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Research Paper

A VARIATIONAL INEQUALITY APPROACH FOR ONE DIMENSIONAL STEFAN PROBLEM

MOJTABA MORADIPOUR

ABSTRACT. In this paper, we develop a numerical method to solve a famous free boundary PDE called the one dimensional Stefan problem. First, we rewrite the PDE as a variational inequality problem (VIP). Using the linear finite element method, we discretize the variational inequality and achieve a linear complementarity problem (LCP). We present some existence and uniqueness theorems for solutions of the underlying variational inequalities and free boundary problems. Finally we solve the LCP numerically by applying a modification of the active set strategy.

MSC(2010): 58E35; 65M70; 91G60.
Keywords: Stefan problem, Variational inequalities, Linear complementarity problems.

1. Introduction

We consider the following partial differential equation called the one dimensional Stephan problem (the oxygen diffusion problem)

$$
\begin{aligned}
&u_t - u_{xx} + 1 = 0, \quad 0 < x < s(t),\\
&u(x,0) = \tfrac{1}{2}(1-x)^2, \quad 0 < x < 1,\\
&u_x(0,t) = 0, \quad t > 0,\\
&u\left(s(t),t\right) = u_x(s(t),t) = 0, \quad t > 0.
\end{aligned} \tag{1.1}
$$

Problem (1.1) is related to the oxygen absorption process in a biological texture and it has been studied in [3, sec. 1.3.10]. In (1.1), $s(t)$ is the unknown free boundary of the problem and it must be computed. The domain of the problem (1.1) has been shown in fig. 1. There is no closed form solution to the problem (1.1) and the solution must be computed numerically. In [1] and references therein, Some numerical techniques have been developed for problem (1.1).

In this paper, we write equation (1.1) as a variational inequality problem, then we discretize and solve the variational inequality. A comprehensive description of variational inequalities can be found in [5] and [7]. Discetization

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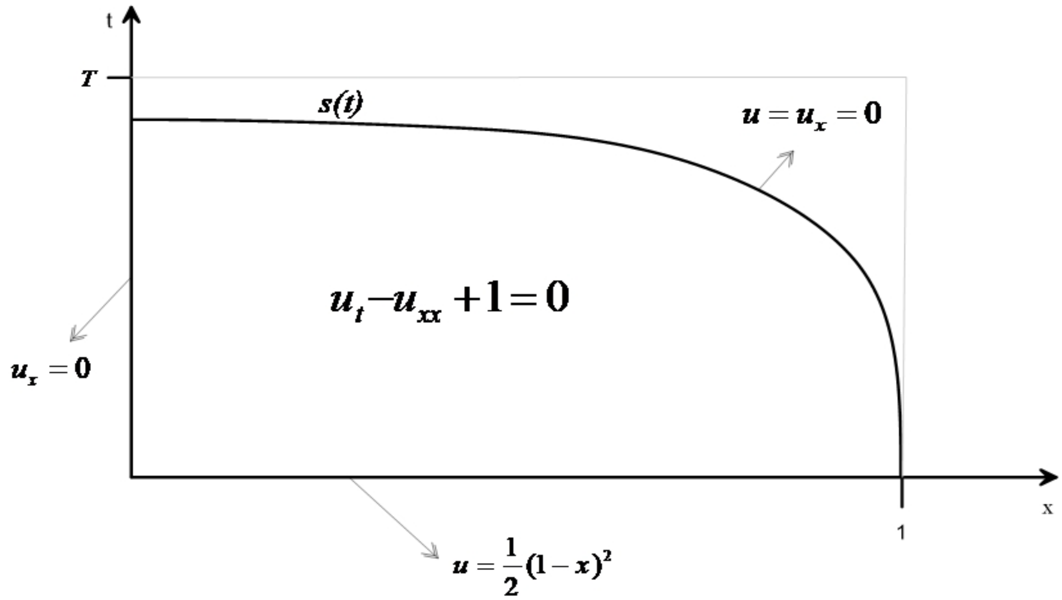

FIGURE 1. The domain of problem (1.1). In the entire of domain, the equation $u_t - u_{xx} + 1 = 0$ holds. Across the free boundary, the solution $u(x, t)$ touches the plane $x - t$ tangentially.

of variational inequalities lead to linear complementarity problems (LCPs). Linear complementarity problems have been described in [2].

There are several numerical methods to solve LCP's. The most famous method to solve LCPs is the projected successive over relaxation (PSOR). The PSOR is an iterative method with oreder of complexity $O(n^3)$. In [11], the authors have applied the PSOR method to solve the LCPs arising form financial mathematics. A naive method to solve LCPs is the active set strategy. The active set strategy has the complexity of order $O(2^n n^3)$ in the worst case. The active set strategy lead us directly to the solution of the LCP, nevertheless it increases the cost of computations. In this paper we use a modification of the active set strategy with order $O(m)$ for m-dimensional matrices.

2. The Stefan problem as a variational inequality

We are aimed to rewrite equation (1.1) as a variational inequality problem. For this purpose, we notice that if $0 < x < s(t)$ then the equation $u_t - u_{xx} + 1 = 0$ holds. If $s(t) < x < 1$ we let $u(x, t) = 0$ and in this region, we have $u_t - u_{xx} + 1 = 0 - 0 + 1 > 0$. From the physics of the Stefan problem, we can assume $u(x, t) \geq 0$; therefore in the entire of domain $(x, t) \in (0, 1) \times (0, t)$ we have $u_t - u_{xx} + 1 \geq 0$. In summary, we have the following system of inequalities (see more details at [3, sec. 6.4.1])

$$
\begin{cases}
u_t - u_{xx} + 1 \geq 0, \quad 0 < x < 1, \\
u(x,t) \geq 0, \quad 0 < x < 1, 0 < t < T, \\
(u_t - u_{xx} + 1)\, u = 0, \quad 0 < x < 1, 0 < t < T, \\
u(x,0) = \frac{1}{2}(1-x)^2, \quad 0 < x < 1, \\
u_x(0,t) = 0, \quad 0 < t < T, \\
u(1,t) = 0, \quad 0 < t < T.
\end{cases} \tag{2.1}
$$

One advantage of equation (2.1) is that the unknown free boundary of the problem $s(t)$ doesn't appear explicitly and we will directly achieve the solution $u(x,t)$. In [3] the finite difference method has been applied to solve (2.1). In what follows, we write the variational form of the problem (2.1). Similar to [11, sec. 4.1], we define a convex subset of $H^1(0,1)$ as follows:

$$
\begin{aligned}
\mathcal{K} = \Big\{ & v(x,t);\ v(.,t) \in H^1(0,1),\ \forall t \in (0,T), \\
& v_x(0,t) = 0, \quad v(1,t) = 0, \\
& v(x,0) = \frac{1}{2}(1-x)^2, \quad v(x,t) \geq 0 \Big\}.
\end{aligned}
$$

The requirements of equation (2.1) imply that $u \in \mathcal{K}$. Multiplying the first inequality of (2.1) by a non negative test function $v \in \mathcal{K}$ yields

$$\int_0^1 (u_t - u_{xx} + 1) v dx \geq 0,$$

from third term of (2.1) we have

$$\int_0^1 (u_t - u_{xx} + 1) u dx = 0,$$

subtracting two equations above we achieve

$$\int_0^1 (u_t - u_{xx} + 1)(v - u) dx \geq 0, \quad \forall v \in \mathcal{K},$$

integration by parts yields

$$\int_0^1 u_t(v-u)dx + u_x(v-u)\Big|_0^1 + \int_0^1 u_x(v_x - u_x)dx + \int_0^1 (v-u)dx \geq 0, \quad \forall v \in \mathcal{K}.$$

Because of boundary conditions of the problem, the integral free term of equation above vanishes; thus the variational form of the problem (1.1) becomes

Problem 2.1. Find $u \in \mathcal{K}$ such that for all $t \in (0,T)$ we have

$$(u_t, v - u) + (u_x, v_x - u_x) + (1, v - u) \geq 0, \quad \forall v \in \mathcal{K}. \tag{2.2}$$

Now, using finite difference method, we discretize the time interval and achieve a sequence of variational inequalities. Suppose that $\{0 = t_0, t_1, \ldots, t_N =$

$T\}$ be an uniform discretization of the time interval $[0, T]$ with time step size δt. Let

$$\bar{\mathcal{K}} = \left\{ v(x);\ v(x) \in H^1(0,1),\ v'(0) = 0,\ v(1) = 0,\ v(x) \geq 0 \right\}, \tag{2.3}$$

we discretize equation (2.2) using the implicit Euler method $u_t(x, t_n) = \frac{u(x,t_n) - u(x,t_{n-1})}{\delta t}$ and obtain

$$\left(\frac{u(x,t_n) - u(x,t_{n-1})}{\delta t}, v(x) - u(x,t_n) \right) + \left(u_x(x,t_n), v'(x) - u_x(x,t_n) \right) + (1, v(x) - u(x,t_n)) \geq 0, \quad \forall v \in \bar{\mathcal{K}},$$

using notation $u^n(x) := u(x, t_n)$ we rewrite the equation above as

$$(u^n, v - u^n) - \left(u^{n-1}, v - u^n\right) + \delta t \left(u^{n\prime}, v' - u^{n\prime}\right) + \delta t(1, v - u^n) \geq 0, \quad \forall v \in \bar{\mathcal{K}}.$$

By defining $b(u, v) = (u, v) + \delta t(u', v')$ the inequality above becomes

Problem 2.2. Find $u^n \in \bar{\mathcal{K}}$ such that

$$b(u^n, v - u^n) \geq (u^{n-1} - \delta t, v - u^n), \quad \forall v \in \bar{\mathcal{K}}. \tag{2.4}$$

The sequence of equations in (2.4) starts with $u^0(x) = u(x, 0) = \frac{1}{2}(1-x)^2$. The next terms $u^1(x), u^2(x), \ldots.$ are obtained by solving the problem (2.2). It can be proved that [11, Theorem 4.1] the bilinear form b in variational inequality (2.4) is continues and coercive. Continuity and coercivity of the bilinear form b is the necessary and sufficient condition for existence and uniqueness of the solution of problem (2.4). Therefore we have the following theorem.

Theorem 2.3. The problem proposed by (2.4) for any $n \in \mathbb{N}$ has a unique solution.

3. Numerical methods for variational inequalities

In this section, using the finite element method, we discretize the variational inequality (2.4). Discretization of the variational inequality (2.4) leads to a variational inequality in finite dimensional space $\mathbb{R}^n$. It can be shown that, in finite dimensional spaces, every variational inequality problem (VIP) is equivalence to a linear complementary problem (LCP) [11, Theorem 2.3]. For more details of the relation between variational inequalities and linear complementary problems, we refer the reader to [2]. In the sequel of this section, we will focus on the numerical solution of the linear complementary problems (LCP's).

3.1. Finite element discretization of variational inequalities.

We set equidistance points $\{0 = x_1, x_2, \ldots, x_M = 1\}$ on the spatial domain $[0, 1]$ with the step size h and introduce the linear finite element (hat functions) as

$$\varphi_j(x) = \begin{cases} \frac{1}{h}(x - x_{j-1}), & x_{j-1} < x < x_j, \\ \frac{1}{h}(x_{j+1} - x), & x_j < x < x_{j+1}. \end{cases}$$

Let $u_h^n = \sum_{j=1}^m u_j^n \varphi_j(x) = \mathbf{u}^{n\top}\mathbf{\Phi}$ be the approximation of $u^n(x)$ when

$$\mathbf{\Phi} = (\varphi_1(x), \varphi_2(x), \ldots, \varphi_m(x))^\top .$$

We suppose that $v_h = \sum_{j=1}^m v(x_j)\varphi_j(x) = \mathbf{v}^\top\mathbf{\Phi}$ be the linear finite element approximation of the test function v. We substitute u_h^n and v_h in equation (2.4) and obtain the following finite dimensional variational inequality

(3.1)

$$\begin{aligned}
&b(\mathbf{u}^{n\top}\mathbf{\Phi}, (\mathbf{v}-\mathbf{u}^n)^\top\mathbf{\Phi}) \geq ((\mathbf{u}^{n-1} - \delta t\ \mathbf{1}_m)^\top\mathbf{\Phi}, (\mathbf{v}-\mathbf{u}^n)^\top\mathbf{\Phi}), \quad \forall \mathbf{v} \geq \mathbf{0},\\
\Rightarrow\ &(\mathbf{v}-\mathbf{u}^n)^\top b(\mathbf{\Phi},\mathbf{\Phi})\mathbf{u}^n \geq (\mathbf{v}-\mathbf{u}^n)^\top(\mathbf{\Phi},\mathbf{\Phi})(\mathbf{u}^{n-1} - \delta t\ \mathbf{1}_m), \quad \forall \mathbf{v} \geq \mathbf{0},\\
\Rightarrow\ &(\mathbf{v}-\mathbf{u}^n)^\top\mathbf{M}\mathbf{u}^n \geq (\mathbf{v}-\mathbf{u}^n)^\top\mathbf{B}(\mathbf{u}^{n-1} - \delta t\ \mathbf{1}_m), \quad \forall \mathbf{v} \geq \mathbf{0},\\
\Rightarrow\ &\left(\mathbf{v}-\mathbf{u}^n, \mathbf{M}\mathbf{u}^n - \mathbf{B}\mathbf{u}^{n-1} - \delta t\mathbf{B}\ \mathbf{1}_m\right) \geq \mathbf{0}, \quad \forall \mathbf{v} \geq \mathbf{0}.
\end{aligned}$$

where $\mathbf{0}$ and $\mathbf{1}_m$ are m-vectors with all entries 0 and 1 respectively. In equation (3.1), all inequalities have meaning element-wise. The coefficients matrix $\mathbf{M} \in \mathbb{R}^{m\times m}$ with entries $\mathbf{M}_{ij} = b(\varphi_j(x), \varphi_i(x))$ can be written as $\mathbf{M} = \mathbf{B} + \delta t\mathbf{A}$ where

$$\mathbf{B}_{ij} = (\varphi_j, \varphi_i) = \int_0^1 \varphi_j(x)\varphi_i(x)dx,$$

and

$$\mathbf{A}_{ij} = (\varphi_j', \varphi_i') = \int_0^1 \varphi_j'(x)\varphi_i'(x)dx.$$

Now according to [11, Theorem 2.3], the alst inequality in (3.1) is equivalent to the following linear complementary problem.

$$\text{(3.2)}\quad \text{Find } \mathbf{u}^n \in \mathbb{R}^m \text{ such that } \begin{cases} \mathbf{u}^n \geq \mathbf{0},\\ \mathbf{M}\mathbf{u}^n - \mathbf{B}\mathbf{u}^{n-1} - \delta t\mathbf{B}\mathbf{1}_m \geq \mathbf{0},\\ \mathbf{u}^{n\top}\left(\mathbf{M}\mathbf{u}^n - \mathbf{B}\mathbf{u}^{n-1} - \delta t\mathbf{B}\mathbf{1}_m\right) = \mathbf{0}. \end{cases}$$

The matrices $\mathbf{A}$ and $\mathbf{B}$ and therefore the coefficients matrix $\mathbf{M}$ are all positive definite and tridiagonal. On the other hand, we know that the positive definiteness of the matix $\mathbf{M}$ is the necessary and sufficient condition for existence and uniqueness of problem (3.2). Thus we have the following theorem.

Theorem 3.1. The linear complementary problem (3.2) for any $n \in \mathbb{N}$ has a unique solution.

4. **The active set strategy**

The standard linear complementary problem is proposed as follows:

Problem 4.1. (Linear complementarity problem in standard form) For a given matrix $\mathbf{M} \in \mathbb{R}^{m\times m}$ and a vector $\mathbf{b} \in \mathbb{R}^m$,

$$\text{(4.1)}\qquad \text{Find } \mathbf{x} \in \mathbb{R}^m \text{ such that } \begin{cases} \mathbf{x} \geq 0,\\ \mathbf{M}\mathbf{x} + \mathbf{b} \geq 0,\\ \mathbf{x}^\top(\mathbf{M}\mathbf{x} + \mathbf{b}) = 0, \end{cases}$$

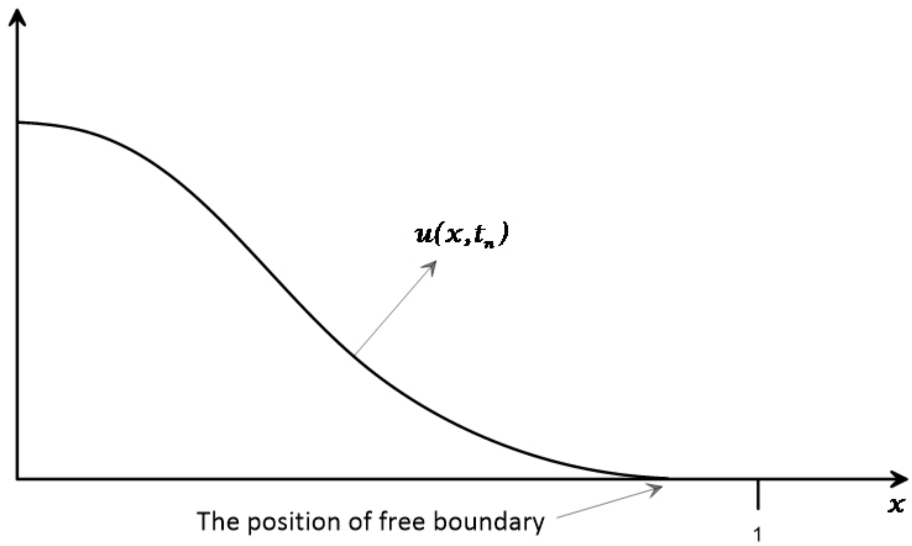

FIGURE 2. Solution $u(x,t)$ at time t_n. Before the position of free boundary, the solution u satisfies the equation $u_t - u_{xx} + 1 = 0$. After the position of free boundary, the solution coincides with x axes ($u(x,t)$ vanishes) and therefore we have $u_t - u_{xx} + 1 = 0 - 0 + 1 > 0$.

where the inequalities have meaning element-wise. Let $\mathbf{y} = \mathbf{M}\mathbf{x} + \mathbf{b}$, the third statement of (4.1) means that for each i, we have $\mathbf{x}_i \mathbf{y}_i = 0$ i.e. at least one of $\mathbf{x}_i, \mathbf{y}_i$ is zero. Given the index set $\mathcal{I} = \{1, 2, \dots, m\}$ we partition $\mathcal{I}$ into two sets

$$\mathcal{A} = \{\ i \mid i \in \mathcal{I} \text{ and } \mathbf{y_i} > 0\},$$

$$\mathcal{F} = \{\ i \mid i \in \mathcal{I} \text{ and } \mathbf{y_i} = 0\}.$$

We rewrite the system $\mathbf{y} = \mathbf{M}\mathbf{x} + \mathbf{b}$ as

$$\begin{bmatrix} \mathbf{y}_{\mathcal{A}} \\ \mathbf{y}_{\mathcal{F}} \end{bmatrix} = \begin{bmatrix} \mathbf{M}_{\mathcal{A}\mathcal{A}} & \mathbf{M}_{\mathcal{A}\mathcal{F}} \\ \mathbf{M}_{\mathcal{F}\mathcal{A}} & \mathbf{M}_{\mathcal{F}\mathcal{F}} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{\mathcal{A}} \\ \mathbf{x}_{\mathcal{F}} \end{bmatrix} + \begin{bmatrix} \mathbf{b}_{\mathcal{A}} \\ \mathbf{b}_{\mathcal{F}} \end{bmatrix}$$

but $\mathbf{y}_{\mathcal{A}} > 0$ implies that $\mathbf{x}_{\mathcal{A}} = 0$ so

$$\begin{bmatrix} \mathbf{y}_{\mathcal{A}} \\ 0 \end{bmatrix} = \begin{bmatrix} \mathbf{M}_{\mathcal{A}\mathcal{A}} & \mathbf{M}_{\mathcal{A}\mathcal{F}} \\ \mathbf{M}_{\mathcal{F}\mathcal{A}} & \mathbf{M}_{\mathcal{F}\mathcal{F}} \end{bmatrix} \begin{bmatrix} 0 \\ \mathbf{x}_{\mathcal{F}} \end{bmatrix} + \begin{bmatrix} \mathbf{b}_{\mathcal{A}} \\ \mathbf{b}_{\mathcal{F}} \end{bmatrix}$$

hence

$$\begin{bmatrix} \mathbf{y}_{\mathcal{A}} \\ 0 \end{bmatrix} = \begin{bmatrix} \mathbf{M}_{\mathcal{A}\mathcal{F}}\mathbf{x}_{\mathcal{F}} + \mathbf{b}_{\mathcal{A}} \\ \mathbf{M}_{\mathcal{F}\mathcal{F}}\mathbf{x}_{\mathcal{F}} + \mathbf{b}_{\mathcal{F}} \end{bmatrix}$$

the elements of solution $\mathbf{x}$ which are correspond to $\mathcal{F}$ are computed by

$$\mathbf{x}_{\mathcal{F}} = -\mathbf{M}_{\mathcal{F}\mathcal{F}}^{-1}\mathbf{b}_{\mathcal{F}}. \tag{4.2}$$

Algorithm 4.1. $\big($**The active set strategy**$\big)$
1. Choose a partition $\{\mathcal{A}, \mathcal{F}\}$ of the index set $\mathcal{I}$
2. Compute $\mathbf{x}_{\mathcal{F}} = -\mathbf{M}_{\mathcal{F}\mathcal{F}}^{-1}\mathbf{b}_{\mathcal{F}}$ and $\mathbf{y}_{\mathcal{A}} = \mathbf{M}_{\mathcal{A}\mathcal{F}}\mathbf{x}_{\mathcal{F}} + \mathbf{b}_{\mathcal{A}}$
3. If $\mathbf{x}_{\mathcal{F}} \geq 0, \mathbf{y}_{\mathcal{A}} \geq 0$ then $\begin{bmatrix} 0 \\ \mathbf{x}_{\mathcal{F}} \end{bmatrix}$ is a solution for (4.1) and stop the algorithm
else choose another partition of $\mathcal{I}$ and go to stage 2.

There are 2^m possible partitions for the index set $\mathcal{I}$. Computing $\mathbf{x}_{\mathcal{F}}$ from (4.2) needs $O(m^3)$ operation in the worst case (for full matrices), hence the complexity order of the active set strategy in the worst case is $O(2^m m^3)$. In the next sections, we develop a modification of the active set strategy with order of complexity $O(m)$ which can extremely speed up the computations.

4.1. **Modification of the active set strategy.** For oxygen diffusion problem, the unknown boundary of the problem, divides the computational domain into two partitions (see figure 2). Before the position of free boundary, the solution u satisfies in the equation $u_t - u_{xx} + 1 = 0$ and the equation $\mathbf{Mx} + \mathbf{b} = 0$ holds. In the right hand side of free boundary, we have the inequality $\mathbf{Mx} + \mathbf{b} > 0$. We define two index sets $\mathcal{A} = \{1, 2, \ldots i-1\}$ and $\mathcal{F} = \{i, i+2, \ldots, m\}$. We choose an initial guess for i then we compute $\mathbf{x}_{\mathcal{F}}$ form formula (4.2) and check the conditions in the third stage of algorithm 4.1. Since $\mathbf{M}$ is a tridiagonal matrix, we use the Thomas algorithm to compute $\mathbf{x}_{\mathcal{F}}$.

Algorithm 4.2. $\big($**Active set strategy for oxigen diffusion problem**$\big)$
1. Choose the partitions $\mathcal{A} = \{1, 2, \ldots i-1\}$ and $\mathcal{F} = \{i, i+1, \ldots, m\}$
2. Solve the system $\mathbf{M}_{\mathcal{F}\mathcal{F}}\mathbf{x}_{\mathcal{F}} = \mathbf{b}_{\mathcal{F}}$ by Thomas algorithm and compute $\mathbf{y}_{\mathcal{A}} = \mathbf{M}_{\mathcal{A}\mathcal{F}}\mathbf{x}_{\mathcal{F}} + \mathbf{b}_{\mathcal{A}}$
3. If $\mathbf{x}_{\mathcal{F}} \geq 0, \mathbf{y}_{\mathcal{A}} \geq 0$ then $\begin{bmatrix} 0 \\ \mathbf{x}_{\mathcal{F}} \end{bmatrix}$ is a solution for (4.1) and stop the algorithm
else set $i := i - 1$ and go to stage 2.

In the third stage of algorithm 4.2 when we decrease i, the dimension of matrix $\mathbf{M}_{\mathcal{F}\mathcal{F}}$ will be increased. If the initial guess of i would be chosen near the free boundary, after a few iterations the solution $\begin{bmatrix} 0 \\ \mathbf{x}_{\mathcal{F}} \end{bmatrix}$ will be found. Since the Thomas algorithm for tridiagonal matrices has the complexity of order $O(m)$, we can state the following theorem.

Theorem 4.2. The algorithm 4.2 to solve the LCP (4.1) only needs $O(m)$ operations.

5. **Numerical Experiments**

In this section, we solve the oxygen diffusion problem (1.1) numerically. We discretize the problem on the computational domain $[0, 1] \times [0, 0.2]$. We

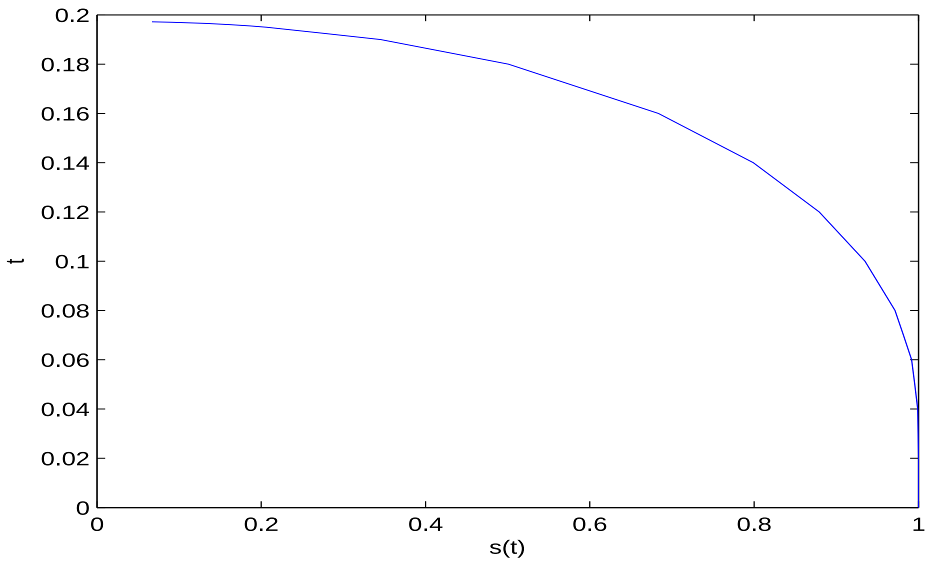

FIGURE 3. The approximation of $s(t)$ the position of unknown free boundary of problem (1.1).

use the time step size $\delta t = 0.01$ and the spatial step size $h = 0.05$ to discretize the computational domain (we set m=21,N=20). To solve the linear complementary problem, we apply the modified active set strategy described in algorithm 4.2. The approximate position of the free boundary $s(t)$ has been shown in fig. 3. Fig. 4 represents the solution $u(x,t)$ at grid points $(x_i, t_j)\big|_{i=1\ldots m, j=1,\ldots,N}$.

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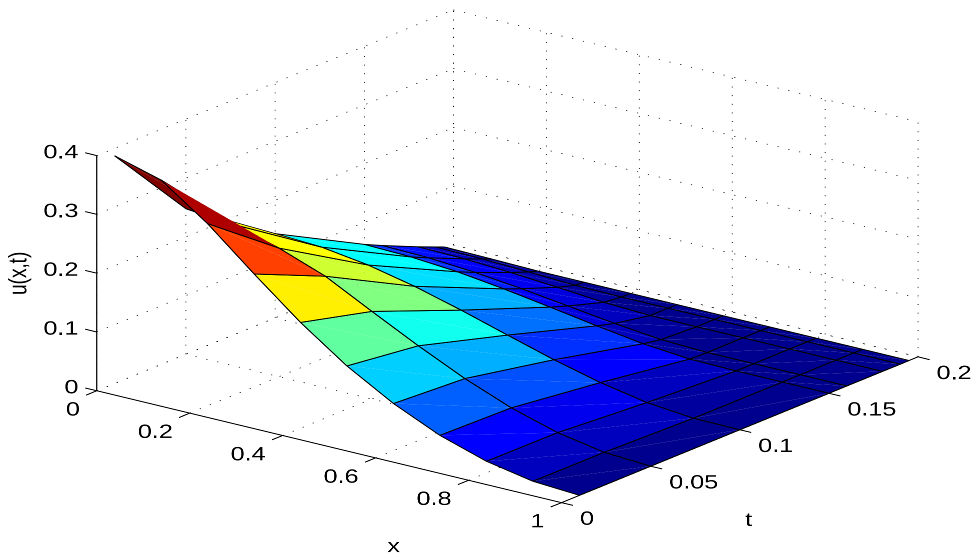

FIGURE 4. Approximation of $u(x,t)$, the solution of equation (1.1) on the computational domain $[0,1] \times [0,0.2]$

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(Mojtaba Moradipour) DEPARTMENT OF MATHEMATICS, LORESTAN UNIVERSITY, KHORRAMABAD, IRAN.

Email address: moradipour.mo@lu.ac.ir