

NUMERICAL SCHEME FOR THE ONE-PHASE 1D STEFAN PROBLEM USING CURVILINEAR COORDINATES

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Abstract. In this paper we present a new approach to solving a one-dimensional, one-phase Stefan problem. The proposed method is based on choosing (a) suitable curvilinear space coordinate/s for the heat-flow equation and the finite difference method. In the final part of this paper, examples of numerical calculations are shown.

Introduction

Moving boundary problems in which the boundary of the domain is not known occur in subjects such as heat flow, hydrology, solute transport or molecular diffusion. Moving boundaries are associated with time dependent problems and the position of the boundary has to be determined as a function of time. Moving boundary problems are often called Stefan problems, with reference to the work of J. Stefan, who investigated the melting of the polar ice cap [1-3].

In the literature there are many well-known methods for solving the Stefan problem. One of them, proposed by Schniewind, is based on the concept that moving boundary moves "from node to node" [4, 5]. A similar approach, where the moving boundary always moves from one grid point to another, was applied by Douglas and Gallie in [6]. These are the methods with variable time step. Murray and Landis suggested a different approach [7]. Their method uses a variable space grid with constant number of space intervals between fixed and moving boundary. Another front-tracking method was proposed by Crank [8]. In his method, the moving boundary will usually be located between two neighbouring grid points. The solution is determined by using a modified finite-difference method which incorporates unequal space intervals near moving boundary. One of the most popular methods of solving moving boundary problems is fixing the moving boundary at the same grid point or line for all time by a suitable coordinate transformation [2, 8].

Our aim is to construct a numerical scheme which allows the use of a constant both the time and the space steps. In this approach we expect the boundary to move along a straight line.

The paper is organized as follows. In the first section we formulate one-dimensional, one-phase Stefan problem in curvilinear coordinates. Numerical scheme

is given in Section 2. Then, two examples of the simulations are presented in Section 3.

1. Mathematical formulation of the problem

Consider a simple version of the Stefan problem describing melting of a semi-infinite sheet:

$$c\rho \frac{\partial u(x,t)}{\partial t} = K \frac{\partial^2 u(x,t)}{\partial x^2}, \quad 0 < x < s(t), \quad t > 0 \quad (1)$$

with initial-boundary conditions

$$u(0,t) = u_0, \quad u(s(t),t) = u_B, \quad t > 0, \quad (2)$$

$$u(0,0) = u_B.$$

and with Stefan condition

$$L\rho \frac{ds(t)}{dt} = -K \frac{\partial u(x,t)}{\partial x} \Big|_{x=s(t)}, \quad s(0) = 0, \quad (3)$$

where K is conductivity, u is temperature, ρ is density, c is specific heat and L is the latent heat required to melt the given material. Assuming constant thermal values and using a simple scaling:

$$X = \frac{x}{l}, \quad \tau = t \frac{K}{c\rho l^2}, \quad U = \frac{u}{u_0}, \quad S = \frac{s}{l} \quad (4)$$

we can formulate the above Stefan problem in non-dimensional variables for finite sheet $0 \leq x \leq l$, where l is some standard length and $\Lambda = cu_0/L$ is dimensionless Stefan number:

$$\frac{\partial U(X,\tau)}{\partial \tau} = \frac{\partial^2 U(X,\tau)}{\partial X^2}, \quad 0 < X < S(\tau) \quad (5)$$

$$U(0,\tau) = 1, \quad U(S(\tau),\tau) = U_B, \quad \tau > 0. \quad (6)$$

$$U(0,0) = U_B$$

$$\frac{dS(\tau)}{d\tau} = -\Lambda \frac{\partial U(X,\tau)}{\partial X} \Big|_{X=S(\tau)}, \quad S(0) = 0. \quad (7)$$

The analytical solution obtained by Neumann [2, 3] for the one-dimensional Stefan problem shows that the liquid/solid interface grows as the square root of

time, namely $S(\tau) \sim \sqrt{\tau}$. By introducing space coordinates $\xi = X^2$ to the system (5)-(7) we obtain relation $S(\tau) \sim \tau$. Using standard operations we transform system (5)-(7) for function $U(X, \tau)$ into the following system for $U(\xi, \tau)$

$$\frac{\partial U(\xi, \tau)}{\partial \tau} = 4\xi \frac{\partial^2}{\partial \xi^2} U(\xi, \tau) + 2 \frac{\partial U(\xi, \tau)}{\partial \xi}, \quad 0 < \xi < S(\tau) \quad (8)$$

$$U(0, \tau) = 1, \quad U(S(\tau), \tau) = U_B, \quad \tau > 0 \quad (9)$$

$$U(0, 0) = U_B$$

$$p = \frac{dS(\tau)}{d\tau} = -4\xi\Lambda \frac{\partial U(\xi, \tau)}{\partial \xi} \Big|_{\xi=S(\tau)=p\tau}, \quad S(0) = 0 \quad (10)$$

where the boundary now moves along a straight line $S(\tau) = p\tau$.

2. Numerical scheme

Now we present a numerical scheme for the system (8)-(10). By $U_{i,j}$ we denote the values of temperature in grid points $(i\Delta\xi, j\Delta\tau)$, where $i := 0, 1, \dots, j$; $j := 0, 1, \dots, n$, $\Delta\xi = 1/n$ with an integer n . To calculate the time step $\Delta\tau$ we use formula:

$$\Delta\tau = (np)^{-1} \quad (11)$$

where parameter p is determined by solving the following transcendental equation:

$$\frac{\Lambda}{\sqrt{\pi}} \left(1 - \frac{u_B}{u_0} \right) = \frac{\sqrt{p}}{2} \exp\left(\frac{p}{4}\right) \operatorname{erf}\left(\frac{\sqrt{p}}{2}\right). \quad (12)$$

To approximate derivatives from formula (8) we use the difference quotients and transform the equation (8) to the following discrete form

$$\frac{U_{i,j} - U_{i,j-1}}{\Delta\tau} = 4i\Delta\xi \frac{U_{i-1,j} - 2U_{i,j} + U_{i+1,j}}{\Delta\xi^2} + 2 \frac{U_{i+1,j} - U_{i,j}}{\Delta\xi}. \quad (13)$$

For $j = 2$ and $i = 1$, value of function U_{12} is determined from formula

$$U_{12} = \frac{4rU_{02} + 6rU_{22} + U_{11}}{1 + 10r}, \quad (14)$$

where parameter $r = \Delta\tau / \Delta\xi = 1/p$.

When $j > 2$ then system of equations (13) can be written in the matrix form

$$\mathbf{A} \cdot \mathbf{U} = \mathbf{B}, \quad (15)$$

where

$$\mathbf{A} = \begin{bmatrix} 10r+1 & -6r & 0 & 0 & \dots & 0 \\ -8r & 18r+1 & -10r & 0 & \dots & 0 \\ 0 & -12r & 26r+1 & -14r & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 & -4(j-1)r & (8(j-1)+2)r+1 \end{bmatrix} \quad (16)$$

$$\mathbf{U} = \begin{bmatrix} U_{1,j} \\ U_{2,j} \\ U_{3,j} \\ \dots \\ U_{j-1,j} \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} U_{1,j-1} + 4rU_0 \\ U_{2,j-1} \\ U_{3,j-1} \\ \dots \\ U_{j-1,j-1} + (4(j-1)+2)rU_B \end{bmatrix}. \quad (17)$$

3. Numerical examples

In this section, two examples of melting processes of ice and aluminum are considered. We apply the numerical scheme formulated above, perform calculations in curvilinear coordinates (ζ, τ) and then convert the results to standard Cartesian coordinates (x, t) .

Example 3.1. In the calculations we assume the following values of parameters for the melting process of ice: $u_B = 273.15$ K, $u_0 = 298.15$ K, $l = 0.1$ m, $c = 4189.9$ J/(kg K), $L = 333400$ J/kg, $\rho = 1000$ kg/m³, $K = 0.5664$ W/(m K). The calculation results are presented in graphs in Figures 1 and 2.

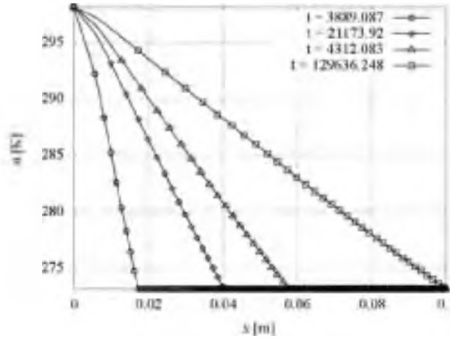


Fig. 1. The calculated temperature distribution in liquid region for Example 3.1 and $n = 300$

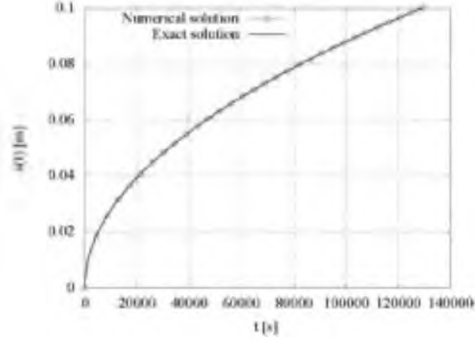


Fig. 2. The comparison of numerical results with the exact solution for Example 3.1 and $n = 300$

Example 3.2. In the second example the melting process of aluminum is considered. The simulation assumes the following values of parameters: $u_B = 931$ K, $u_0 = 1073$ K, $l = 0.1$ m, $c = 1130.44$ J/(kg K), $L = 396000$ J/kg, $\rho = 2380$ kg/m³, $K = 215$ W/(m K). The calculation results are presented in graphs in Figures 3 and 4.

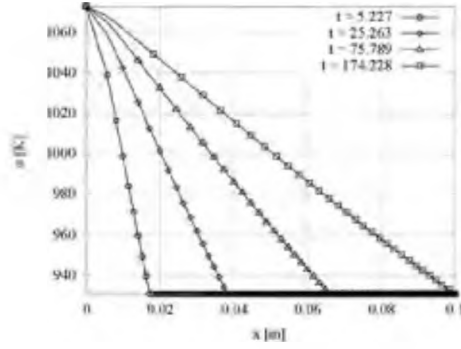


Fig. 3. The calculated temperature distribution in liquid region for Example 3.2 and $n = 300$

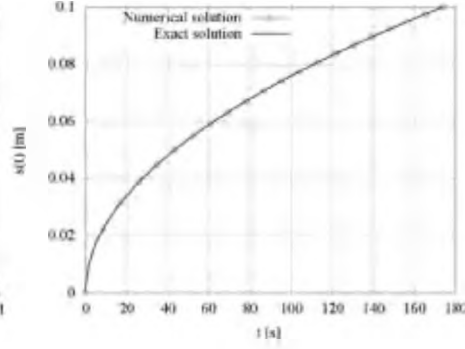


Fig. 4. The comparison of numerical results with the exact solution for Example 3.2 and $n = 300$

Conclusions

In this paper we presented a new approach to solve the one-phase 1D Stefan problem. The introduced method is based on the finite difference method for the heat-flow equation in new space coordinates. This approach allows us to use a rectangular grid with the constant time and space steps. We compared numerical results obtained for 300 steps with the exact solution and received average relative error: 0.126% for Example 3.1 and 0.207% for Example 3.2 respectively.

Let us note that classical moving boundary problems were extensively studied in literature (compare [1-10] and the references given therein). Most of these problems can only be solved using numerical methods. The motivation of the proposed approach is its further application to fractional versions of the Stefan problem [11-14]. In the literature certain exact solutions to some simple cases of this problem were developed. However, in principle, they depend on parameters hidden in complicated function equations which are very difficult to solve. Similar to the standard theory of heat or solute transfer, the general fractional moving boundary problems could be solved only using numerical approach. However, the standard numerical schemes developed for classical Stefan problems are not effective in the case of models including fractional derivatives which are non-local operators. The constructed numerical scheme simplifies the grid and seems more suitable to model complicated non-local operators appearing in fractional moving

boundary problems. The extension and application of the proposed method to the fractional case will be the subject of our further investigations.

Acknowledgments

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