fixed source point

2.1. The problem. We are concerned with a partial differential diffusion-reaction system with a source term written in the form [3]

$$\begin{cases} \dfrac{\partial u}{\partial t} = \alpha_1 \dfrac{\partial^2 u}{\partial x^2} - \beta uv + q(t)\delta(x-\eta), & x \in]0, L[, t \in]0, T], \\ \dfrac{\partial v}{\partial t} = \alpha_2 \dfrac{\partial^2 v}{\partial x^2} - \beta uv, & x \in]0, L[, t \in]0, T], \\ \dfrac{\partial w}{\partial t} = \alpha_3 \dfrac{\partial^2 w}{\partial x^2} + \beta uv, & x \in]0, L[, t \in]0, T], \end{cases} \tag{1}$$

where L and T are two positive real constants and δ is the Dirac delta function. The dependent variables u, v and w could be interpreted as the concentration of a given substance, $\alpha_i > 0$, $i = 1, 2, 3$, its diffusion coefficient (u and v are the reagent and w the product of the reaction), and β the velocity of the reaction. The function $q(t)$ indicates how much u is added to the system at point $x = \eta$.

In order to define the numerical method, we first replace the Dirac delta function in (1) by a suitable discrete delta function d_ϵ using the mollifier ideas [2], [4]. One possibility, consists in choosing the Peskin's discrete delta function, or "hat function", with support $]-\epsilon, \epsilon[$

$$d_\epsilon(x) = \begin{cases} (\epsilon - |x|)/\epsilon^2, & |x| \le \epsilon, \\ 0, & \text{otherwise}, \end{cases}$$

obtaining the approximate problem

$$\begin{cases} \dfrac{\partial u}{\partial t} = \alpha_1 \dfrac{\partial^2 u}{\partial x^2} - \beta uv + q(t)d_\epsilon(x-\eta), & x \in]0, L[, t \in]0, T], \\ \dfrac{\partial v}{\partial t} = \alpha_2 \dfrac{\partial^2 v}{\partial x^2} - \beta uv, & x \in]0, L[, t \in]0, T], \\ \dfrac{\partial w}{\partial t} = \alpha_3 \dfrac{\partial^2 w}{\partial x^2} + \beta uv, & x \in]0, L[, t \in]0, T]. \end{cases} \tag{2}$$

Let us now consider the boundary conditions

$$u(0,t) = c_0^1 \text{ and } \frac{\partial u}{\partial x}(L,t) = 0, t \in [0, T], \tag{3}$$

$$v(0,t) = c_0^2 \text{ and } \frac{\partial v}{\partial x}(L,t) = 0, t \in [0, T], \tag{4}$$

$$w(0,t) = c_0^3 \text{ and } \frac{\partial w}{\partial x}(L,t) = 0, t \in [0,T], \tag{5}$$

as well as the initial condition

$$u(x,0) = 0, v(x,0) = 0, w(x,0) = 0, \forall x \in]0,L[. \tag{6}$$

Note that, from equations (2)–(6) it is possible to compute u, v and w as function of q and c_0^1, c_0^2, and c_0^3.

2.2. Discrete solution. Convergence. In order to study the finite difference scheme which discretize the initial boundary value problem (IBVP) (2)–(6) we consider the approach suggested by Verwer and Sanz-Serna [6]. To prove the convergence of the discretized solution to the exact solution we need to establish the consistency and stability of both spatial and time discretization.

2.2.1. *Spatial discretization.* Let us consider the space discretization on the equidistant grid

$$\Omega_h = \{x_0 = 0, x_j = x_{j-1} + h, j = 2, ..., M-1, x_M = L, h = \frac{L}{M}\},$$

for a given integer $M \geq 2$. Consider now the standard second order finite differences for discretizing the second order derivatives and represent by $U_j(t)$, $V_j(t)$ and $W_j(t)$ the resulting approximations for $u(x_j,t)$, $v(x_j,t)$ and $w(x_j,t)$, $j = 1, ..., M$. The semi-discrete, continuous in time approximation to the IBVP (2)–(6) is given by, $j = 1, ..., M$,

$$\begin{cases} \dfrac{d}{dt}U_j = \alpha_1 h^{-2}(U_{j+1} - 2U_j + U_{j-1}) - \beta U_j V_j + q(t)\delta_h(x_j - \eta), & t \in]0,T], \\ \dfrac{d}{dt}V_j = \alpha_2 h^{-2}(V_{j+1} - 2V_j + V_{j-1}) - \beta U_j V_j, & t \in]0,T], \\ \dfrac{d}{dt}W_j = \alpha_3 h^{-2}(W_{j+1} - 2W_j + W_{j-1}) + \beta U_j V_j, & t \in]0,T], \end{cases} \tag{7}$$

where $U_0 = c_0^1$, $V_0 = c_0^2$, $W_0 = c_0^3$ and $U_{M+1} = U_{M-1}$, $V_{M+1} = V_{M-1}$ and $W_{M+1} = W_{M-1}$, according to the boundary conditions. The source point η should be one of the discretization points, for instance, $\eta = x_p$, $p \in \{1, ..., M\}$.

Let $Y_j = [U_j, V_j, W_j]^T$ and $Y = [Y_1^T, ..., Y_M^T]^T$. Then, the system (7) may be written in the form

$$\frac{d}{dt}Y = F(t, Y) = (K + \beta G(Y))Y + Q(t) + \bar{c_0}, \tag{8}$$

where K is the block tridiagonal matrix

$$K = h^{-2}\begin{bmatrix} -2A & A & & & \\ A & -2A & A & & \\ & \ddots & \ddots & \ddots & \\ & & A & -2A & A \\ & & & 2A & -2A \end{bmatrix}, \qquad A = \begin{bmatrix} \alpha_1 & & \\ & \alpha_2 & \\ & & \alpha_3 \end{bmatrix},$$

and

$$G(Y) = \operatorname{diag}\left(G_1(Y_1), ..., G_M(Y_M)\right), G_j(Y_j) = \begin{bmatrix} -V_j & 0 & 0 \\ 0 & -U_j & 0 \\ V_j & 0 & 0 \end{bmatrix}, j = 1, .., M,$$

$Q(t)$ is the vector of all components equal to zero except the one that corresponds to the position of U_p where it is equal to $\frac{q(t)}{h}$ and $\bar{c_0} = [c_0^1, c_0^2, c_0^3, 0, \dots, 0]^T$.

Let us prove the convergence of Y to $y_h = [u_h, v_h, w_h]^T$ in the maximum norm $\|\cdot\|_\infty$, where $y_h(t) = \mathcal{R}_h y(x, t)$, $\mathcal{R}_h$ is the natural restriction operator to the spatial grid and $y = [u, v, w]^T$ is the exact solution of the IBVP (2)–(6) written in the form

$$\begin{cases} \dfrac{\partial y}{\partial t} = A\dfrac{\partial^2 y}{\partial x^2} + \beta g(y)y + q(t)d_h(x-\eta), & x \in]0, L[, t \in]0, T], \\ y(0, t) = c_0, \dfrac{\partial y}{\partial x}(L, t) = 0, & t \in]0, T], \\ y(x, 0) = 0, & x \in]0, L[, \end{cases} \tag{9}$$

where $c_0 = [c_0^1, c_0^2, c_0^3]^T$, $\bar{q}(t) = [q(t), 0, 0]^T$ and $g(y)y = [-uv, -uv, uv]^T$.

Following Verwer and Sanz-Serna [6], let us consider the logarithmic norm $\mu_\infty[\cdot]$ associated to the maximum norm, which is defined, for a real square matrix B by

$$\mu_\infty[B] = \max_i (b_{ii} - \sum_{j \neq i} |b_{ij}|).$$

Let

$$S_h(t) = \{\xi : \xi = (1-\theta)y_h(t) + \theta Y(t)\}$$

and μ_{max} defined by

$$\mu_{max} \geq \max_{\xi \in S_h(t)} \mu_\infty[F'(t,\xi)], \qquad t \in [0,T],$$

where

$$F'(t,\overline{Y}) = K + \beta \text{diag}(G_j), \qquad G_j = \begin{bmatrix} -\overline{V}_j & -\overline{U}_j & 0 \\ -\overline{V}_j & -\overline{U}_j & 0 \\ \overline{V}_j & \overline{U}_j & 0 \end{bmatrix}, j = 1,..,N,$$

represents the Jacobian matrix of F and $\overline{Y}$ is in the segment $S_h(t)$. If such μ_{max} exists then we may conclude that

$$\|y_h(t) - Y(t)\|_\infty \leq C(t,\mu_{max})\|T_h(t)\|_\infty, \qquad t \in [0,T],$$

where

$$C(t,\mu_{max}) = \frac{e^{\mu_{max}} - 1}{\mu_{max}}$$

depends only on t and μ_{max} and $T_h(t)$ is the local truncation error defined by

$$T_h(t) = F(t, y_h(t)) - \frac{d}{dt} y_h(t).$$

So, if μ_{max} exists and the discretization is consistent, i.e., $\|T_h(t)\|_\infty \to 0$ as $h \to 0$ uniformly in t, then $\|y_h(t) - Y(t)\|_\infty \to 0$.

If the solution Y of (7) has fourth order piecewise continuous derivatives and since we define our grid in order to contain the injection points, we obtain a second order approximation in the form (see [2], [4])

$$\frac{d}{dt}Y_j(t) = A\delta_2 Y_j(t) + \mathcal{O}(h^2), \qquad j \in \{1,\dots,M\}\backslash\{p\},$$

$$\frac{d}{dt}Y_p(t) = A\delta_2 Y_p(t) + \frac{q(t)}{h} + \mathcal{O}(h^2),$$

where δ_2 represents the second order centered finite difference operator and p is such that $x_p = \eta$.

We will now prove the stability of the spatial discretization by proving the existence of μ_{max}. Let $\overline{Y}$ be a point in the segment $S_h(t)$. Since $\mu_\infty[K] = 0$, we have

$$\mu_\infty[F'(t,\overline{Y})] \leq \beta \mu_\infty[\text{diag}(G_j)] \leq \beta \max_j (\overline{U}_j + \overline{V}_j),$$

which proves the existence of a μ_{max} independent of h.

2.2.2. *Time discretization.* Let us consider the explicit Euler scheme to perform the time integration. Then, the approximations to the solution of (8) on the uniform grid defined in $[0, T]$ with step size Δt, i.e., $t^0 = 0$, $t^N = T$, and $\Delta t = t^n - t^{n-1}$, $n = 1, \ldots, N$, are given by

$$Y^{n+1} = Y^n + \Delta t F(t^n, Y^n), \qquad n = 0, ..., N-1. \tag{10}$$

Since the method is consistent, to prove the convergence we must prove that the method is C-stable with respect to the maximum norm. The method is C-stable if a positive real number $\Delta t_0 = \Delta t_0(h)$ and a real constant C_0, independent of Δt and h exists, such that, for each $\Delta t \in]0, \Delta t_0]$ and each two solutions of the method Y and $\widetilde{Y}$

$$\|Y^{n+1} - \widetilde{Y}^{n+1}\|_\infty \leq (1 + C_0 \Delta t)\|Y^n - \widetilde{Y}^n\|_\infty.$$

In our case,

$$Y^{n+1} - \widetilde{Y}^{n+1} = (I + \Delta t F'(t^n, \xi))(Y^n - \widetilde{Y}^n),$$

where $\xi = \theta Y^n + (1-\theta)\widetilde{Y}^n$, $\theta \in [0, 1]$, and I is the identity matrix. Then

$$\|Y^{n+1} - \widetilde{Y}^{n+1}\|_\infty = \|I + \Delta t F'(t^n, \xi)\|_\infty \|Y^n - \widetilde{Y}^n\|_\infty.$$

If

$$\Delta t \leq \frac{h^2}{2\alpha}, \qquad \alpha = \max_{i=1,2,3}\{\alpha_i\}, \tag{11}$$

we may easily conclude that $C_0 = \mu_{max}$ and so the method is C-stable. We proved the following result.

Theorem 1. *Let us consider y the solution of the differential system (9) and Y the numerical approximation given by the numerical method*

$$Y^{n+1} = Y^n + \Delta t \left((K + \beta G(Y^n))Y^n + Q^n + \bar{c_0} \right), \quad n = 0, ..., N-1, \tag{12}$$

where $Q^n = Q(t^n)$, $n = 0, ..., N$. If the stability condition (11) holds, the method is convergent, i.e,

$$\lim_{h, \Delta t \to 0} \|y(t^i, x_j) - Y_i^j\|_\infty = 0.$$

2.3. Numerical results. Let us consider the problem (9) with $L = 5$, $T = 1$, $\alpha = [2, 1, 2]^T$, $\beta = 0.5$, $c_0 = [40, 100, 0]^T$ and $q(t) = 40$, for $t \in [0, 1]$. Using the numerical scheme (12) with $h = 1/10$ and $\Delta t = 1/1000$ we obtain its numerical solution. We plot in Figure 1 the variation of u, v and w concentration for $x \in [0, 5]$, $t \in [0, 1]$ and $\eta = 2$.

To illustrate the influence of the source point location, η, into the concentration of u, v and w, we apply the method for two different values of η and $t = 1$. The results obtained are plotted in Figure 2.

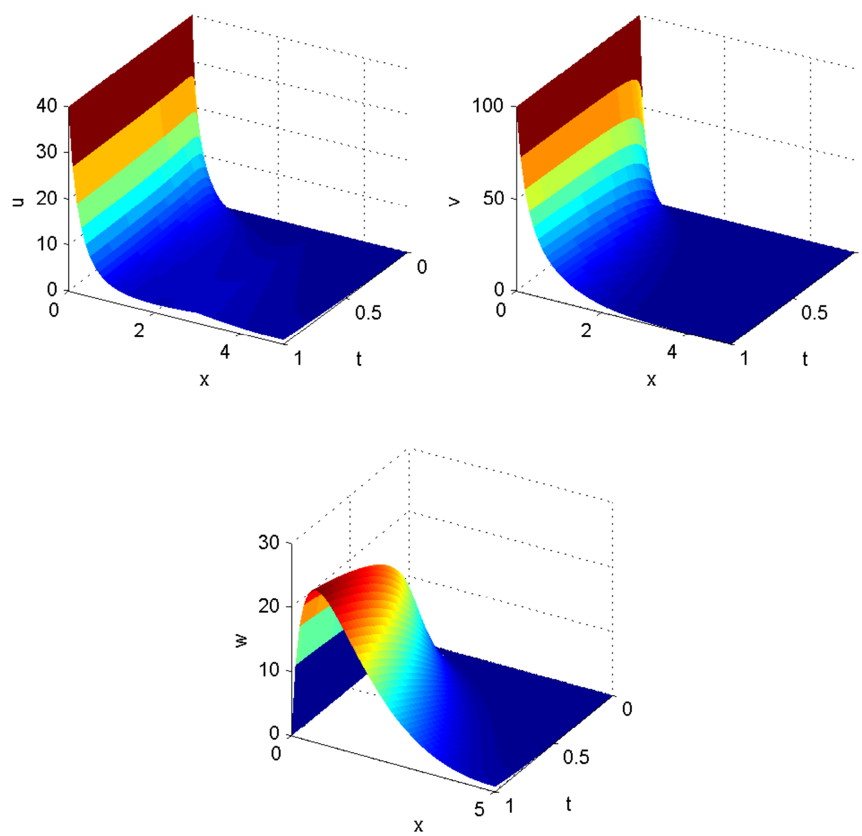

FIGURE 1. Spatial and time variation of u, v and w concentration ($\eta = 2$)

3. Optimized source point

3.1. Objective function. Consider now the problem (2)–(6) being $y(x, \bar{t}; \eta)$ its exact solution at time $\bar{t} \in]0, T]$. An approximation to this solution can be found using directly the method (12), $\bar{t} \in]0, T]$. Let η be the control variable, which can be calculated solving the optimization problem defined by

$$\max_{\eta \in [0,L]} f(u, v, w, \eta) = \int_0^L w(x, \bar{t}) dx, \qquad \bar{t} \in]0, T], \tag{13}$$

and subjected to (2)–(6). This corresponds to maximize the total amount of substance w produced at time $\bar{t}$.

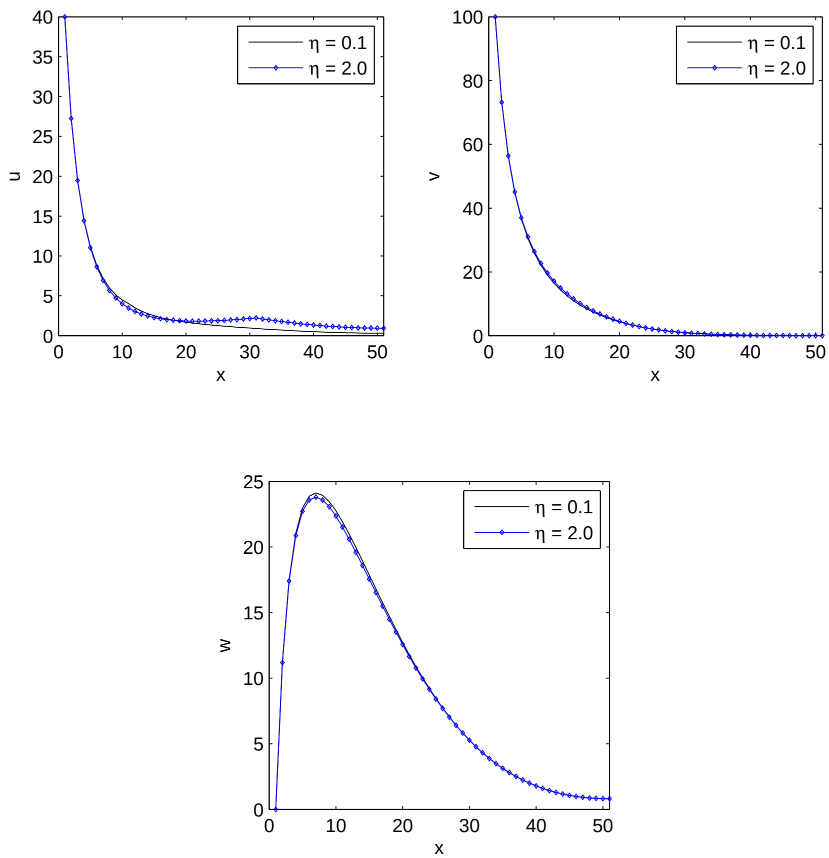

FIGURE 2. u, v and w concentration at time $t = 1$, for different locations of the source point

Using (12) and a discretization of (13) we can obtain an aproximation to the optimal value for η. This procedure requires a large computational effort to find the optimal value, since both time and space discretizations origin a huge number of variables $(3MN + 1)$ which do not allow an acceptable precision. Our aim is to follow a new strategy that reduce the computational costs.

3.2. The algorithm. In order to solve the problem (2)–(6), (13) we first discretize the differential system (2)–(6) as explained in Section 2 and compute the solution Y^n, $n = 1, ..., M$, from (12). Next, we aproximate the function f in order to obtain an explicit expression to be optimized. With this purpose, we considered a family of parameterized functions that are well fitted to the numerical results obtained with fixed η. The parameters, depending on η, can be computed using the least squares technique. Then, with several values for η, we obtain curves that approximate the parameters as function of η. In this way we obtain a function, depending only on η, that approximates f and which can be easily optimized using numerical methods [5], reducing significantly the computational effort.

The steps mentioned before define the algorithm that we propose for the solving problem (2)–(6), (13) and can be easily implemented.

The choice of a suitable family of functions is essential for a correct fitting. In the present case, and according to the numerical results obtained in the last section, we propose the family of functions

$$\bar{y}(x;\eta) := [\bar{u}(x;\eta), \bar{v}(x;\eta), \bar{w}(x;\eta)]^T = [c_0^1 e^{-b_1 x}, c_0^2 e^{-b_2 x}, (a_3 x + c_0^3) e^{-b_3 x}]^T, \tag{14}$$

to approximates $y(x, \bar{t}; \eta)$. The parameters b_1, b_2, b_3 and a_3 depend on η but can be computed using the least squares technique. The problem can now be solved with a great reduction of calculations.

As shown in Figure 3, where, for $\bar{t} = 1$ and $\eta = 2.0$, the exact solution $y(x, \bar{t}; \eta)$ as well as the corresponding numerical solution $\bar{y}(x;\eta)$ are plotted, the family of functions (14) is a good choice. The parameters b_1, b_2, b_3 and a_3, for $\eta = 2.0$, were obtained by the least squares technique. For a more detailed study of the error see Table 1, which also contains the error for $\eta = 0.1$. Here, $\|\cdot\|$ is the euclidian norm and $\bar{y}_h = [\bar{u}_h, \bar{v}_h, \bar{w}_h]^T = \mathcal{R}_h \bar{y}(x;\eta)$, where $\mathcal{R}_h$ is the restriction operator to the mesh points and U^N, V^N, W^N are the components of Y^N.

In conclusion, the optimal value for η may be obtained by solving

$$\max_{\eta \in [0,L]} f(\bar{y}(x;\eta)) \tag{15}$$

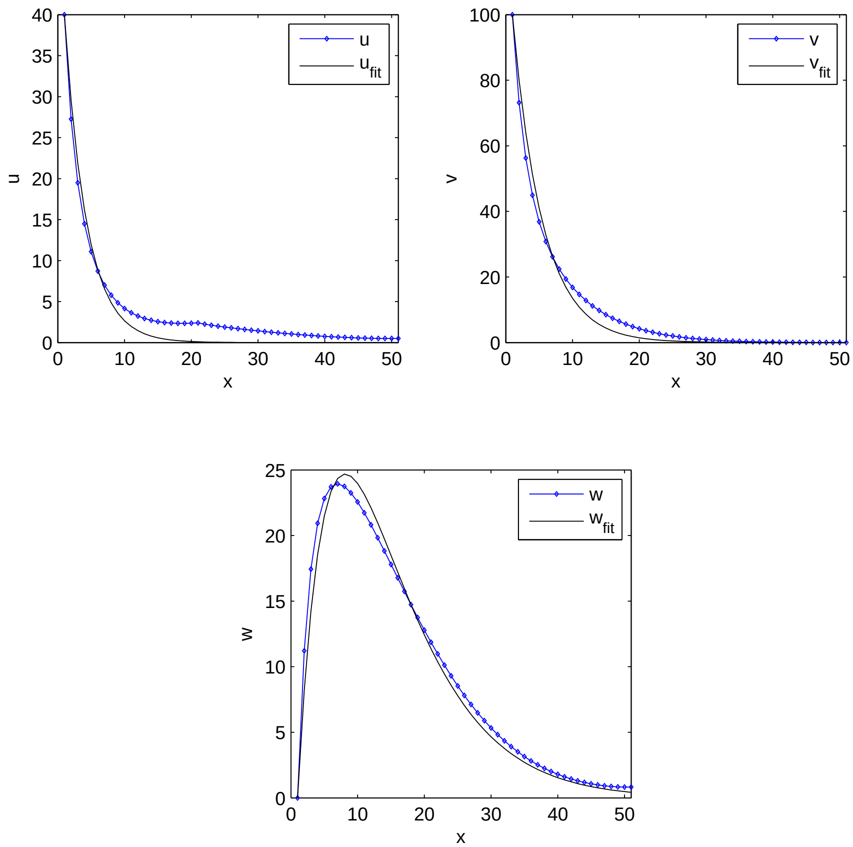

FIGURE 3. Least squares approximation of $y(x,1;2)$ by curves of the type $y_{fit} := \bar{y}(x;2)$.

	$\|\|U^N - \bar{u}_h\|\|$	$\|\|V^N - \bar{v}_h\|\|$	$\|\|W^N - \bar{w}_h\|\|$
$\eta = 0.1$	0.1418	0.3985	0.1328
$\eta = 2.0$	0.2038	0.3709	0.1330

TABLE 1. Error for the fitted solution obtained by the least squares method on the mesh points.

where $\bar{y}(x;\eta)$ is the fitted function of Y^n obtained by (12). So, replacing (14) in (15) we obtain a funtion that depend only on η and will be denoted by

$$\bar{f}(\eta) := f(\bar{y}(x;\eta)) = \int_0^L \bar{w}(x;\eta)dx = a(\eta)(1 - e^{-b(\eta)L}(1 + b(\eta)L))/(b(\eta)^2). \tag{16}$$

η	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5
$a(\eta)$	95.609	95.435	94.752	94.235	94.019	94.000	94.059	94.127	94.173
$b(\eta)$	1.4206	1.4118	1.4052	1.4039	1.4066	1.4108	1.4146	1.4174	1.4191
$\|\|W^N - \bar{w}_h\|\|$	0.1312	0.1287	0.1304	0.1330	0.1343	0.1345	0.1342	0.1338	0.1335

TABLE 2. Variation of a and b, obtained by the least squares procedure with η and the respective error in w.

η	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5
$\bar{f}(\eta)$	47.094	47.537	47.581	47.431	47.203	46.960	46.733	46.540	46.391
$I_{\bar{w}}(0,L)$	47.059	47.547	47.646	47.469	47.182	46.902	46.682	46.532	46.450
$I_w(0,L)$	48.612	49.037	49.119	48.969	48.721	48.468	48.262	48.117	48.035

TABLE 3. Approximations of the objective function f: $\bar{f}$, exact value of $\int_0^L \bar{w}(x;\eta)dx$; $I_{\bar{w}}(0,L)$, approximation of $\int_0^L \bar{w}(x;\eta)dx$ by the rectangular rule; $I_w(0,L)$, approximation of $\int_0^L w(x;\bar{t},\eta)dx$ by the rectangular rule.

Here, $a(\eta)$ and $b(\eta)$ are the fitting coefficients for each η.

3.3. Numerical results. Let us return to the problem (2)–(6), where L, T, α, β, c_0 and $q(t)$ assume the same values as in Section 2.3. In that section we obtained an approximation for the solution of the considered problem fixing some values of η. Now we will obtain the optimal value of η by using the described algorithm.

In what concern the parameters $a(\eta)$ and $b(\eta)$, for different values of η, we obtained the values in Table 2. We note that the variation of the discrete functions $a(\eta)$ and $b(\eta)$ are small.

In order to optimize (15), we need explicit formulae for $a(\eta)$ and $b(\eta)$ which can be obtained by fitting the values in Table 2 by curves of type $\mu_1 e^{-\mu_2\eta} + \mu_3\eta + \mu_4$. Then we obtain an explicit expression of the objective function $\bar{f}$.

Solving (15) we conclude that the best location for the source point is giving by $\eta = 1.317422$ and the value of the objective function is $\bar{f}(\eta) = 47.595661$. These values are in agreement with the values in Table 3.

4. Conclusion

In this paper we propose a method to approximate the solution an optimal control problem which is difficult to solve. The procedure is based on the synergy between the numerical methods and optimization. In short, the numerical methods are used to deal with the differential equation and provide the data to approximate the objective function, using the least squares method, which will be at last optimized.

Some numerical results are also present. The specific example considered in this work can be interpreted in terms of chemical reactions [3].

References

[1] A. Araújo, F. Patrício and José L. Santos, Optimal solution of a diffusion equation with a discrete source term, *DMUC Report*, **07-33** (2007), to appear in Communications in Numerical Methods in Engennering. DOI: 10.1002/cnm.1204

[2] R.P. Beyer and R.J. Leveque, Analysis of a one-dimensional model for the immersed boundary method, *SIAM J. Numer. Anal.*, **29** (1992) 332–364.

[3] R. Dilão, The reaction-diffusion approach to morphogenesis, *Proc. Symp. Math. Comp. Biol.* **4(1)** (2005) 325–364.

[4] J.D. Kandilarov and L.G. Vilkov, The immersed interface method for a nonlinear chemical diffusion equation with local sites of reactions, *Numerical Algorithms*, **36** (2004) 285–307.

[5] S. Nash and A. Sofer, *Linear and Nonlinear Programming*, Mc. GrawHill, 1996.

[6] J. G. Verwer and J. M. Sanz-Serna, Convergence of method of lines approximations to partial differential equations, *Computing*, **33(3-4)** (1984) 297–313.

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