

TWO NUMERICAL METHODS FOR HEAT CONDUCTION PROBLEMS WITH PHASE CHANGE

by

Lin XING^a, Lianghai QU^{a,*}, Jianguo XU^a, and Feng LING^b

^a College of Science, Zhongyuan University of Technology, Zhengzhou, Henan, China

^b School of Mathematics and Statistics, Zhaoqing University, Zhaoqing, Guangdong, China

Original scientific paper

<https://doi.org/10.2298/TSCI1804787X>

A fixed-space-step method and a fixed-time-step method are presented, respectively, for solving the Stefan problems with time-dependent boundary conditions. The evolution of the moving interface and the temperature distribution in the phase change domain are simulated numerically by using two methods for melting in the half-plane and outward spherical solidification. Numerical experiment results show that the numerical results obtained from the two methods are in good agreement for the different test examples, and the two methods can be applied to solve Stefan problems in engineering practice.

Key words: *phase change, heat conduction, moving interface, temperature field, numerical solution*

Introduction

The Stefan problem or the moving boundary problem can be defined as a parabolic partial differential equation with associated initial and boundary conditions which has to be solved in a time-dependent space domain with the moving interface [1-3]. Owing to the unknown position of the moving interface and the non-linear form of the thermal energy balance equation at the interface, the Stefan problem is usually solved by numerical methods or approximate analytical methods [4-6]. Caldwell and Kwan [7] presented a brief review of five key numerical methods for 1-D Stefan problems for simple geometries including plane, cylindrical and spherical, and obtained the numerical results of spherical and cylindrical phase change problem with fixed boundary condition from four methods including the enthalpy method, boundary immobilization method, perturbation method and heat balance integral method. Qu *et al.* [8] established a finite difference method to solve the Stefan problem with periodic boundary condition and analyzed the effects of the oscillating surface temperature on the motion of the moving interface and the temperature distribution.

In the present paper, the fixed-space-step method and the fixed-time-step method are presented for solving the Stefan problems with time-dependent boundary conditions. The evolution of the moving interface and the temperature field in the phase change domain are simulated numerically for melting in the half-plane and outward spherical solidification. The numerical results are compared with those obtained by other numerical methods.

* Corresponding author, e-mail: qulianghai263@sina.com

Melting in a semi-infinite domain

Consider 1-D single-phase melting of ice in a semi-infinite domain due to the time-dependent boundary temperature. The dimensionless formulation of this problem [9] is:

$$\frac{\partial^2 T(x, t)}{\partial x^2} = \frac{\partial T(x, t)}{\partial t}, \quad 0 < x < R(t) \quad (1)$$

$$\frac{dR(t)}{dt} = -\text{Ste} \frac{\partial T(x, t)}{\partial x}, \quad x = R(t) \quad (2)$$

subject to the initial and boundary conditions:

$$T(x, t) = 0, \quad x = R(t), t > 0 \quad (3)$$

$$T(x, t) = f(t), \quad x = 0, t > 0 \quad (4)$$

$$R(t) = 0, \quad t = 0 \quad (5)$$

where Ste is the Stefan number given by $(\bar{C}\Delta\bar{T}_{\text{ref}})/\bar{h}$, where \bar{C} is the specific heat capacity, \bar{h} – the latent heat, and $\Delta\bar{T}_{\text{ref}}$ – the reference temperature.

Fixed-space-step method

We establish a finite difference scheme to solve the system (1)-(5) by considering the needed time corresponding to the forward-moving constant distance of the moving interface each time [8]. Let Δx be the forward-moving distance of the phase change interface each time, namely the constant space step size. Thus $R_j = j\Delta x$ is the position of the moving interface at $t = t_j$, with $t_0 = 0$ and $j = 0, 1, 2, \dots$. Using a backward difference scheme for the time derivative and a central difference scheme for the space derivative, eqs. (1) and (2) in discrete form can be expressed as:

$$aT_{j-1}^N - (2a + b)T_j^N + aT_{j+1}^N = -bT_j^{N-1}, \quad j = 1, 2, \dots, N - 1 \quad (6)$$

$$b = -\text{Ste} \frac{T_{N-2}^N - 4T_{N-1}^N + 3T_N^N}{2\Delta x} \quad (7)$$

where $\Delta t_{N-1} = t_N - t_{N-1}$, $a = 1/\Delta x$, and $b = \Delta x/\Delta t_{N-1}$.

The initial and boundary conditions (3)-(5) in discrete form are, respectively:

$$T_N^N = 0 \quad (8)$$

$$T_0^N = f(t_N) \quad (9)$$

$$R(t_0) = R_0 = 0 \quad (10)$$

Fixed-time-step method

We establish a finite difference scheme to solve the system (1)-(5) by computing the forward-moving distance of the moving interface corresponding to the constant time step each time. Let Δt be the constant time step, and R_j is the position of the moving interface at $t = j\Delta t$, with $t_0 = 0$ and $j = 0, 1, 2, \dots$. Using a backward difference scheme for the time derivative and a non-equidistant Lagrange three-point interpolation formula for the space derivative, eqs. (1) and (2) in discrete form can be expressed as:

$$\frac{2\Delta x_j T_{j-1}^N - 2(\Delta x_{j-1} + \Delta x_j) T_j^N + 2\Delta x_{j-1} T_{j+1}^N}{\Delta x_{j-1} \Delta x_j (\Delta x_{j-1} + \Delta x_j)} = \frac{T_j^N - T_j^{N-1}}{\Delta t}, \quad j = 1, 2, \dots, N-1$$

$$\frac{\Delta x_{N-1}}{\Delta t} = -\text{Ste} \frac{(\Delta x_{N-1})^2 T_{N-2}^N - (\Delta x_{N-2} + \Delta x_{N-1})^2 T_{N-1}^N + \Delta x_{N-2} (\Delta x_{N-2} + 2\Delta x_{N-1}) T_N^N}{\Delta x_{N-2} \Delta x_{N-1} (\Delta x_{N-2} + \Delta x_{N-1})}$$

where $\Delta x_{j-1} = R_j - R_{j-1}$, $j = 1, 2, \dots, N$. Introducing two variables $c_j = \Delta x_{j-1} \Delta x_j$ and $d_j = \Delta x_{j-1} + \Delta x_j$, the two equations above can then be transformed into the following form:

$$2\Delta t \Delta x_j T_{j-1}^N - (2\Delta t d_j + c_j d_j) T_j^N + 2\Delta t \Delta x_{j-1} T_{j+1}^N = -c_j d_j T_j^{N-1}, \quad j = 1, 2, \dots, N-1 \quad (11)$$

$$\Delta x_{N-1} = -\Delta t \text{Ste} \frac{(d_{N-1} - \Delta x_{N-2})^2 T_{N-2}^N - (d_{N-1})^2 T_{N-1}^N + \Delta x_{N-2} (2d_{N-1} - \Delta x_{N-2}) T_N^N}{c_{N-1} d_{N-1}} \quad (12)$$

The initial and boundary conditions (3)-(5) in discrete form are, respectively:

$$T_N^N = 0 \quad (13)$$

$$T_0^N = f(t_N) = f(N\Delta t) \quad (14)$$

$$R(t_0) = R_0 = 0 \quad (15)$$

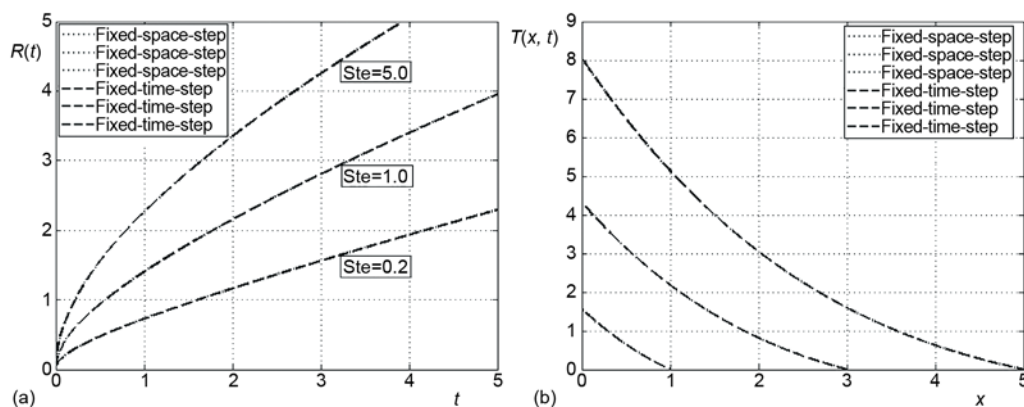
Numerical results and discussion

In order to initialize our numerical procedures and to circumvent the singularity at $t = 0$, the exact temperature distribution and the corresponding position of the moving interface given by the exact solution are used at t_1 and t_2 after $t_0 = 0$ for all numerical calculations [9]. We consider one-dimensional melting problem in a semi-infinite domain due to the boundary temperature $T(0, t) = f(t) = 1 + t$, we simulate numerically the evolution of the moving boundary and the temperature distribution in the phase change process by using two methods and compare the computational accuracy of the numerical results.

Table 1 shows the position of the moving boundary at five different times for three different values of the Stefan number. Here, the constant space step size $\Delta x = 0.001$ is used for the fixed-space-step method and the constant time step size $\Delta t = 0.001$ is used for the fixed-time-step method. In the case of $\text{Ste} = 0.2$, the position of the moving boundary obtained from these two methods are respectively $R(t) = 2.2937$ and $R(t) = 2.2938$ at $t = 5.000$, which absolute error is only about 0.0001. But in the case of $\text{Ste} = 5.0$, the position of the moving boundary obtained from these two methods are, respectively, and $R(t) = 5.7840$ and $R(t) = 5.7835$ at $t = 5.000$, which absolute error is about 0.0005. Thus the position of the moving boundary obtained from these two methods is very close and the absolute error is less than 0.0015, as can be seen from tab. 1. Figure 1(a) shows the evolution of the moving interface as a function of time for three different values of the Stefan number, and fig. 1(b) shows the temperature distribution in the phase change domain for $\text{Ste} = 1.0$ when the moving interface moves to $R(t) = 1.0, 3.0$, and 5.0, respectively. It can be seen from fig. 1 that the results obtained from the two methods agree very well. The evolution of the moving interface depends very strongly upon the Stefan number. For the larger Stefan number, the velocity of the moving interface is larger. On the other hand, in the case of the boundary condition $T(x = 0, t) = f(t) = 1 + t$, the temperature in the whole phase change domain is changing clearly as the domain grows.

Table 1. Comparison of the position of the moving interface using two numerical methods for melting in the half-plane

Ste	t	Fixed-space-step	Fixed-time-step	Error
0.2	1.000	0.7303	0.7303	0.0000
0.2	2.000	1.1646	1.1646	0.0000
0.2	3.000	1.5604	1.5605	0.0001
0.2	4.000	1.9348	1.9349	0.0001
0.2	5.000	2.2937	2.2938	0.0001
1.0	1.000	1.4033	1.4027	0.0006
1.0	2.000	2.1559	2.1556	0.0003
1.0	3.000	2.8071	2.8069	0.0002
1.0	4.000	3.4011	3.4009	0.0002
1.0	5.000	3.9552	3.9551	0.0001
5.0	1.000	2.2624	2.2609	0.0015
5.0	2.000	3.3511	3.3502	0.0009
5.0	3.000	4.2520	4.2514	0.0006
5.0	4.000	5.0518	5.0513	0.0005
5.0	5.000	5.7840	5.7835	0.0005

**Figure 1. Evolution of the moving interface and temperature distributions in the phase change domain for two numerical methods for melting in the half-plane; (a) evolution of the moving interface, (b) temperature distributions for Ste = 1.0**

Outward spherical solidification

Consider the outward spherical solidification of a saturated liquid due to the time-dependent boundary temperature. The governing equation of this problem [7] is:

$$\frac{1}{r} \frac{\partial^2 [rT(r, t)]}{\partial r^2} = \frac{\partial T(r, t)}{\partial t}, \quad t > 0, \quad 1 < r < R(t) \quad (16)$$

subject to the initial and boundary conditions:

$$\frac{dR(t)}{dt} = \text{Ste} \frac{\partial T(r, t)}{\partial r}, \quad r = R(t) \quad (17)$$

$$T(r, t) = f(t), \quad r = 1, \quad t > 0 \quad (18)$$

$$T(r, t) = 1, \quad r = R(t), \quad t > 0 \quad (19)$$

$$R(t) = 1, \quad t = 0 \quad (20)$$

Fixed-space-step method

Let Δr be the constant space step, and $R_j = 1 + j\Delta r$ is the position of the moving interface at $t = t_j$, with $t_0 = 0$ and $j = 0, 1, 2, \dots$. Using a backward difference scheme for the time derivative and a central difference scheme for the space derivative, eq. (16) in discrete form can be expressed as:

$$\frac{1}{r_j} \frac{r_{j+1} T_{j+1}^N - 2r_j T_j^N + r_{j-1} T_{j-1}^N}{(\Delta r)^2} = \frac{T_j^N - T_j^{N-1}}{\Delta t_{N-1}}, \quad j = 1, 2, \dots, N-1 \quad (21)$$

where $\Delta t_{N-1} = t_N - t_{N-1}$, $N = 1, 2, \dots$. The Stefan condition (17) at $r_N = 1 + N\Delta r$ in discrete form is:

$$\frac{\Delta r}{\Delta t_{N-1}} = \text{Ste} \frac{3T_N^N - 4T_{N-1}^N + T_{N-2}^N}{2\Delta r} \quad (22)$$

Introducing two variables $a = 1/\Delta r$ and $b = \Delta r/\Delta t_{N-1}$, eqs. (21) and (22) can be transformed into the following form:

$$\left(a + \frac{1}{r_j}\right) T_{j+1}^N - (2a + b) T_j^N + \left(a - \frac{1}{r_j}\right) T_{j-1}^N = -b T_j^{N-1}, \quad j = 1, 2, \dots, N-1 \quad (23)$$

$$b = \text{Ste} \frac{3T_N^N - 4T_{N-1}^N + T_{N-2}^N}{2\Delta r} \quad (24)$$

The initial and boundary conditions (18)-(20) in discrete form are, respectively:

$$T_0^N = f(t_N) \quad (25)$$

$$T_N^N = 1 \quad (26)$$

$$R_0 = R(t_0) = 1 \quad (27)$$

The set of eqs. (23)-(27) are the finite difference scheme of the set of partial differential eqs. (16)-(20) for the spherical solidification.

Fixed-time-step method

Let Δt be the constant time step, and R_j is the position of the moving interface at $t_j = j\Delta t$, with $t_0 = 0$ and $j = 0, 1, 2, \dots$. Using a backward difference scheme for the time deriv-

ative and a non-equidistant Lagrange three-point interpolation formula for the space derivative, eqs. (16) and (17) in discrete form can be expressed as:

$$\frac{2}{R_j} \frac{-(\Delta r_j)^2 T_{j-1}^N + [(\Delta r_j)^2 - (\Delta r_{j-1})^2] T_j^N + (\Delta r_{j-1})^2 T_{j+1}^N}{\Delta r_{j-1} \Delta r_j (\Delta r_{j-1} + \Delta r_j)} + \frac{2\Delta r_j T_{j-1}^N - 2(\Delta r_{j-1} + \Delta r_j) T_j^N + 2\Delta r_{j-1} T_{j+1}^N}{\Delta r_{j-1} \Delta r_j (\Delta r_{j-1} + \Delta r_j)} = \frac{T_j^N - T_j^{N-1}}{\Delta t}, \quad j = 1, 2, \dots, N-1$$

$$\frac{\Delta r_{N-1}}{\Delta t} = Ste \frac{(\Delta r_{N-1})^2 T_{N-2}^N - (\Delta r_{N-2} + \Delta r_{N-1})^2 T_{N-1}^N + [2\Delta r_{N-2} \Delta r_{N-1} + (\Delta r_{N-2})^2] T_N^N}{\Delta r_{N-2} \Delta r_{N-1} (\Delta r_{N-2} + \Delta r_{N-1})}$$

where $\Delta r_{N-1} = R_N - R_{N-1}$, $N = 1, 2, \dots$. Introducing two variables $c_j = \Delta r_{j-1} \Delta r_j$ and $d_j = \Delta r_{j-1} + \Delta r_j$, the two equations above can then be transformed into the following form:

$$2\Delta r_j \Delta t (R_j - \Delta r_j) T_{j-1}^N - d_j [2R_j \Delta t + 2\Delta t (d_j - 2\Delta r_j) + R_j c_j] T_j^N + 2\Delta r_{j-1} \Delta t (R_j + \Delta r_{j-1}) T_{j+1}^N = -R_j c_j d_j T_j^{N-1}, \quad j = 1, 2, \dots, N-1 \tag{28}$$

$$\Delta r_{N-1} = Ste \frac{(d_{N-1} - \Delta r_{N-2})^2 T_{N-2}^N - (d_{N-1})^2 T_{N-1}^N + [2c_{N-1} + (\Delta r_{N-2})^2] T_N^N}{c_{N-1} d_{N-1}} \Delta t \tag{29}$$

Thus, the set of eqs. (28), (29), and (25)-(27) are the other finite difference scheme of the set of partial differential eqs. (16)-(20) for the spherical solidification.

Numerical results and discussion

For $Ste = 0.2$ and the boundary condition $T(r = 1, t) = f(t) \equiv 0$, fig. 2(a) shows the evolution of the moving interface as a function of time for the outward spherical solidifying problem, and fig. 2(b) shows the temperature distribution in the phase change domain when the moving interface moves to $R(t) = 1.2, 1.5$, and 1.8 , respectively. Here, the constant space step size $\Delta r = 0.001$ is used for the fixed-space-step method and the constant time step size

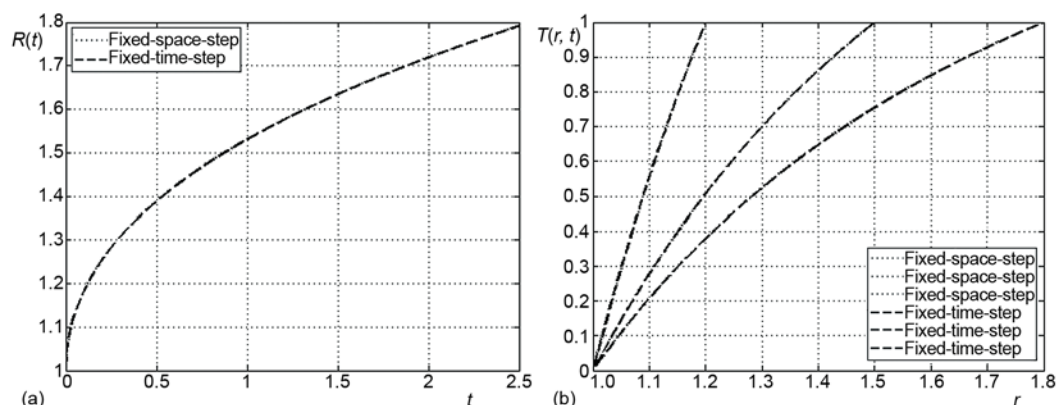


Figure 2. Evolution of the moving interface and temperature distributions in the phase change zone for two numerical methods for outward spherical solidification with $Ste = 0.2$ and $f(t) \equiv 0$; (a) evolution of the moving interface, (b) temperature distributions

$\Delta t = 0.001$ is used for the fixed-time-step method. It can be seen from tab. 2 that the results obtained from the two methods agree well with those obtained by the enthalpy method and the perturbation method [10], and the absolute error among the results is less than 0.001. Thus one may conclude that the fixed-space-step method and the fixed-time-step method are feasible and effective to solve the spherical solidifying problem.

Table 2. Comparison of the position of the moving interface for two numerical methods for outward spherical solidification with $Ste = 0.2$ and $f(t) \equiv 0$

t	Fixed-space-step	Fixed-time-step	Enthalpy [10]	Perturbation [10]
0.200	1.2540	1.2537	1.2547	1.2547
0.400	1.3504	1.3503	1.3509	1.3511
0.600	1.4216	1.4216	1.4222	1.4223
0.800	1.4800	1.4801	1.4805	1.4806
1.000	1.5303	1.5304	1.5309	1.5310
1.200	1.5750	1.5751	1.5756	1.5756
1.400	1.6154	1.6156	1.6160	1.6160
1.600	1.6525	1.6527	1.6531	1.6531
1.800	1.6868	1.6870	1.6874	1.6875
2.000	1.7190	1.7192	1.7195	1.7196

In the case of $Ste = 0.2$ and the boundary condition $T(r = 1, t) = f(t) = -t^2$, fig. 3(a) shows the evolution of the moving interface as a function of time for the outward spherical solidifying problem, and fig. 3(b) shows the temperature distribution in the phase change domain when the moving interface moves to $R(t) = 1.2, 1.6,$ and 2.0 , respectively. For this test example, the size of the phase change domain is increasing linearly as time goes on after $t = 1.5$, namely the velocity of the moving interface as a function of time becomes almost constant after a time step. On the other hand, the temperature in the phase change domain is

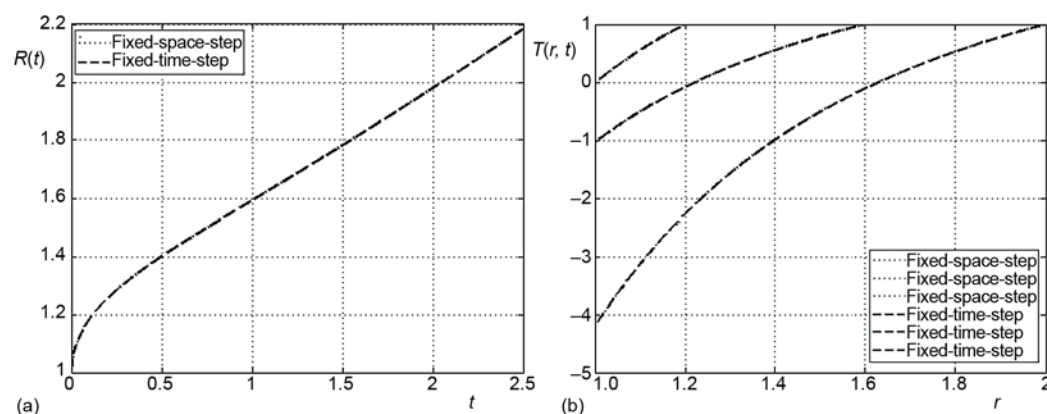


Figure 3. Evolution of the moving interface and temperature distributions in the phase change zone for two numerical methods for outward spherical solidification with $Ste = 0.2$ and $f(t) = -t^2$; (a) evolution of the moving interface, (b) temperature distributions

changing rapidly, and the temperature difference increases from about 2 to 5.2 when the moving interface moves from $R(t) = 1.6$ to $R(t) = 2.0$, as shown in fig. 3(b). Obviously, this phenomenon is caused by the boundary condition $T(r = 1, t) = f(t) = -t^2$.

Conclusions

By considering the needed time corresponding to the forward-moving constant distance of the moving interface and the forward-moving distance of the moving interface corresponding to the constant time step each time, we present the fixed-space-step method and the fixed-time-step method, respectively. Four finite difference schemes are established for solving Stefan problems. The evolution of the moving interface and the temperature distribution in the phase change domain are simulated numerically for melting in the half-plane and outward spherical solidification. Numerical experiment results show that the numerical results obtained from these two methods are in good agreement for the different test examples, and these two methods can be applied to solve two Stefan problems in engineering practice.

Acknowledgment

The work is supported by Key Scientific Research Project in Colleges and Universities of Henan Province (no. 15A140045), Science and Technology Project of China Textile Industry Association (no. 2015020) and the National Natural Science Foundation of China (no. 41271076).

References

- [1] Javierre, E., et al., A Comparison of Numerical Models for One-Dimensional Stefan Problems, *Journal of Computational and Applied Mathematics*, 192 (2006), 2, pp. 445-459
- [2] Rajeev, Kushwaha, M. S., An Approximate Approach for a Stefan Problem with Periodic Boundary Condition, *Journal of Engineering Computers & Applied Sciences*, 1 (2012), 1, pp. 66-73
- [3] Qu, L. H., et al., An Approximate Method for Solving Melting Problem with Periodic Boundary Conditions, *Thermal Science*, 18 (2014), 5, pp. 1679-1684
- [4] Vrankar, L., et al., Moving-Boundary Problems Solved by Adaptive Radial Basis Functions, *Computers & Fluids*, 39 (2010), 9, pp. 1480-1490
- [5] Tadi, M., A Four-Step Fixed-Grid Method for 1D Stefan Problems, *Journal of Heat Transfer*, 132 (2010), 11, pp. 114502.1-114502.4
- [6] Mitchell, S. L., Myers, T. G., Application of Standard and Refined Heat Balance Integral Methods to One-Dimensional Stefan Problems, *SIAM Review*, 52 (2010), 1, pp. 57-86
- [7] Caldwell, J., Kwan, Y. Y., Numerical Methods for One-Dimensional Stefan Problems, *Communications in Numerical Methods in Engineering*, 20 (2004), 7, pp. 535-545
- [8] Qu, L. H., et al., Numerical Study of One-Dimensional Stefan Problem with Periodic Boundary Conditions, *Thermal Science*, 17 (2013), 5, pp. 1453-1458
- [9] Mitchell, S. L., Vynnycky, M., Finite-Difference Methods with Increased Accuracy and Correct Initialization for One-Dimensional Stefan Problems, *Applied Mathematics and Computation*, 215 (2009), 4, pp. 1609-1621
- [10] Caldwell, J., Kwan, Y. Y., A Brief Review of Several Numerical Methods for One-Dimensional Stefan Problems, *Thermal Science*, 13 (2009), 2, pp. 61-72