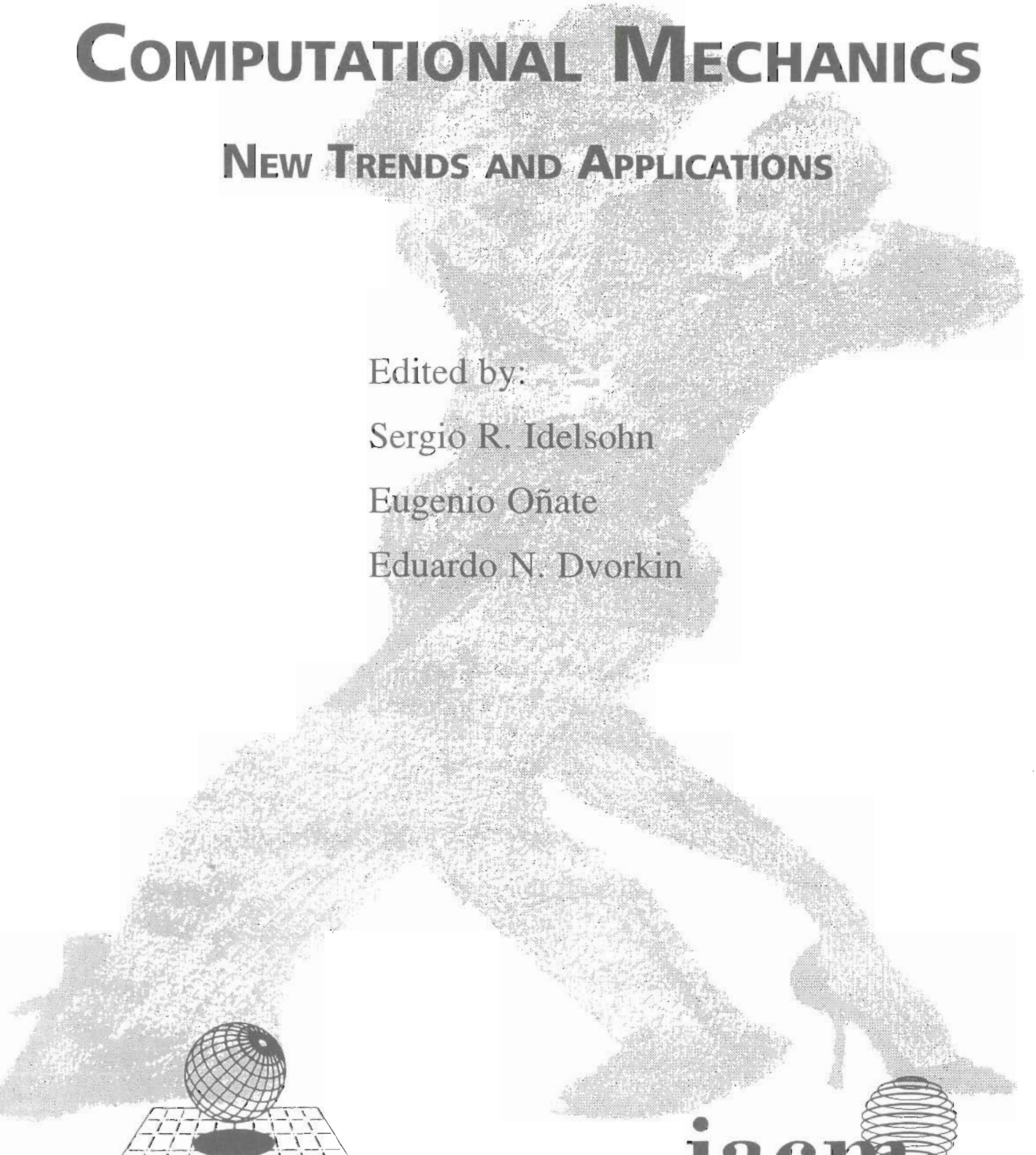
COMPUTATIONAL MECHANICS

NEW TRENDS AND APPLICATIONS

Sergio R. Idelsohn, Eugenio Oñate and Eduardo N. Dvorkin (Eds.)



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PREFACE

This CD ROM Proceedings contain the papers presented at the *Fourth World Congress on Computational Mechanics* (IV WCCM) held in the city of Buenos Aires (Argentina) on June 29-July 2, 1998. The first three congress in the series where held in Austin (1986), Stuttgart (1990) and Tokyo (1994). The 1998´Congress incorporated the XIX Ibero-Latin-American Conference on Computational Methods in Engineering (CILAMCE). This joint event was held under the auspices of the International Association for Computational Mechanics (IACM) and was jointly organized by the Argentinean Association for Computational Mechanics (AMCA) and the Spanish Association for Numerical Methods in Engineering (SEMNI).

The continuous importance of this research topic is demostrated by the fact that the number of papers has increased from 400 papers presented in the first congress to over 1000 papers in the Buenos Aires meeting.

The developments that have taken place in the different theoretical and engineering application fields of the broad area of Computational Mechanics are illustrated by the contents of these CD-ROM proceedings. The 700 papers included represent a Compendium of nearly 14.000 pages. The papers are clasified into the following main areas: (i) Mathematical Modelling and Numerical Methods, (ii) Solid and Structural Mechanics, (iii) Solid Materials Modeling, (IV) Fluid Mechanics (V) Heat Transfer and Fluid-Structure Interaction, (VI) Inverse Problems and Optimizations (VII) Software Development, Algorithms and Programming and (VIII) Applications Fields including problems in Biomechanics, Computational Physics, Electromagnetics, Environmental Sciences, Geomechanis, Forming Processes, Chemical Engineering, Robotics and Educational aspects of Computational Mechanics, among others.

The CD-ROM proceedings are printed directly from electronic versions of the manuscripts provided by the authors. The editors therefore can not accept responsability for any inaccuracies, comments or opinions contained in the papers.

Finally the editors wish to thank the authors for their participation and cooperation in making the IV WCCM a success.

S. Idelsohn, E. Oñate and E. Dvorkin,
Buenos Aires, June 1998

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NUMERICAL RESULTS FOR A ONE- PHASE SUPERCOOLED STEFAN PROBLEM WITH CONSTANT HEAT FLUX ON THE FIXED FACE

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Key words: Stefan problem, free boundary, supercooled liquid, finite difference. .

Abstract. *Generally the practice applications about phase-change problems (Stefan problem) haven't accurate solutions. Then it is neccesary to have numerical methods for their analysis. The goal of this paper is to compare some numerical methods to compute the interphase of a one-phase supercooled liquid with a constant heat flux on the fixed face and to determine when there exist a blow-up or an extinction time for the corresponding solution.*

1 INTRODUCTION

1.1 The general case of non-negative flux

Let us consider the following free boundary problem (P1): find a triple (T, s, z) such that

(i) $T > 0$;
(ii) $s(t)$ is a positive continuous function in $[0, T)$, $s \in C^1(0, T)$;
(iii) $z(x, t)$ is a bounded function, continuous in $0 \le x \le s(t)$, $0 \le t < T$, such that $z_x(x, t)$ is bounded in the same domain and continuous, with the possible exception of a finite number of points on the parabolic boundary, $z_{xx}(x, t)$ and $z_t(x, t)$ are continuous in $0 < x < s(t)$, $0 < t < T$;
(iv) the following conditions are satisfied:

$$z_{xx} - z_t = 0, \qquad D_T = \{(x,t): 0 < x < s(t),\ 0 < t < T\} \tag{1i}$$

$$z(x, 0) = 0, \qquad 0 < x < 1; \qquad s(0) = 1; \tag{1ii}$$

$$z_x(0, t) = g(t), \qquad 0 < t < T; \tag{1iii}$$

$$z(s(t), t) = 0, \qquad z_x(s(t), t) = -\dot{s}(t), \qquad 0 < t < T. \tag{1iv}$$

We are concerned with the case in which *g(t)* is a non negative piecewise continuous function in $(0, +\infty)$, bounded in every interval $(0, t)$, $t > 0$.

The problem (P1) with this hypothesis is called a *one-phase supercooled Stefan Problem* in one spatial dimension. It is well known that, with this hypothesis, the problem (P1) has a unique solution[2] and one of the following cases must occur[2, 3, 6]:

(A) the problem (P1) has a solution with arbitrarily large T;
(B) there exists a time $T_B > 0$ such that $\lim_{t \to T_B^-} s(t) = 0$;
(C) there exists a time $T_C > 0$ such that

$$\inf_{t \in (0, T_C)} s(t) > 0 \quad \text{and} \quad \liminf_{t \to T_C^-} \dot{s}(t) = -\infty .$$

Some simple properties of the solution of (P1) are summarized in the following Lemma[1] :

<u>Lemma 1</u>: (i) If (T_C, s, z) solves (P1) and $\liminf_{t \to T_C^-} \dot{s}(t) = -\infty$, $\lim_{t \to T_C^-} s(t) > 0$

then there exists a $t \le T_C$ such that $\int_0^t g(u)du \ge 1$.

(ii) If the case (C) occurs, then $\int_0^{T_C} g(t)dt > 1$.

(iii) If (T_B, s, z) solves (P1) and $\lim_{t \to T_B^-} s(t) = 0$, then $\int_0^{T_B} g(t)dt = 1$.

(iv) If there exists $T_0 > 0$ such that $\int_0^{T_0} g(t)dt = 1$ and $g(t) \le 1$, $0 < t < T_0$, then (B) occurs with $T_B = T_0$.

(v) The problem (P1) has a (unique) solution for arbitrarily large T if and only if

$$\int_0^{t} g(t)dt < 1 \quad \text{for any} \quad t > 0 .$$

1.2 The case with constant flux

We consider the case in which the flux $z_x(0, t)$ is constant in time, say $g(t) = K > 0$. As a trivial consequence of (v) of Lemma 1, no global solutions exist in this case, so that either (B) or (C) must occur. Moreover, for a given positive K, the solution exists for any $t < \frac{1}{K}$ and if $K \le 1$ then (B) must occur. The following lemma gives some sufficient conditions on K so that the solution is in case (B) or (C)[1, 4].

Lemma 2: (i) A $K_1 > 0$ exists such that $K > K_1$ implies (C) for the solution of (P1). The following estimate holds for K_1:

$$K_1 < 2.221297 .$$

(ii) Let $K_2 > 0$ be the solution of $K(1-\frac{8}{p^2}\exp(-\frac{p^2}{8}(1+\frac{1}{K^2}))) = 1$. Then $K \le K_2$ implies (B). An estimate for K_2 is $K_2 > 1.091465$.

The goal of this paper is to verify numerically the results given in Lemma 2 and also to investigate the behavior of the solution when the values for the constant heat flux K are in the interval (1.091465, 2.221297). From the numerical experiences, we can observe that the solution is in case (B).

2. NUMERICAL ANALYSIS

In order to approximate the solution z(x,t) of problem (P1) we use first an implicit method with variable space grid[5] and then an explicit method with variable time and space grid[5]. The number of space intervals between x = 0 and x = s(t) is kept constant and equal to N for all time. Thus $\Delta x = \frac{s(t)}{N}$ is different in each time step and the moving boundary is always on the N-th. grid line. The variable $U_{i,j}$ will approximate $z(x_i, t_j)$ where $x_i = i\Delta x$ and $t_j = j\Delta t$, while s_j will approximate $s(t_j)$.

2.1 Implicit Method

Using an implicit scheme, the equations of (P1) become:

$$U_{i,j} = (iq_j - r_j)U_{i-1,j+1} + (1+2r_j)U_{i,j+1} - (iq_j + r_j)U_{i+1,j} \quad i=1,..,N-1; \quad j=0,1,2,.... \tag{2i}$$

$$s_0 = 1, \tag{2ii}$$

$$U_{i,0} = 0, \quad i = 0,..,N, \tag{2iii}$$

$$U_{0,j+1} = U_{1,j+1} - K\Delta x_{j+1}, \quad j = 0, 1, 2,... \tag{2iv}$$

$$U_{N,j+1} = 0, \quad j = 0, 1, 2,... \tag{2v}$$

$$s_{j+1} = s_j + \frac{\Delta t}{\Delta x_j} U_{N-1,j}, \quad j = 0, 1, 2,... \tag{2vi}$$

where $r_j = \frac{\Delta t_j}{\Delta x_{j+1}^2}$ and $q_j = \frac{s_{j+1} - s_j}{2s_j + 1}$, j = 0, 1, 2,.....

2.2 Explicit Method

Using an explicit scheme, the equations of (P1) become:

$$U_{i,j+1} = (r_j - iq_j)U_{i-1,j} + (1-2r_j)U_{i,j} + (iq_j + r_j)U_{i+1,j} \quad i=1,..,N-1; \quad j=0,1,2,... \tag{3i}$$

$$s_0 = 1, \tag{3ii}$$

$$U_{i,0} = 0, \quad i = 0,..,N \tag{3iii}$$

$$U_{0,j+1} = U_{1,j+1} - K\Delta x_{j+1}, \qquad j = 0, 1, 2,... \quad (3iv)$$

$$U_{N,j+1} = 0, \qquad j=0, 1, 2,... \quad (3v)$$

$$s_{j+1} = s_j + \frac{\Delta t_j}{\Delta x_j} U_{N-1,j}, \qquad j = 0, 1,2.. \quad (3vi)$$

where $r_j = \dfrac{\Delta t_j}{\Delta x_j^2}$ and $q_j = \dfrac{s_{j+1} - s_j}{2 s_j}$, j = 0, 1, 2,....

3. NUMERICAL RESULTS

To obtain the numerical results we use the following algorithms:

Algorithm for the Implicit Method:
Step 0_ Give initial and boundary conditions for the temperature and the free boundary;
Step 1_ Compute s_1 using (2vi);
Step 2_ Compute $U_{i,1}$ solving the system (2i);
Step 3_ Compute $U_{0,1}$ using (2iv);
Step 4_ Evaluate ¿$s_1 \geq 0$? * NO, then STOP,

* YES, turn to Step 1.

Algorithm for the Explicit Method:
Step 0_ Give initial and boundary conditions for the temperature and the free boundary;
Step 1_ Compute s_1 using (3vi);
Step 2_ Compute $U_{i,1}$ using (3i);
Step 3_ Compute $U_{0,1}$ using (3iv);
Step 4_ Evaluate ¿$s_1 \geq 0$? * NO, then STOP,

* YES, turn to Step 1.

The language used to program the above algorithms was Turbo Pascal 7.0. Now we show the graphics obtained though the software Origin 3.0 for different values of the constant heat flux K. We have taken N = 10 and we have considered 4300 components for the discrete free boundary vector in the implicit scheme, and 32000 components in the explicit scheme.

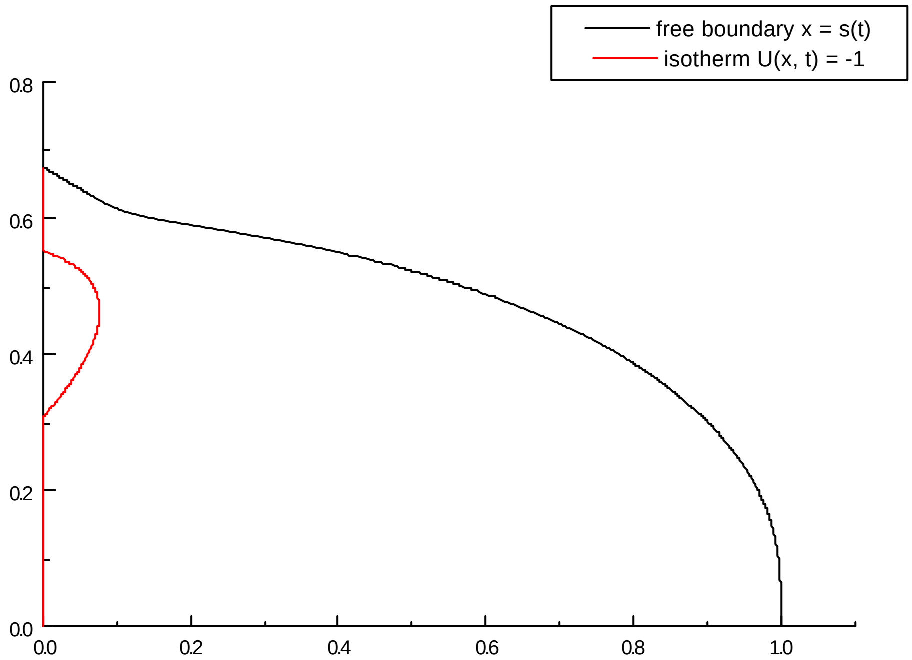

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Fig 1: Heat constant flux K= 1.5 with implicit method

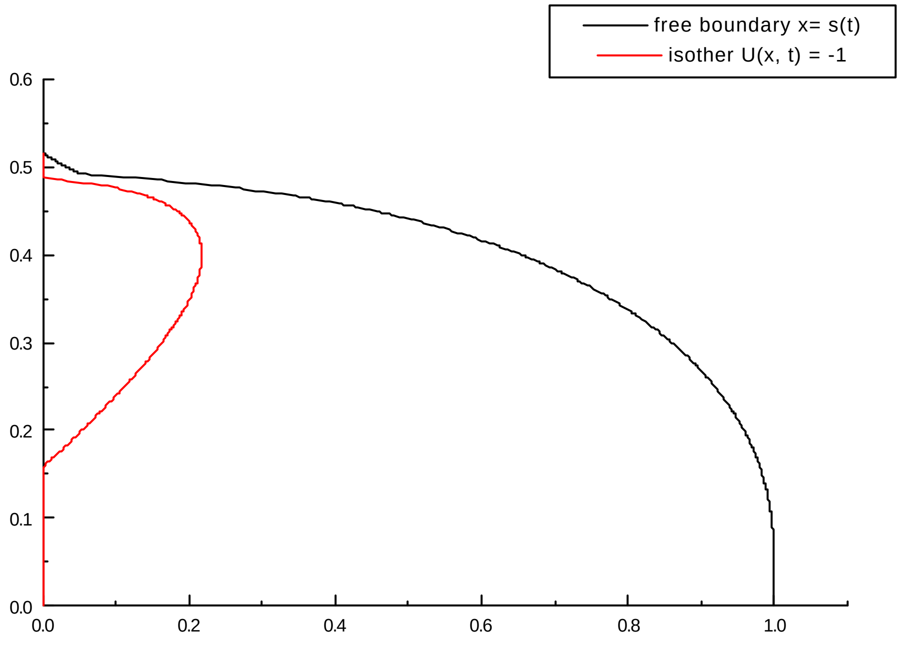

Fig 2: Heat constant flux K= 2.0 with implicit method

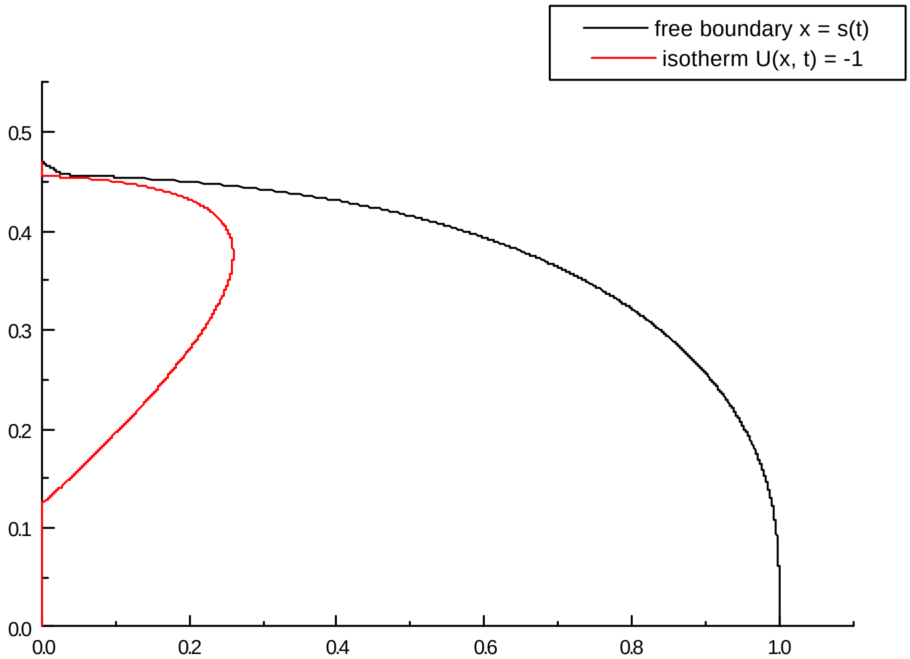

Fig 3: Heat constant flux K= 2.22 with implicit method.

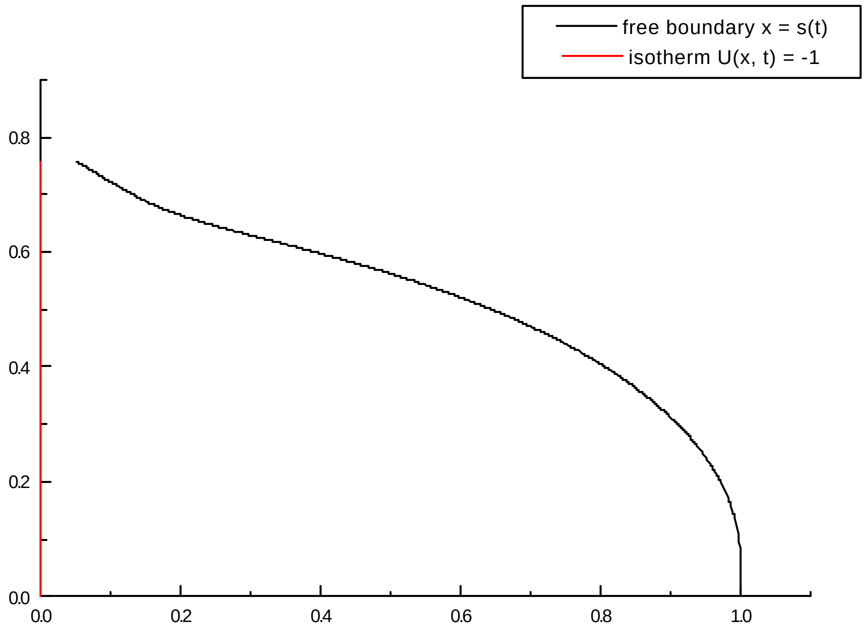

Fig 4: Heat constant flux K= 1.5 with explicit method.

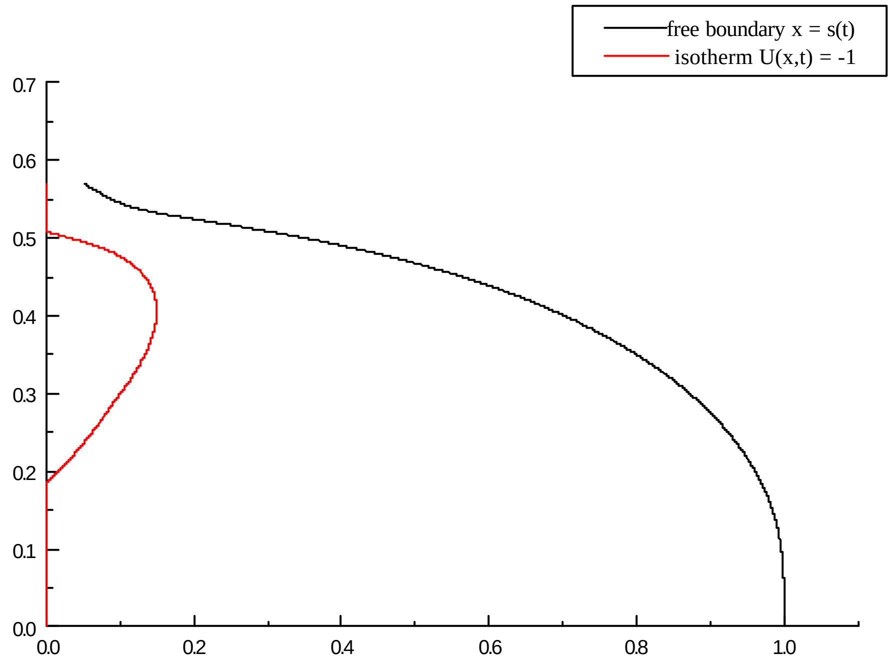

Fig 5: Constant heat flux K= 2.0 with explicit method.

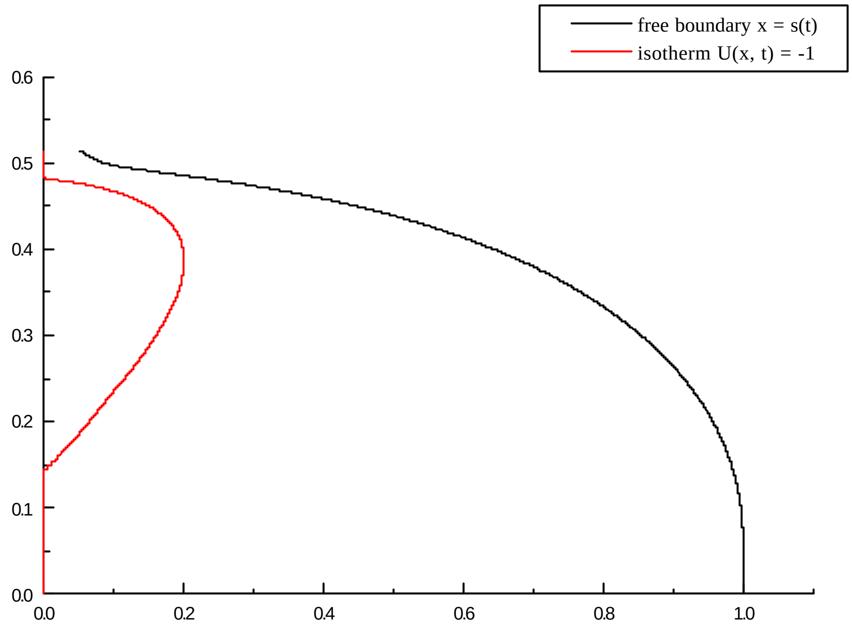

Fig 6: Heat constant flux K= 2.22 with explicit method.

Proposition 3: Taking into account the numerical results given by figures 1 to 6 we can state the following result:

$$K \leq 2.221297 \text{ implies case (B).}$$

Remark: We have also used an explicit and an implicit method with an inmovilized domain (through the substitution $y = \frac{x}{s(t)}$) which transforms the spatial domain (0, s(t)) into the fixed domain (0, 1). In this case we can use a constant Δx, and we have obtained similar results to that obtained through the above methods.

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