A NOVEL ALGORITHM FOR SOLVING THE CLASSICAL STEFAN PROBLEM

by

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A novel algorithm for solving the classic Stefan problem is proposed in the paper. Instead of front tracking, we preset the moving interface locations and use these location coordinates as the grid points to find out the arrival time of moving interface respectively. Through this approach, the difficulty in mesh generation can be avoided completely. The simulation shows the numerical result is well coincident with the exact solution, implying the new approach performes well in solving this problem.

Key words: *Stefan problem, moving interface, finite difference method, numerical simulation*

Introduction

Classical Stefan problems involving melting or solidification, and generally referred to as ‘phase-change’ or ‘moving-boundary’ problem are important in many engineering applications [1-12], *i. e.*, in the freezing of food, the solidification or the melting of metals in the casting. Since the solid-liquid interface is time-dependent and must be determined as a part of the solution, the problems are highly nonlinear and become complicated. Therefore, these problems in the most cases are required to be solved numerically.

In the last decades various numerical techniques have been developed to solve moving boundary problem. In these methods the unknown interface position is mostly taken as part of the solution, to cause the difficulty in mesh generation to the numerical process. In the paper by presetting the positions where the moving interface will reach at different time and using these position coordinates as the grid nodes, we calculate the arrival time of the moving interface respectively. Through this approach, the difficulty in the mesh generation can be avoided completely. The algorithm is also very straightforward and efficient for its finite difference formulation.

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Governing equations and numerical scheme

Melting in a half-space (one-region problem) will be used as an example to demonstrate the numerical scheme.

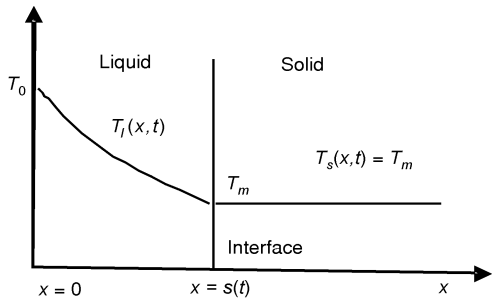

Figure 1. The melting in a half-space (one-region problem)

A solid at the solidification temperature T_m is confined to a half-space $x > 0$. At time $t = 0$, the temperature of the boundary surface at $x = 0$ is raised to T_0 which is higher than T_m and maintained at that temperature for times $t > 0$. As a result melting starts at the surface $x = 0$ and the solid-liquid interface moves in the positive x-direction. Figure 1 shows the coordinates and the temperature profiles. The solid phase is assumed to be at a constant temperature T_m throughout, the temperature is unknown only in the liquid phase and then the problem becomes a one-region problem. At time $t > 0$ the task is to calculate the temperature distribution in the liquid phase and to obtain the location of the moving interface.

The mathematical formulation for this problem is given as:

$$\frac{\partial^2 T_l}{\partial x^2} = \frac{1}{a_l}\frac{\partial T_l}{\partial t} \quad \text{in} \quad 0 < x < s(t),\ t > 0 \tag{1}$$

$$T_l(x,t) = T_0 \quad \text{at} \quad x = 0,\ t > 0 \tag{2}$$

and for the interface as

$$T_l(x,t) = T_m \quad \text{at} \quad x = s(t),\ \ t > 0 \tag{3}$$

$$-k_l \frac{\partial T_l}{\partial x} = \rho r \frac{ds}{dt} \quad \text{at} \quad x = s(t),\ \ t > 0 \tag{4}$$

where T_l is the temperature of liquid phase, k_l and a_l are thermal conductivity and diffusivity of liquid respectively, ρ is the density at solid-liquid interface, and r is the latent heat.

Suppose the positions where the moving interface will reach at different times are known and are at equally spaced intervals (or non-uniform spaced intervals). As shown in figs. 2-4, these positions are denoted by s_2, s_3, … , s_{n+1}, corresponding to the arrival time $t_1 = = \Delta t_1$, $t_2 = \Delta t_2$, … , $t_n = \Delta t_n$, but the arrival times are unknown, *i. e.*, time variables t_1, t_2, …, t_n, are to be determined. Then, these position coordinates will be used as the mesh grids. Let $s_1 = = x_1 = 0$, $x_i = s_i$ and $\Delta x = x_i - x_{i-1} = s_i - s_{i-1}$ ($i = 2, 3, 4 \ldots n$) denote space step.

For one-region problem, we just need to add the position of moving interface at different time, step by step on the melting side at an equal space interval, and use these position coordinates as the mesh grids to calculate the arrival time respectively. The numerical procedure for several of time steps is illustrated as below:

(1) Determination of time step t_1

In the paper throughout, forward or backward difference formulation and central difference formulation are used for the first and second-order derivatives, respectively.

As shown in fig. 2, star mark denotes the position where the moving interface reaches at time step t_1. The finite difference form of eq. (4) is:

$$-k_l \frac{T_2^1 - T_1^1}{\Delta x} = \rho r \frac{\Delta x}{t_1} \qquad (5)$$

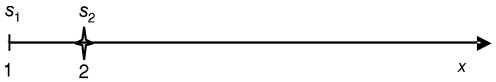

Figure 2. The mesh sketch to determine time step t_1

Here $\Delta x = s_2 - s_1$. The superscript and subscript denote the time step and grid numbers, respectively. We note that $T_1^1 = T_0$ and $T_2^1 = T_m$ are known, so the temperatures of the nodes on the melting side are already known. Introducing $\Omega_l = \rho r \Delta x^2 / k_l$ and solving eq. (5) we have:

$$t_1 = \frac{\Omega_l}{T_0 - T_m} \qquad (6)$$

(2) Determination of time step t_2

Taking similar steps above, the discrete form for eq. (4) is (see fig. 3):

$$T_2^2 = T_m + \frac{\Omega_l}{t_2} \qquad (7)$$

Since $T_1^2 = T_0$ and $T_3^2 = T_m$ are known, so only the temperature of node 2 is to be determined

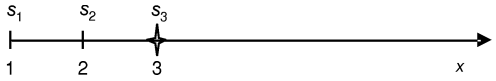

Figure 3. The mesh sketch to determine time step t_2

The discrete form of eq. (1) at node 2 is:

$$\frac{T_2^2 - T_2^1}{t_2} = a_l \left(\frac{T_1^2 - 2T_2^2 + T_3^2}{\Delta x^2} \right) = a_l \left(\frac{T_0 - 2T_2^2 + T_m}{\Delta x^2} \right)$$

It can be rewritten as:

$$(2 + R_l / t_2) T_2^2 = (T_m + T_0) + R_l T_2^1 / t_2$$

where $R_l = \Delta x^2 / a_l$, then we have the following equations:

$$T_2^2 = T_m + \Omega_l / t_2 \qquad (8)$$

$$(2 + R_l / t_2) T_2^2 = (T_m + T_0) + R_l T_2^1 / t_2 \qquad (9)$$

Eqs. (8-9) are nonlinear. The algorithm for solving above equations will be discussed later.

(3) Determination of time step t_k

Similarly, the following equations can be obtained (see fig. 4):

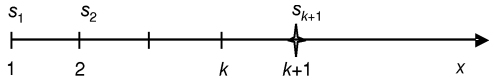

Figure 4. The mesh sketch to determine time step t_k

$$T_k^k = T_m + \frac{\Omega_l}{t_k} \tag{10}$$

$$\mathrm{C} \quad \mathrm{T} = \mathrm{D} \tag{11}$$

where

$$\mathrm{C} = \begin{bmatrix} (2+R_l/t_k) & -1 & 0 & & \\ -1 & (2+R_l/t_k) & -1 & 0 & \\ \multicolumn{5}{c}{\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots} \\ & -1 & (2+R_l/t_k) & -1 & 0 \\ & & -1 & (2+R_l/t_k) & \end{bmatrix}, \quad \mathrm{T} = \begin{bmatrix} T_2^k \\ T_3^k \\ \ldots\ldots \\ T_{k-1}^k \\ T_k^k \end{bmatrix}, \quad \mathrm{D} = \begin{bmatrix} T_0 + R_l T_2^{k-1}/t_k \\ R_l T_3^{k-1}/t_k \\ \ldots\ldots\ldots\ldots \\ .R_l T_{k-1}^{k-1}/t_k \\ T_m \ + \ R_l T_k^{k-1}/t_k \end{bmatrix}$$

It should be noted that the matrix in eq. (11) is a tridiagonal matrix, which is characterized by predominantly main diagonal elements, so eq. (11) can be readily solved.

The solution procedure involves

(1) Using a guessing value t_k^* to calculate the matrix [D] and [C], respectively.

(2) Solving eq. (11) with Thomas algorithm to obtain the node temperatures.

(3) Taking eq. (10) as the convergence criterion:

$$\mathrm{Ref} = \left| T_k^k - T_m - \Omega_l / t_k^* \right| \le \varepsilon \tag{12}$$

(4) If eq. (12) is not satisfied, a new t_k^* is assumed again. Repeat the above steps until convergence is reached. In the paper the dichotomizing search technique is used to obtain the ultimate value t_k.

The example of melting process of aluminum is considered. The melting temperature of aluminum is T_m = 931 K. $\Delta x = \Delta s = 0.005$ m and T_0 = 1073 K are used and the other physical parameters are given as follow [13]: $r = 396 \cdot 10^3$ J/kg, ρ_l = 2380 kg/m^3, k_l = = 215 Wm/K, c_l = 1130.44 Jkg/K. The convergence criterion is $\varepsilon = 1 \cdot 10^{-3}$.

According to the exact solution of half-space (one-region problem) [14], the location of the moving interface is given by:

$$s(t) = 2\lambda\sqrt{a_l t} \tag{13}$$

where the parameter λ is determined by the following transcendental equation:

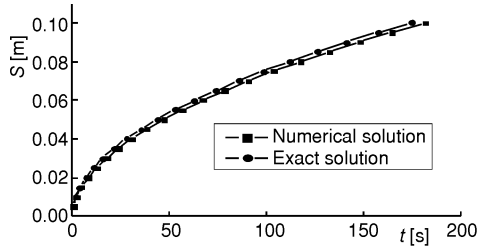

Figure 5. The comparison of numerical results with the exact solution

$$\lambda \exp(\lambda^2)\mathrm{erf}(\lambda) = \frac{c_l (T_0 - T_m)}{r\sqrt{\pi}} \tag{14}$$

Through solving eq. (14), we can obtain λ = = 0.4237. To further indentify the model performance, the comparison of the numerical results with the exact ones is shown in fig. 5.

From the fig. 5, it can be found that the numerical result is well coincident with the exact solution, implying the new approach

performed well in solving this problem. The absolute error and relative error of the numerical result in 20 time steps is 7.35 seconds and 4.22%, respectively (elapsed time is 174.2 seconds).

The temperature distribution is shown in fig. 6. Due to the high thermal conductivity of aluminum, the temperature distribution in liquid region is almost in linear profile.

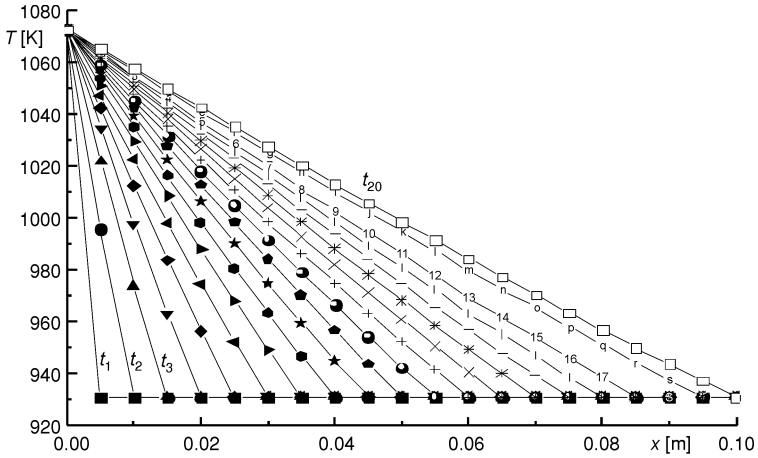

Figure 6. The calculated temperature distribution in liquid region

Conclusion

A novel algorithm for solving the classic Stefan problem is presented in the paper. The algorithm is also verified to be straightforward and efficient for its finite difference formulation. The numerical scheme for two-region problem will be further discussed in another paper.

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