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# MAT

## SERIE A : CONFERENCIAS, SEMINARIOS Y TRABAJOS DE MATEMÁTICA

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#### VI SEMINARIO SOBRE PROBLEMAS DE FRONTERA LIBRE Y SUS APLICACIONES

#### Primera Parte

**Domingo A. Tarzia (Ed.)**

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**CONDITIONS TO OBTAIN A WAITING TIME FOR A  
DISCRETE TWO-PHASE STEFAN PROBLEM**

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**RESUMEN**

En este trabajo se considera un problema unidimensional de conducción de calor no-estacionario, con condiciones de borde mixtas. Con un esquema en diferencias finitas implícito se obtienen condiciones suficientes para asegurar que la solución será positiva en un paso de tiempo, si es positiva en el paso de tiempo anterior. También se deduce, empleando un esquema en diferencias finitas explícito, la expresión de la temperatura en cada paso de tiempo, como un polinomio en la variable  $\lambda = \alpha \frac{\Delta t}{\Delta x^2}$ , con coeficientes dados como una función de los datos del problema. Se pueden así establecer condiciones suficientes sobre los datos que aseguran la existencia de un tiempo de espera, a partir del cual comienza el cambio de fase.

**PALABRAS CLAVE**

Conducción del calor, Cambio de fase, Problema de Stefan, Análisis Numérico, Frontera Libre.

**ABSTRACT**

In this paper we consider a one-dimensional non-stationary heat conduction problem, with initial datum and with mixed boundary conditions. We obtain, with an implicit finite difference scheme, some sufficient conditions, so that the discrete solution is positive at any moment if it is positive at the previous time step. We also deduce, with an explicit finite difference scheme, the discrete expression of the temperature at each time step, as a polynomial in the variable  $\lambda = \alpha \frac{\Delta t}{\Delta x^2}$ , with coefficients given as function of the problem dates. So we can establish some sufficient conditions on the data in order to obtain the existence of a waiting time at wich a phase-change begins.

**KEYWORDS**

Heat Conduction, Phase-change, Stefan Problem, Numerical Analysis, Free-Boundary.

**AMS subject classification:** 65M06, 80A22

**1.- INTRODUCTION**

In this paper we consider a one-dimensional heat conduction problem in a finite (or semi-infinite) slab of a material that is initially in the liquid phase, at a temperature  $\theta_0(x)$  greater than the phase change temperature, having a heat flux  $q(t)$  on the left face  $x = 0$  and a temperature condition on the right face  $x = x_0$ .

We can state the problem through the following equations ( $0 < x_0 \leq +\infty$ ):

$$\rho c \frac{\partial \theta}{\partial t} - k \frac{\partial^2 \theta}{\partial x^2} = 0, \quad 0 < x < x_0, \quad t > 0, \quad (1.1)$$

$$\theta(x,0) = \theta_0(x) > 0, \quad 0 \leq x \leq x_0, \quad (1.2)$$

$$k \frac{\partial \theta}{\partial x}(0,t) = q(t) > 0, \quad t > 0, \quad (1.3)$$

$$\theta(x_0,t) = b(t), \quad t > 0, \quad (1.4)$$

The constants  $\rho$ ,  $c$  and  $k$  represent the mass density, the specific heat and the thermal conductivity respectively. For the case  $x_0 = +\infty$  we change the condition (1.4) by  $\theta(+\infty,t) = \theta_0(+\infty) > 0$ , for  $t > 0$ .

Without loss of generality we assume that the phase-change temperature of the material is  $0^\circ\text{C}$ . In accordance with the data  $\theta_0$ ,  $q$  and  $b$ , it can happen that [6]:

(a) the heat conduction problem is defined for all time  $t > 0$ .

(b) there exists a waiting time  $t^* < +\infty$  such that another phase (i.e. the solid phase) appears for  $t \geq t^*$  and then we have a two-phase Stefan problem. In this case, there exists a free boundary  $x = s(t)$ , which separates the liquid and solid phases, with  $s(t^*) = 0$ .

If the temperature on the right face  $x = x_0$  is a constant  $b(t) = b > 0$ , and the flux on the left face  $x = 0$  is  $q(t) = q > 0$ , also a constant, then the stationary solution is given by:

$$\theta_\infty(x) = \frac{q}{k} (x - x_0) + b.$$

In this case a necessary condition to obtain a stationary two-phase Stefan problem is given by [5]:

$$q > \frac{kb}{x_0}.$$

Taking into account that the solution of problem (1.1) – (1.4) with data  $b > 0$  and  $q > 0$  tends to  $\theta_\infty = \theta_\infty(x)$  when  $t$  goes to infinity [2], in [6] was considered the problem of finding the relation between the heat flux  $q > 0$  on  $x = 0$  and a time  $t_1$  such that another phase appears for  $t \geq t_1$ . The following results were obtained:

**Theorem 1:** [1]

*Suppose the initial temperature verifies the conditions  $b \geq \theta_0 \geq 0$  in  $[0, x_0]$  and  $\theta_0(x_0) = b$ . If we consider the  $t, q$  plane and we define the following set:*

$$Q = \left\{ (t, q) / q > f(t), t > 0 \right\},$$

where

$$f(t) = \frac{bk}{x_0 [1 - \exp(-\frac{\alpha \pi^2 t}{4x_0^2})]} , \alpha = \frac{k}{\rho c} \tag{1.5}$$

then we have a two-phase problem for all  $(t, q) \in Q$ .

The goal of this paper is to obtain a discrete expression for the inequation  $q > f(t)$ , obtained in the above theorem.

In section 2 we get some conditions on the data which guarantees the positivity of the discrete solution, i.e. no phase-change occurs.

In section 3, we express the discrete temperature at the face  $x = 0$  as a polynomial in the variable  $\lambda = \alpha \frac{\Delta t}{\Delta x^2}$  (with  $\Delta t$  the temporal step and  $\Delta x$  the spatial step) and we obtain an inequality for the heat flux  $q$ , as a function of data coefficients  $\theta_0$ ,  $k$  and  $\alpha$ . In other words, we can determine if there exists a waiting time from which the other phase, the solid phase, appears .

**2. AN APPROXIMATION WITH AN IMPLICIT FINITE DIFFERENCE METHOD**

We set up a mesh with step  $\Delta x = \frac{x_0}{N}$  ( $N$  is a natural number) for the spatial variable  $x$  and with step  $\Delta t$  for the temporal variable  $t$ . We note with  $U_i^j$  an approximate value of the temperature  $\theta$  at the point  $(x, t) = (i\Delta x, j\Delta t)$  for  $i = 0, 1, \dots, N$  and  $j = 1, 2, 3, \dots$ , that is  $U_i^j \approx \theta(x_i, t_j)$ .

We use an implicit finite difference schema, so we can state problem (1.1) – (1.4) in a matrix form :

$$\mathbf{A} \mathbf{U}^j = \mathbf{U}^{j-1} + \mathbf{c}^j \tag{2.1}$$

where  $\mathbf{A}$  is the following  $N-1$ -dimensional square matrix

$$\mathbf{A} = \begin{pmatrix} 1 + \lambda & -\lambda & 0 & : & : & 0 \\ -\lambda & 1 + 2\lambda & -\lambda & 0 & : & 0 \\ 0 & -\lambda & : & : & : & 0 \\ 0 & : & : & : & : & 0 \\ : & & & & : & -\lambda \\ 0 & 0 & 0 & : & -\lambda & 1 + 2\lambda \end{pmatrix} \tag{2.2}$$

$\lambda = \alpha \frac{\Delta t}{\Delta x^2}$  is a parameter,  $\mathbf{U}^j = (U_1^j, U_2^j, \dots, U_{N-1}^j)^t$  is a  $N-1$ -dimensional vector and  $\mathbf{c}^j$  is the  $N-1$ -dimensional vector

$$\mathbf{c}^j = ( -\lambda \frac{\Delta x}{k} q(t_j), 0, \dots, 0, \lambda b(t_j) )^t \tag{2.3}$$

This regressive finite difference schema is unconditionally stable and it converges to the solution of the continuous problem with a rate of convergence  $O(\Delta t + \Delta x^2)$  [3].

We are interested in the relationship between the data, so that if the discrete temperature  $U_i^j$  is positive ( $i = 0, 1, \dots, N$ ), then the discrete temperature  $U_i^{j+1}$  in the next time step is also positive.

We will see some definitions which will be useful in the sequel:

**Definition:**

- i) A matrix  $\mathbf{M} = (m_{ij})$  is said to be **positive** if all of its elements  $m_{ij}$  are non-negatives ( $m_{ij} \geq 0 \ \forall i, j$ ). In particular, a vector  $\mathbf{v} = (v_i)$  is said to be **positive** if  $v_i \geq 0, \forall i$ .
- ii) A square real matrix  $\mathbf{M}$  is said to be **monotone** if it is invertible and its inverse is positive.

Moreover (see [1]):

$$\mathbf{M} \text{ is monotone} \Leftrightarrow \{\mathbf{v} \in \mathbb{R}^n: \mathbf{M}\mathbf{v} \geq 0\} \subset \{\mathbf{v} \in \mathbb{R}^n: \mathbf{v} \geq 0\} \quad (2.4)$$

Taking into account the above equivalence, we can prove the following properties [4]:

**Theorem 2:**

- i) The matrix  $\mathbf{A}$ , defined in (2.2), is monotone.
- ii) The inverse matrix  $\mathbf{A}^{-1}$  is positive.

**Theorem 3:**

Let  $q$ ,  $\theta_0$  and  $b$  be positive constants ( $\theta_0 = b, \mathbf{c}^j = \mathbf{c}, \forall j$ ) and  $\mathbf{U}^j = (U_1^j, U_2^j, \dots, U_{N-1}^j)^t$  which satisfies the schema (2.1) for  $j = 1, 2, \dots$ . Then, if at the time  $t_j = j\Delta t$ ,  $\mathbf{U}^j$  is positive and the inequality

$$q < \frac{\rho c U_1^j \Delta x}{\Delta t} \quad j = 1, 2, \dots \quad (2.5)$$

holds, then  $\mathbf{U}^{j+1}$  is also positive.

**3. SOME CONDITIONS TO OBTAIN A WAITING TIME FOR THE DISCRETE PROBLEM**

If we use an explicit finite difference schema we get that the discrete temperature  $U_i^j$  which approximates  $\theta(x_i, t_j)$  satisfies:

$$U_i^j = U_i^{j-1} + \lambda(U_{i+1}^{j-1} - 2U_i^{j-1} + U_{i-1}^{j-1}) \quad i = 1, \dots, N-1, j = 1, 2, 3, \dots \quad (3.1)$$

$$U_i^0 = \theta_0(x_i) \quad i = 0, 1, \dots, N \quad (3.2)$$

$$U_0^j = U_1^j - \frac{\Delta x}{k} q(t_j) \quad j = 1, 2, 3, \dots \quad (3.3)$$

$$U_N^j = b(t_j) \quad j = 1, 2, 3, \dots \quad (3.4)$$

This method is not as efficient as that consider in the above section, because it is conditionally stable and it converges to the solution of problem (1.1) – (1.4) with a convergence rate  $O(\Delta t + \Delta x^2)$  only if [3]:

$$\lambda \leq \frac{1}{2} \tag{3.5}$$

Nevertheless we use here this method, because in this way it is possible to obtain an explicit expression for the discrete temperature at the left face  $x = 0$  for all time step  $j\Delta t$ , as a function of the initial and the boundary dates. So we can establish sufficient conditions in order to obtain a waiting time in the discrete problem. We have [4]:

**Theorem 4:**

*If the data  $b, q$  and  $\theta_0$  are constants,  $b = \theta_0$  and (3.5) holds, then, when we consider the scheme (3.1) – (3.4), the values  $U_i^m$  of the discrete temperature obtained, verify the following properties:*

i)  $U_i^m \leq U_{i+1}^m \quad i = 1, \dots, N-1, m = 0, 1, 2, 3, \dots \tag{3.6}$

ii)  $U_i^m \geq U_i^{m+1} \quad i = 1, \dots, N, m = 0, 1, 2, 3, \dots \tag{3.7}$

As a consequence of the above theorem, in order to determine the moment from which the solid phase appears in the discrete problem, it suffices to find the value of  $j$  such that  $U_0^j < 0$ .

In the following theorem, we express the discrete temperature as a polynomial in the variable  $\lambda$  [4]:

**Theorem 5:**

*Under the hypothesis of Theorem 4 it results*

$$U_i^1 = \theta_0 \quad i = 1, 2, \dots, N - 1 \tag{3.8}$$

$$U_i^j = \theta_0 - q \frac{\Delta x}{k} P_i^j(\lambda) \quad i = 1, 2, \dots, j - 1 \quad j = 2, 3, \dots \tag{3.9}$$

$$U_i^j = \theta_0 \quad i = j, j + 1, \dots, N-1 \quad j = 2, 3, \dots \tag{3.10}$$

where

$$P_i^j(x) = \sum_{m=i}^{j-1} a_m(i,j) x^m \quad \text{and} \quad a_m(i,j) = (-1)^{m+i} b_m c_{im} d_{jm} \tag{3.11}$$

with

$$b_1 = 1 \quad b_m = \frac{(2m-3)!! 2^{m-1}}{m} \quad m = 2, 3, \dots$$

$$c_{im} = \frac{(2i-1)}{(m-i)! (m+(i-1))!} \quad m = i, i + 1, \dots, j - 1 \tag{3.12}$$

$$d_{jm} = \frac{(j-1)!}{(j-(m+1))!} \quad m = i, i + 1, \dots, j - 1$$

**Theorem 6:**

*Under the hypothesis of Theorem 4 it results*

$$U_{\circ}^j = \theta_{\circ} - q \frac{\Delta x}{k} P_{\circ}^j(\lambda) \quad j = 1, 2, \dots \quad (3.13)$$

where the polynomial  $P_{\circ}^j$  is given by:

$$P_{\circ}^j(x) = \sum_{m=0}^{j-1} a_m(j) x^m \quad (3.14)$$

with  $a_0(j) = 1$   $a_1(j) = j - 1$  (3.15)

$$a_m(j) = \frac{(-1)^{m+1} 2^{m-1} (2m-3)!! (j-1)!}{(m!)^2 (j-(m+1))!} \quad m = 2, \dots, j-1$$

**Corollary 7:**

If  $q > \frac{\theta_{\circ} k}{\Delta x P_{\circ}^j(\lambda)}$  then there exists a waiting time  $t_j = j\Delta t$  such that the problem (3.1) – (3.4) is a two-phase problem for all  $t > t_j$ .

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