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SOLUTION OF THE NON-LINEAR PARABOLIC PROBLEMS USING NONLINEAR COMPLEMENTARITY ALGORITHM (FDA-NCP)

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Abstract. Parabolic type problems involving a variational and complementarity formulation arise in mathematical models of several applications in Engineering, Economy, Biology and different branches of Physics. These kinds of problems present several analytical and numerical difficulties related, for example, to time evolution and moving boundary.

In this work we implement a numerical method based on the finite difference scheme for time evolution and nonlinear complementarity algorithm (FDA-NCP) for solving the problem at each time step. We use the implicit finite difference scheme with adaptative time step implementation which allows us to use bigger time steps and speed up the simulations. One of the advantages using the FDA-NCP is its global convergence.

This method was applied to simple non-linear parabolic partial differential equation, which describes oxygen diffusion problem inside one cell. This equation was rewritten in the quasi-variational form. The main problem consists in tracking the moving boundary that represents the oxygen penetration depth inside the cell.

1 INTRODUCTION

The parabolic type problems involving variational formulation and complementarity problems appear in many applications. For example the liquid flow at the inner domain, diffusion, heat flow including phase change and chemical reactions are modeled as parabolic type moving boundary problems, see (Crank, 1984). Different examples arise in Engineering and Economics, see (Ferris and Pang, 1997).

Since the analytic solutions of these kinds of non-linear problems are difficult to obtain, one can transform them into the variational formulation in order to obtain an approximate solution. Many works cited below work particular case of oxygen diffusion using the linear model. In this paper we address more general case, which is interesting for many applications.

The diffusion of oxygen into absorbing tissue was first studied in (Crank and Gupta, 1972). First the oxygen is allowed to diffuse into a medium, some of the oxygen can be absorbed by the medium and the concentration of oxygen at the surface of the medium is maintained constant. This phase of the problem continues until a steady state is reached in which the oxygen does not penetrate any further into the medium. During the second phase the surface is sealed so that no oxygen passes in or out, the medium continues to absorb the available oxygen already in it and, as consequence, the boundary marking the furthest depth of penetration in the steady state starts to recede towards the sealed surface.

The major challenge is that of tracking the movement of the moving boundary during this stage of the process as well as determining the distribution of oxygen throughout the medium at any instant in time. This type of problem is known as an implicit moving boundary problem, see (Crank, 1984).

There is a number of analytical and numerical methods used to obtain the solution of this problem, we recall some of them here. In (Crank and Gupta, 1972) the approximate analytical solution is used for starting times, when the moving boundary is moving slowly. When the speed of the moving boundary has increased the numerical scheme with a fixed grid network is used. The concentration is calculated at each grid point using the Euler equation. For the grid near the moving boundary, a Lagrange type formula is used and the location of the moving boundary is determined using a Taylor series expansion.

In (Hansen and Hougaard, 1974) the integral equation was used for the function defining the position of the moving boundary and an integral formula for the concentration distribution. The integral equation is solved asymptotically during the entire motion of the moving boundary whereas the concentration integral is solved asymptotically for small times and computed by numerical quadrature at later times.

In (Gupta and Kumar, 1981) a Crank-Nicolson implicit finite difference scheme with variable time step was used avoiding the large number of time steps generally required for the methods in (Crank and Gupta, 1972) and (Hansen and Hougaard, 1974). Due to the implicit boundary condition, an integral equation is used to determine the time steps.

One semi-analytical method is proposed in (Gupta and Banik, 1989), it solves the implicit moving boundary problems using the constrained integral method. The problem of the diffusion of oxygen in a sphere was studied as an example of an implicit moving boundary problem. The distribution of the oxygen concentration was assumed to be a polynomial of even degree, in which four unknown functions should be determined as a part of the required solution. These unknowns were expressed in terms of the concentration at the outer surface of the sphere, which is still unknown and to be determined. Finally, the number of unknowns were reduced to two: the concentration at the outer surface and the position of the moving boundary. There are

some recent works dealing with the problem of oxygen diffusion using modifications of the constrained integral method, see (Ahmed, 2006; Çatal, 2003). In (Boureghda, 2006) the oxygen diffusion problem was studied analytically.

In this work we propose a numerical method based on a combination of the implicit central space finite difference scheme, (Strikwerda, 1989) and a nonlinear complementarity algorithm, (Mazorche, 2007). This approach allows us to use bigger time steps and for each one of them we expect better convergence compared to usual finite difference schemes using Newton's method, see (Strikwerda, 1989) and (Chapiro and Marchesin, 2008). In order to speed up the evaluation we use time adaptative implementation were the choice of the next time step is made based on the information given by the nonlinear complementarity algorithm. Some results of this method addressing linear problems were presented in Mazorche et al. (2010).

Other methods dealing with complementarity problems can be found in (Chen and Mangasarian, 1996; Cottle et al., 1980; Mazorche and Herskovits, 2005).

This paper is organized as follows. In Section 2 we introduce the physical model of oxygen diffusion. In Section 3 we describe the non-complementarity algorithm used to solve the problem at each time step and the finite difference scheme used for time evaluation. In Section 4 we describe the obtained results comparing them with the existing data. Finally, in Section 6 we present some conclusions.

2 PHYSICAL FORMULATION

The oxygen diffusion problem appears in many applications. In (Crank and Gupta, 1972) the linear mathematical model of biological diffusion examines the oxygen injection into the sick cell and diffusion of injected oxygen inside it. Another example appears from the study of the reaction kinetic of coke oxidation in porous media, see (Chapiro, 2009). Here we study a one dimensional particular case involving oxygen diffusion that possesses a moving boundary. For simplicity, the oxygen is allowed to diffuse into a medium which absorbs and immobilizes oxygen at constant rate. The concentration of oxygen at the surface of the medium is maintained constant. A moving boundary marks the limit of oxygen penetration.

The process is assumed to consist of two levels. The first phase of the problem continues until a steady state is reached in which there is no oxygen transfer into the medium, see Figure 1, left. The oxygen absorption is considered.

At the second phase the surface of the medium is sealed so that no more oxygen passes in or out. The medium continues to absorb the available oxygen already diffusing in it and, as a consequence, the boundary marking the depth of penetration in the steady state recedes towards the sealed surface, see Figure 1, right. The major problem is that of tracing this movement of the boundary and determining the distribution of oxygen as a function of time. A secondary problem is associated with numerical techniques that has to deal with the discontinuity in the derivative boundary condition which results from the abrupt sealing of the outer surface.

Following (Crank, 1984) we denote by $C(X,T)$ the concentration of oxygen free to diffuse at a distance X from the outer surface of the medium at a time T. D is the constant diffusion coefficient, $r(C)$ is the rate of consumption of oxygen per unit volume of the medium (is assumed constant for $C(X,T) > 0$). The steady state is defined by a solution of

$$D\frac{d^2C}{dX^2} - r(C) = 0, \tag{1}$$

where C satisfies the conditions $C = \partial C/\partial X = 0$, for $X_0 \leq X$, where X_0 corresponds to the most extent oxygen penetration, and the outer surface $C = C_0 = const.$, for $X = 0$. The

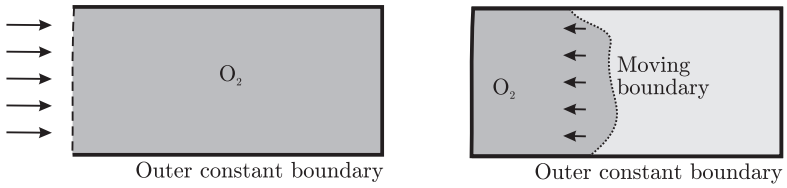

Figure 1: Schematic representation of the oxygen diffusion into the media sample. The first stage is represented on the left. Here the oxygen enters the sample until equilibrium is reached. During the second phase, on the right, the sample is sealed and the oxygen inside diffuses and is absorbed by the medium generating the moving boundary.

required solution for constant $r(C) = r_0$ is given by:

$$C = \frac{r_0}{2D}(X - X_0)^2, \quad X_0 = \sqrt{\frac{2DC_0}{r_0}}. \tag{2}$$

After the surface $X = 0$ has been sealed, the position of the receding boundary is denoted by $X_0(T)$ and the problem to be solved becomes:

$$\frac{\partial C}{\partial T} = D\frac{\partial^2 C}{\partial X^2} - r(C), \quad 0 \leq X \leq X_0, \tag{3}$$

$$\frac{\partial C}{\partial X} = 0, \quad X = 0, \quad 0 \leq T, \tag{4}$$

$$C = \frac{\partial C}{\partial X} = 0, \quad X = X_0(T), \quad 0 \leq T, \tag{5}$$

$$C = \frac{r_0}{2D}(X - X_0)^2, \quad 0 \leq X \leq X_0, T = 0, \tag{6}$$

where $T = 0$ is the moment when the surface is sealed. By making the changes of variables:

$$x = \frac{X}{X_0}, \quad t = \frac{D}{X_0^2}T, \quad c = \frac{C}{2C_0}, \tag{7}$$

and denoting by $s(t)$ the value of x corresponding to $X_0(T)$, the above system is reduced to the following non-dimensional form:

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} - f(c), \quad 0 \leq x \leq s(t), \tag{8}$$

$$\frac{\partial c}{\partial x} = 0, \quad x = 0, \quad 0 \leq t, \tag{9}$$

$$c = \frac{\partial c}{\partial x} = 0, \quad x = s(t), \quad 0 \leq t, \tag{10}$$

$$c = \frac{1}{2}(1 - x)^2, \quad 0 \leq x \leq 1, \quad t = 0, \tag{11}$$

where c is the concentration of oxygen free to diffuse. In Crank and Gupta (1972) and others works cited in the introduction the function $f(c) = -1$. In this work we introduce one small non-linearity and consider the case $f(c) = -1 - c(1 - c)$.

Following (Baiocchi and Pozzi, 1975) we transform the system (8) - (11) into a variational approach

$$\frac{\partial c}{\partial t} - \frac{\partial^2 c}{\partial x^2} + 1 + c(1-c) \geq 0, \quad c \geq 0, \tag{12}$$

together with the equality

$$\left(\frac{\partial c}{\partial t} - \frac{\partial^2 c}{\partial x^2} + 1 + c(1-c) \right) c = 0. \tag{13}$$

The inequality (12) is satisfied as equality by (8) inside the region $0 < x < s(t)$. When $s(t) \leq x \leq 1$ by (10) we get $c = 0$ and thus (12) is equivalent to $1 > 0$. The inequality $c \geq 0$ follows from (11). The equality (13) is valid because for any $x \in [0, 1]$ one of the factors vanishes.

Remark: *The equivalence of the solution of the system equations in the variational approach* (12)-(13) *and the weak solution of the Stefan problem described by the system* (8)-(11) *for the linear case are studied in (Baiocchi and Pozzi, 1975) and (Baiocchi and Capelo, 1984). The formal demonstration of this result for the non-linear case is left to the future work.*

3 NUMERICAL SCHEME

In this section we describe how to solve the system (12)-(13) numerically. We use Finite Difference Scheme (FDS) for the time evaluation and a nonlinear complementarity algorithm to solve the problem at each time level. In this way the implementation is very adaptative, we can change the finite difference scheme and the algorithm separately.

Although the Finite Element Method (FEM) is better to simulate the Neumann boundary conditions we use FDS. There are two reasons for this. The implementation of FDS is simpler than the FEM. All papers found and to which we compare our algorithm use FDS and as we want to find out the gain we get when using nonlinear complementarity algorithms we have to use the same type of schemes. We use both the classical Cranck-Nicolson scheme and central space scheme.

For each time step we use an interior point algorithm for complementarity problems (FDA-NCP) developed by (Mazorche, 2007). Next we present a brief description of the problem of complementarity and the algorithm FDA-NCP.

3.1 Nonlinear complementarity algorithm

Let $F : D \subset \mathbb{R}^M \rightarrow \mathbb{R}^M$ be a nonlinear vector function defined on the domain D. The nonlinear complementarity problem consists in finding $c \in \mathbb{R}^M$ such that:

$$F(c) \geq 0, \quad c \geq 0 \quad \text{and} \quad c \circ F(c) = 0, \tag{14}$$

where $c \geq 0$ means that each component of the vector c is nonnegative, and "$\circ$" denote the entrywise Hadamard product for vectors, given by $(c \circ y)_i = c_i\, y_i$. In our case the two inequalities in (14) correspond to (12) and the Hadamard product is described by (13).

Defining the feasible set $\Upsilon = \{c \in \mathbb{R}^M \mid c \geq 0, F(x) \geq 0\}$, it is easy to see that c is a solution of the problem (14) if and only if c is in the feasible set and $c \circ F(c) = 0$.

FDA-NCP is an iterative algorithm to find the solution of problem (14). It starts from an initial point in Υ and generates a sequence of points in Υ that converge to the required solution. It first defines a search direction and performs a line search along that direction to find a point

with lower value for the potential function $\Phi(c) = \sum_{i=1}^{n} c_i\, F_i(c)$. That point is defined to be the next point of the sequence and the algorithm returns to the first step till a convergence criterion is satisfied. The search direction is based on Newton's direction for the nonlinear system of equations $c \circ F(c) = 0$. To obtain a convergence to the solution, Newton's direction is modified by a restoration direction, as done in (Herskovits, 1998). The present approach is supported by strong theoretical studies by (Mazorche and Herskovits, 2009).

The following notation will be employed to describe the algorithm FDA-NCP: $F^k = F(c^k)$, $M^k = \nabla(c \circ F(c))$, $\Phi^k = \Phi(c^k)$, $\nabla\Phi^k = \nabla\Phi(c^k)$ and $\lambda^k = \Phi^k/M$.

FDA-NCP

Data: $c^0 \in \mathrm{int}(\Upsilon)$, $k = 0$, $\epsilon > 0$, $E = [1, ..., 1]^T$, $\nu, \nu_1 \in (0, 1)$, $\alpha \in (0, 1/2)$.

Step 1: Computation of the search direction d^k

Find d^k solving the following linear system of equations:

$$M^k\, d^k \;\; = -c^k \circ F^k + \alpha\, \lambda^k\, E. \tag{15}$$

Step 2: Line search

Set t as the first number in the sequence $\{1, \nu, \nu^2, \nu^3, ...\}$ that satisfies:

$$\begin{aligned} c^k + t\, d^k \quad & \geq 0; \\ F(c^k + t\, d^k) \quad & \geq 0; \\ \Phi^k + t\, \nu_1\, (\nabla\Phi^k . d^k) \quad & \geq \Phi(c^k + t\, d^k). \end{aligned} \tag{16}$$

Step 3: Update

Set $c^{k+1} = c^k + t\, d^k$ and $k = k + 1$.

Step 4: Stop criterion

If $\|c^k \circ F^k\| \leq \epsilon$ stop, else go to step 1.

In (Mazorche and Herskovits, 2009) it has been shown that the search direction d^k is well defined in Υ when function F verifies some usual regularity assumptions.

3.2 Finite difference scheme

Explicit schemes can only use very small time steps because of the CFL restriction. Implicit schemes allow for larger time steps and may be unconditionally stable, but they are computationally more expensive. As the quality of the solution is tied to its stability, we choose to solve the system implicitly.

We consider the homogeneous grid for the variable x with $M + 1$ points, where x_0 and x_M are the boundary points of the interval where the calculation takes place. The grid spacing is $h = x_{m+1} - x_m = 1/M$ and the grid position m corresponds to $x = m\Delta x$. Analogously the time is denoted by t with time index denoted by n and the time step is Δt. However, we consider time step-adaptative finite difference schemes, so Δt may change from one grid level to another. Generally we get $\Delta t = \Delta t_n$ and the time index n corresponds to $t = \sum_{i=1}^{n} \Delta t_n$.

Using the presented notation we denote the differential operator from the left side of the inequality (12) as $F(c)$ and rewrite it in the discrete form

$$F_\Delta(c) = \frac{c_m^{n+1} - c_m^n}{\Delta t} - \frac{c_{m-1}^{n+1} - 2c_m^{n+1} + c_{m+1}^{n+1}}{2\Delta x^2} - \frac{c_{m-1}^n - 2c_m^n + c_{m+1}^n}{2\Delta x^2} + f_\Delta, \tag{17}$$

where $f_\Delta = 1$ in the linear case and $f_\Delta = (c_m^n(1-c_m^n) + c_m^{n+1}(1-c_m^{n+1}))/2$ in the non-linear. Substituting the differential operator $F(c)$ in (12) by the discrete operator $F_\Delta(c)$, multiplying the inequality by Δt and isolating the terms for time step $n+1$ on the left we obtain the equation describing the numerical scheme. In what follows we use $\mu = \Delta t/\Delta x^2$. The evaluation equation for the grid points $m = 0$ and $m = M$ can not be described with (17) because of the boundary conditions.

3.2.1 First phase of the problem

For the first phase of the problem, as described in Section 2, the concentration of oxygen at the left end of the interval (x=0) is constant and is modeled with Dirichlet boundary conditions $c_0 = c_L$. The right side of the interval (x=1) is sealed and is modeled as Neumann boundary condition $\partial c/\partial x(x_M) = 0$. We use the ghost point method at the right boundary in order to implement this condition. This method consists in increasing the grid by one point x_{N+1} and use the Dirichlet condition. The value of the concentration at x_{N+1} is determined using the boundary condition:

$$0 = \frac{\partial c}{\partial x}(x_M, t) \approx \frac{c_{M+1}^{n+1} - c_M^{n+1}}{\Delta x}. \tag{18}$$

It follows that $c_{M+1}^{n+1} = c_M^{n+1}$, substituting c_{M+1}^{n+1} into (17) for $m = M$ we obtain

$$-\frac{\mu}{2}c_{M-1}^{n+1} + \left(1+\frac{\mu}{2}\right)c_M^{n+1} \geq \frac{\mu}{2}c_{M-1}^{n} + \left(1-\frac{\mu}{2}\right)c_M^{n} - \Delta t f_\Delta, \tag{19}$$

The problem has M variables and can be rewritten in matrix form with the inequality is assumed to be satisfied for each element.

3.2.2 Second phase of the problem

During the second phase of the problem the left end of the sample is sealed, proceeding analogously to the previous case we introduce x_{-1} and determine the value of concentration at x_{-1} using the boundary condition:

$$0 = \frac{\partial c}{\partial x}(x_0, t) \approx \frac{c_0^{n+1} - c_{-1}^{n+1}}{\Delta x}. \tag{20}$$

It follows that $c_{-1}^{n+1} = c_0^{n+1}$, substituting c_{-1}^{n+1} into (17) for $m = 0$ we obtain:

$$\left(1+\frac{\mu}{2}\right)c_0^{n+1} - \frac{\mu}{2}c_1^{n+1} \geq \left(1-\frac{\mu}{2}\right)c_0^{n} + \frac{\mu}{2}c_1^{n} - \Delta t f_\Delta, \tag{21}$$

The right side is exactly the same as described in (19). Now the problem in matrix form with Neumann conditions at both sides is:

$$A\,[c_1^{n+1},\ c_2^{n+1},\ \cdots,\ c_M^{n+1}]^T \geq B\,[c_1^n,\ c_2^n,\ \cdots,\ c_M^n]^T - \overline{\Delta t f_\Delta}^T, \tag{22}$$

where

$$A = \begin{bmatrix} 1+\mu & -\mu & 0 & \cdots & 0 \\ -\frac{\mu}{2} & 1+\mu & -\frac{\mu}{2} & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & -\frac{\mu}{2} & 1+\mu & -\frac{\mu}{2} \\ 0 & \cdots & 0 & -\frac{\mu}{2} & 1+\mu \end{bmatrix}, \quad B = \begin{bmatrix} 1-\mu & \mu & 0 & \cdots & 0 \\ \frac{\mu}{2} & 1-\mu & \frac{\mu}{2} & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & \frac{\mu}{2} & 1-\mu & \frac{\mu}{2} \\ 0 & \cdots & 0 & \frac{\mu}{2} & 1-\mu \end{bmatrix} \tag{23}$$

and

$$\overline{\Delta t f_\Delta}^T = [\Delta t f_\Delta^1,\ \cdots,\ \Delta t f_\Delta^2,\ \Delta t f_\Delta^M - \mu c_L]^T. \tag{24}$$

Remark: *There are some other possibilities to discretize the space derivative at the boundary point, for example one can consider* $\partial c/\partial x \approx (c_1 - c_{-1})/2\Delta x$. *This choice can have a big impact in the stability of the scheme, see (Strikwerda, 1989) and (K.W. and D.F., 2005).*

3.2.3 Adaptative time step implementation

The routine merging FDA-NCP algorithm described in Section 3.1 and the finite difference scheme described in Section 3.2 was implemented in the following way.

Step 0: We start with the initial concentration distribution c_n^0, $n = 0, 1, \ldots, N$ and the first time step Δt_0.

Step 1: Next we use (22) (analogous equation if we are simulating the first phase of the problem) in order to obtain the operator $F_\Delta(c)$ in the discrete form.

Step 2: Use FDA-NCP algorithm to solve (14) with $F_\Delta(c)$. The number of iterations of FDA-NCP is used to determine the next time step length.

Step 3: Use the solution obtained in **step 2** as the concentration $c(x)$ at the next time step. Repeat the algorithm from the **step 1** until reaching the final time.

4 NUMERICAL RESULTS: LINEAR CASE

In this Section we present the results of some numerical simulations addressing the linear case described in Section 3. In all the iterations the FDA-NCP algorithm utilizes the linear search step equal to 1. This fact indicates that the FDA-NCP algorithm converges quadratically to the solution of the problem and agrees with the theoretical results presented in (Mazorche and Herskovits, 2009).

4.1 First phase

The first phase of the problem was used to test our algorithm. The implementation uses the Dirichlet boundary condition $c(x_0) = c_L = 0.5$ at the left and the Neumann boundary condition $\partial c/\partial x(x_0) = 0$ at the right side of the interval. The initial condition corresponds to the medium filled with oxygen. Simulations results can be seen on Figure 2.

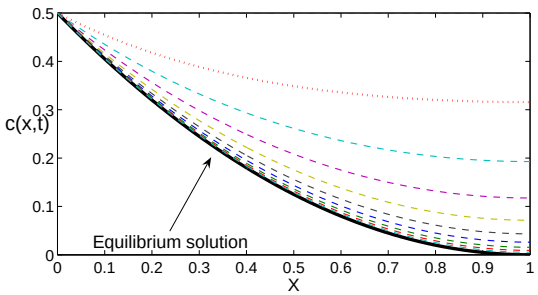

Figure 2: The plot represents the simulation of the first phase of the oxygen diffusion problem. Oxygen concentration at different times: the initial concentration (dotted), some iterations (dashed) and the equilibrium solution given by (11) (solid).

In order to better represent the physics of our problem it would be interesting to consider the medium with no oxygen as the initial condition. Unfortunately any oxygen distribution below the equilibrium solution is not in the feasible set for the FDA-NCP algorithm. In order to simulate this situation we substitute the nonlinear complementarity algorithm by the Extragradient method with constant step length, see (Tinti, 2005). The simulation results can be seen on Figure 3.

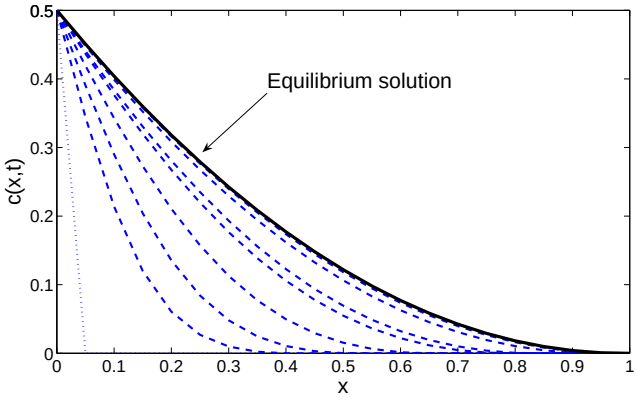

Figure 3: The plot represents the simulation of the first phase of the oxygen diffusion problem. Oxygen concentration at different times: the initial concentration (dotted), some iterations (dashed) and the equilibrium solution given by (11) (solid).

4.2 Second phase

Next, we simulate the second phase of the problem using Neumann boundary conditions at the left and right sides of the interval $\partial c/\partial x(x_0) = 0$ and $\partial c/\partial x(x_N) = 0$. We compare our result with the one obtained in (Crank and Gupta, 1972) using semi-analytical techniques on Figure 4.

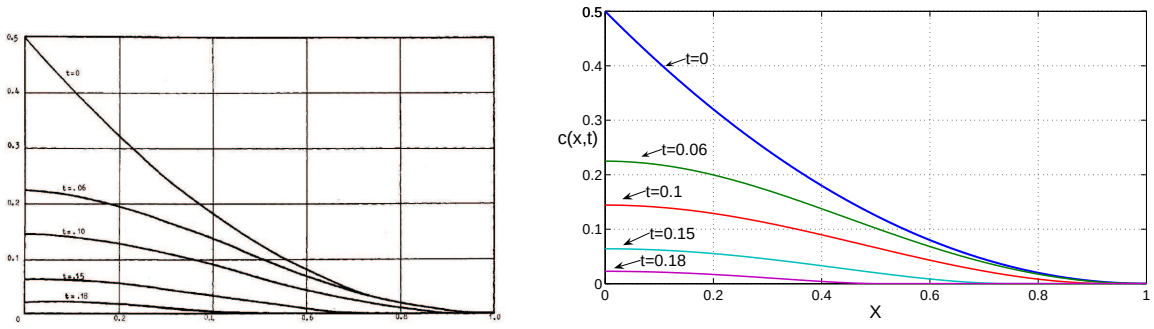

Figure 4: Both plots represent the simulation of the second phase of the oxygen diffusion problem. The oxygen concentration is represented for different times (from upper to lower) $t = 0$, $t = 0.06$, $t = 0.1$, $t = 0.15$ and $t = 0.18$. The left Figure corresponds to the results obtained in (Crank and Gupta, 1972); the right Figure corresponds to our simulations.

We can describe the moving boundary behavior in time as shown on Figure 5. We compare the moving boundary position at different times in Table 1.

Table 1: Moving boundary position. In this table we compare the results of the present work to: A: (Ahmed, 2006); HH: (Hansen and Hougaard, 1974); CG: (Crank and Gupta, 1972); G: (Gupta, 1973); GK: (Gupta and Kumar, 1981). CN-cub and CN-lin correspond to Cranck-Nicolson scheme with cubic and linear interpolation, CSBT corresponds to implicit central space scheme with cubic interpolation.

Time	CN-cub	CN-lin	CSBT	A	HH	CG	G	GK
0.0	1.0000	1.0000	1.0000	1.0000	1.00000	-	-	-
0.02	1.0000	1.0000	1.0000	0.9992	1.00000	-	-	-
0.04	1.0000	1.0000	1.0000	0.9983	0.99918	0.9988	0.9988	0.9950
0.06	0.9840	0.9935	0.9900	0.9921	0.99918	0.9905	0.9903	0.9899
0.08	0.9640	0.9729	0.9620	0.9663	0.97155	0.9650	0.9613	0.9623
0.10	0.9303	0.9400	0.9260	0.9313	0.93501	0.9312	0.9301	0.9249
0.12	0.8730	0.8799	0.8720	0.8750	0.87916	0.8747	0.8719	0.8703
0.14	0.7928	0.8004	0.7940	0.7937	0.79891	0.7912	0.7882	0.7916
0.16	0.6748	0.6880	0.6780	0.6784	0.68337	0.6756	0.6682	0.6825
0.18	0.4942	0.5042	0.5000	0.4909	0.50109	0.4849	0.4766	0.4768
0.19	0.3419	0.3509	0.3520	0.3401	0.34537	-	-	-
0.195	0.2049	0.2193	0.2340	0.2012	0.20652	-	-	-

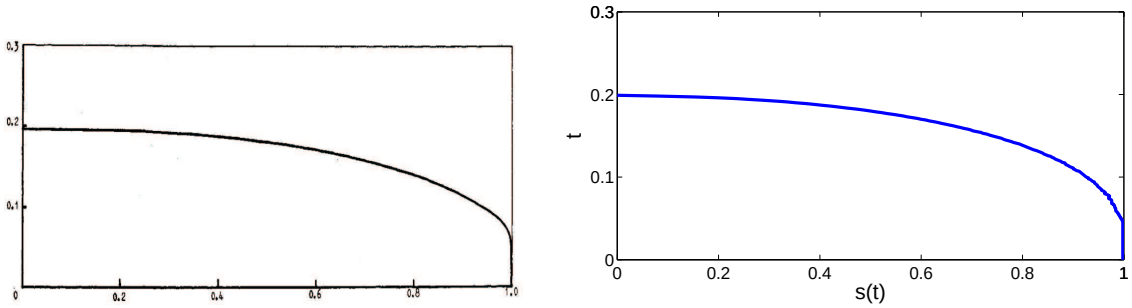

Figure 5: Both plots represent the moving boundary position $s(t)$ on the horizontal coordinate and time t on the vertical one. The left Figure corresponds to the results obtained in (Crank and Gupta, 1972) and the right Figure corresponds to our simulations.

5 NUMERICAL RESULTS: NON-LINEAR CASE

In this Section we present the results of some numerical simulations of the non-linear case described in Section 3. As before, in all the iterations the FDA-NCP algorithm utilizes the linear search step equal to 1.

There is no literature describing the non-linear case simulated in this text. In order to validate our algorithm we use classical Crank-Nicolson finite difference scheme with adaptative time step. At each time the moving boundary was obtained by truncation and new Cauchy problem was formulated.

For this case we simulate the second phase of the problem using Neumann boundary conditions at the left and right sides of the interval $\partial c/\partial x(x_0) = 0$ and $\partial c/\partial x(x_N) = 0$. We compare the result using the (FDA-NCP) with the classical Crank-Nicolson scheme on Figure 6.

We can describe the moving boundary behavior in time as shown on Figure 7.

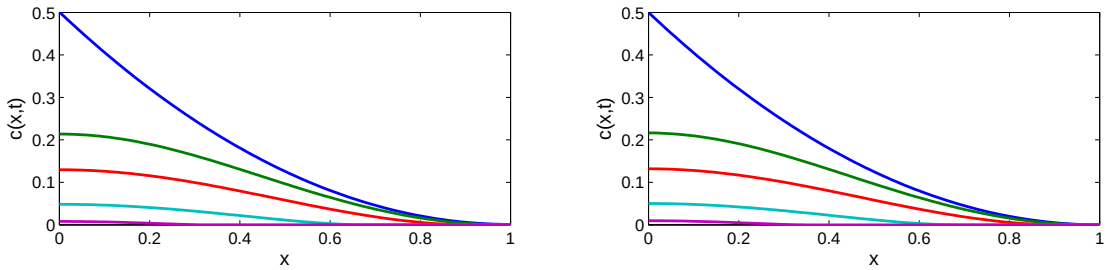

Figure 6: Both plots represent the simulation of the second phase of the non-linear oxygen diffusion problem. The oxygen concentration is represented for different times (from upper to lower) $t = 0$, $t = 0.06$, $t = 0.1$, $t = 0.15$ and $t = 0.18$. Left Figure corresponds to the results obtained using the (FDA-NCP); the right Figure corresponds to the classical Crank-Nicolson scheme.

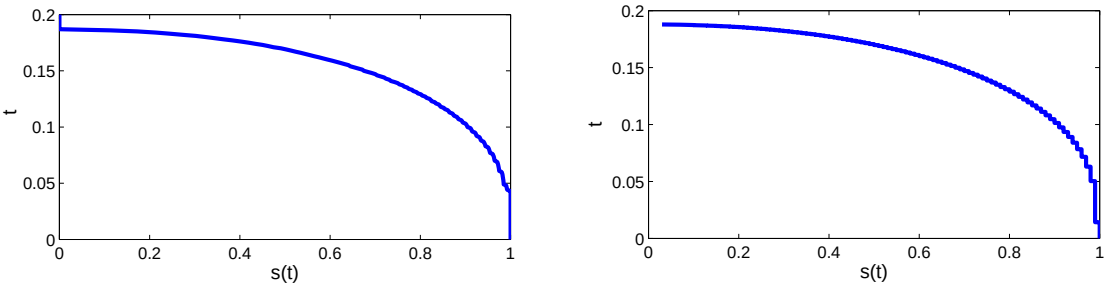

Figure 7: Both plots represent the moving boundary position $s(t)$ on the horizontal coordinate and time t on the vertical one. Left Figure corresponds to the results obtained using the (FDA-NCP); the right Figure corresponds to the classical Crank-Nicolson scheme.

6 CONCLUSIONS

In this work we propose a numerical method based on the implicit finite difference scheme and nonlinear complementarity algorithm which can be applied to linear and non-linear parabolic problems involving a variational formulation present in many applications. To illustrate this idea we apply it to the oxygen diffusion problem.

We simulated both phases of the oxygen diffusion problem. The first phase was used to test our algorithm. We started with some oxygen concentration close to the outer boundary. During the simulations the concentration converges to the equilibrium solution (11) as expected, see Figures 2 and 3.

In order to simulate the second phase of the problem we start with the equilibrium solution of the first phase and obtain the evolution over time of the oxygen concentration. The results show good agreement with (Crank and Gupta, 1972) as shown on Figure 4.

Finally, we obtain the moving boundary position $s(t)$ as a function of time. Numerical results obtained with the algorithm proposed in this paper show good agreement with those presented in (Crank and Gupta, 1972), see Figure 5 and with other ones as shown in Table 1. For the non-linear case the results were compared to the simulation using classical Crank-Nocolson scheme.

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