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Finite difference solution of one-dimensional Stefan problem with periodic boundary conditions

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Abstract

A finite difference method is used to solve the one-dimensional Stefan problem with periodic Dirichlet boundary condition. The temperature distribution, the position of the moving boundary and its velocity are evaluated. It is shown that, for given oscillation frequency, both the size of the domain and the oscillation amplitude of the periodically oscillating surface temperature, strongly influence the temperature distribution and the boundary movement. Furthermore, good agreement between the present finite difference results and numerical results obtained previously using the nodal integral method is seen.

Keywords: Moving boundary problem; Stefan problem; Finite difference method

1. Introduction

Moving boundary problems or Stefan problems involving heat and mass transfer in materials undergoing phase change arise in many physical processes, such as melting of ice, recrystallization of metals, binary alloy melting and solidification induced by pulsed-laser irradiation, evaporation of droplets, oxygen diffusion problem, particle dissolution in solid media, etc. Such a process covers a wide range of applications in which phase changes from solid, liquid or vapour states. The material is assumed to undergo a phase change with a moving boundary that has to be tracked as part of the solution. Owing to the unknown location of the phase change interface and the nonlinear form of the thermal energy balance equation at the interface, analytical solutions are difficult to obtain except for a limited number of special cases.

Due to difficulties in obtaining analytical solutions, various numerical techniques are often employed [1]. Numerical techniques are specially known to have difficulties with time-dependent boundary conditions, and very fine mesh size and small time steps are often needed for accurate solutions. Because these are often computer intensive—only a few results for the Stefan problem with time-dependent boundary conditions are available in the literature. Solutions of such Stefan problems include linear, exponential and periodical variation of the surface temperature or the flux with time [2–4]. The Stefan problem with periodically (in time) oscillating temperature on the fixed boundary is important for practical cases involving melting and solidification of ice over the diurnal cycle, and in industrial processes with cyclical surface temperature or heat flux variation. The position of the moving boundary, its velocity and the temperature distribution within the domain are important for these applications. A comparative study of various numerical methods for moving boundary problems has been made by Furzeland [3].

There are two main approaches to the solution of the Stefan problem. One is the front-tracking method, where the position of the phase boundary is continuously tracked. As for example, the heat balance integral method [5] explicitly tracks the motion of isotherms (the phase boundary being one of them). Alternatively, variable grid methods (variable space grid and variable time step) provide the way to track the phase front

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explicitly [6]. However, these methods are poorly suited to multi-dimensional problems due to the difficulties with algorithms of implementation and large computational cost. Another approach is to use a fixed-domain formulation. For example, the isotherm migration method, uses temperature as independent variable [7]. A more common one is the enthalpy method in which enthalpy rather than temperature is an independent variable [8,9]. Alternatively, using a suitable coordinate transformation, one may immobilise the moving front at the expense of solving a more complicated problem [10–12].

Various numerical methods have been applied to the Stefan problem including finite element, finite difference and integral methods. Several finite element methods have been developed and successfully applied to the Stefan problem with various boundary and initial conditions [10,13–15]. Solutions reported in the literature using the finite difference methods for solving the moving boundary problem include the one-dimensional Stefan problem describing the evaporation processes [16,17], the process of melting of solid [18], oxygen diffusion problem [12] and the dissolution of stoichiometric multi-component particles in ternary alloys [19]. On the other hand, a coupling integral equation approach has been used by Mennig and Özişik [2] for solving the Stefan problem describing the melting/solidification process as well as the nodal integral (NI) approach applied by Rizwan-uddin [4,11] to the Stefan problem describing the melting of solids, where these phase-change problems involve time-dependent boundary conditions. Generally, in terms of accuracy and efficiency, the choice between various finite element, finite difference and integral methods for the solution of a particular Stefan problem is not always clear, due to their specific advantages and limitations.

In this paper we consider the one-dimensional Stefan problem with periodic Dirichlet boundary condition, and use the finite difference approach in order to determine the temperature distribution and phase boundary during the process.

2. Formulation

The dimensionless formulation of the Stefan problem for the liquid region of a melting solid at the phase change temperature in an invariant domain ($0 \leqslant x \leqslant 1$) is [4,11]

$$\frac{\partial^2 T(x,t)}{\partial x^2} + xR(t)\frac{\mathrm{d}R(t)}{\mathrm{d}t}\frac{\partial T(x,t)}{\partial x} = R^2(t)\frac{\partial T(x,t)}{\partial t}, \quad 0 \leqslant x \leqslant 1, \tag{1}$$

$$R(t)\frac{\mathrm{d}R(t)}{\mathrm{d}t} = -\mathrm{Ste}\frac{\partial T(x,t)}{\partial x}, \quad x = 1, \tag{2}$$

subject to the initial and boundary conditions

$$\begin{aligned} &R = 0, \quad t \leqslant 0, \\ &T = f(t), \quad x = 0, \ t > 0, \\ &T = 0, \quad x = 1, \ t > 0, \end{aligned} \tag{3}$$

where $T(x,t)$ is the temperature distribution, R is the position of the moving boundary, Ste is the Stefan number given by $(C_\mathrm{l}\Delta T_\mathrm{ref})/h_\mathrm{sl}$, with C_l—the specific heat capacity of liquid, h_sl—the latent heat and ΔT_ref—a reference temperature [20].

As the solid melts with time, the moving boundary $R(t)$ moves to the right. If the temperature in the solid region ($x > 1$) is assumed to be spatially uniform and constant in time, equal to the phase change temperature, as here, then the problem is usually referred to as the single-phase Stefan problem.

The time-dependent surface temperature boundary condition is assumed to be of the form $T(x=0,t) \equiv f(t) = [1 + \varepsilon\sin(\omega t)]$, the same form used earlier by Rizwan-uddin [4], where ε is the surface temperature oscillation amplitude and ω is the oscillation frequency. Thus, we have three physical parameters (Ste, ε and ω) in this model. In order to solve the Stefan problem defined by Eqs. (1)–(3) Rizwan-uddin [4] employed the nodal integral method.

3. Finite difference method

We now report, to solve this Stefan problem using the finite difference method. We employ an explicit finite difference method. Using a forward difference scheme for the time derivative and a central difference scheme for the space derivative, Eq. (1) in discretized form can be expressed as

$$T_{i,m+1} = T_{i,m} + \frac{kx_i\dot{R}_m}{2hR_m}(T_{i+1,m} - T_{i-1,m}) + \frac{k}{h^2R_m^2}(T_{i+1,m} - 2T_{i,m} + T_{i-1,m}), \tag{4}$$

where $T_{i,m} \equiv T(x_i, t_m)$, h ($\equiv \Delta x$) is the constant space grid size such that $x_i = ih$, with $i = 0, 1, \ldots, N$ ($x_0 = 0$, $x_N = 1$), $t_m = t_0 + mk$, where k ($\equiv \Delta t$) is the time step and t_0 is the time at which the numerical process is initialised. A truncation error for this scheme is $\mathrm{O}(k) + \mathrm{O}(h^2)$.

The temperature distribution at the origin ($x = 0$) is easily obtained using Eq. (3), which in discretized form is

$$T_{i,m} \equiv f(t_m) = [1 + \varepsilon\sin(\omega t_m)], \quad i = 0, \ m = 0, 1, 2, \ldots \tag{5}$$

For the temperature distribution at $0 < x < 1$ ($i = 1, 2, \ldots, N-1$, $m = 0, 1, 2, \ldots$,) Eq. (4) will be used. The temperature distribution at $x = 1$ according to (3) is

$$T_{i,m} = 0, \quad i = N, \quad m = 0, 1, 2, \ldots \tag{6}$$

The Stefan condition (2) at $x = 1$ ($i = N$) in discretized form is

$$R_{m+1} = R_m - \frac{k\mathrm{Ste}}{2hR_m}(3T_{N,m} - 4T_{N-1,m} + T_{N-2,m}), \quad m = 0, 1, 2, \ldots, \tag{7}$$

where the following three point backward scheme [3,17] is used for the temperature gradient at the moving interface ($x = 1 = N\Delta x$):

$$\left.\frac{\partial T}{\partial x}\right|_{x=R} = \frac{3T_N - 4T_{N-1} + T_{N-2}}{2\Delta x} + \mathrm{O}(\Delta x^2). \tag{8}$$

Initial condition (3) in discretized form is

$$R_0 = 0. \tag{9}$$

4. Numerical results and discussion

In the case of $\varepsilon \neq 0$, the exact solution of this Stefan problem is not known. For $\varepsilon = 0$ or $T(x = 0, t) = 1$, the exact solution of the problem defined by Eqs. (1)–(3) is [21]

$$T(x,t) = 1 - \frac{\mathrm{erf}(x\lambda)}{\mathrm{erf}(\lambda)}, \quad R(t) = 2\lambda\sqrt{t}, \tag{10}$$

where the value of λ is determined from the following transcendental equation:

$$\sqrt{\pi}\lambda \mathrm{e}^{\lambda^2}\mathrm{erf}(\lambda) = \mathrm{Ste}. \tag{11}$$

In order to initialize our numerical procedures and to circumvent the singularity at $t = 0$, i.e. $R(t) = 0$, the exact temperature distribution and the corresponding position of the moving boundary given by Eq. (10) are used at a short time interval t_{in} after $t = 0$ for the time-dependent problem ($T(x = 0, t) = [1 + \varepsilon\sin(\omega t)]$). One should mention here that the same initialization procedure has been used previously by Rizwan-uddin both for the Stefan problem treated in the present paper [4] and for the Stefan problem with temperature on the left boundary ramped linearly ($T(x = 0, t) = (1 - 0.2t)$) [11].

We solve the Stefan problem defined by Eqs. (1)–(3) with periodic boundary condition at $x = 0$ using the finite difference method, for three different Stefan numbers $\mathrm{Ste} = 0.2$, 1.0 and 2.0 and two oscillation amplitudes $\varepsilon = 0.5$ and 0.9. The initial time $t_{\mathrm{in}} = 0.01$, a constant grid size $h(\equiv \Delta x = 1/N) = 0.1$ (number of grid points $N = 10$ is adopted) and the time step $k(\equiv \Delta t) = 0.00002$ are used for all numerical calculations. One should mention here that, for $\mathrm{Ste} = 1.0$ and 2.0, larger time steps $k = 0.0001$ and grid size $h = 0.1$ also guarantee stability of our difference schemes applied. For $\mathrm{Ste} = 0.2$, using the time step $k = 0.0001$ and grid size $h = 0.2$, we also achieve stability of our difference schemes. It should be noted that such a choice of smaller time step and finer grid size has been made in order to get more accurate numerical solutions of the Stefan problem analyzed. The values of λ obtained from the solution of the transcendental Eq. (11) are 0.30642, 0.62006 and 0.80060 for $\mathrm{Ste} = 0.2$, 1.0 and 2.0 [2], respectively.

In order to have validation of the accuracy of our finite difference method, first we compare the present results for moving boundary position with numerical results obtained previously by Rizwan-uddin [4] with the nodal integral method. In Fig. 1a the computational values for moving boundary position are plotted for three different Stefan numbers for an oscillation amplitude of 0.5 and frequency $\pi/2$, as a function of time. The nodal integral and finite difference results are so close as to be indistinguishable in the graphs. Fig. 1b shows the present results for the position of the moving boundary for three different Stefan numbers for larger oscillation amplitude of 0.9 and frequency $\pi/2$. For both oscillation amplitudes analyzed, the growth of the moving boundary depends very strongly upon Ste. It is seen from Fig. 1 that in the first stage of moving boundary evolution, the effect of the oscillating boundary temperature clearly impacts the growth rate of the moving boundary, and in the second stage the moving boundary evolves essentially as the square root of time, corresponding to a steep increase in the temperature on the left boundary. The moving boundary in the first stage has superimposed humps corresponding to the forcing period T. Further time evolution of the moving boundary results in diminishing of superimposed humps which occurs faster for smaller ε and larger Ste. A comparison of $f(t)$ and the corresponding $R(t)$ from Fig. 1 shows that as the domain size increases, the moving boundary takes longer to respond to the temperature variation taking place at the left boundary. Consequently, the increasing delay results in $T(x = 0, t)$ and $\mathrm{d}R(t)/\mathrm{d}t$ to alternately become in phase and out of phase in time, as can be seen from Fig. 2. A very strong decrease in the velocity of the moving boundary for a short time period ($t \lesssim 2$) after $t = 0$ is seen for all Ste analyzed. It is important to note that in the case of the larger oscillation amplitude $\varepsilon = 0.9$ and the smallest Stefan number $\mathrm{Ste} = 0.2$ analyzed, the velocity of the moving boundary periodically becomes zero, i.e. periodically there is no movement of the right boundary, as can be seen from Fig. 2b. This means that sufficiently large oscillation amplitude of $T(x = 0, t)$ applied to material with small Stefan number, may result in periodical termination of the melting process. On the other hand, for materials with larger Stefan number ($\mathrm{Ste} = 1.0$ and 2.0), the melting process occurs without termination. Thus one may conclude

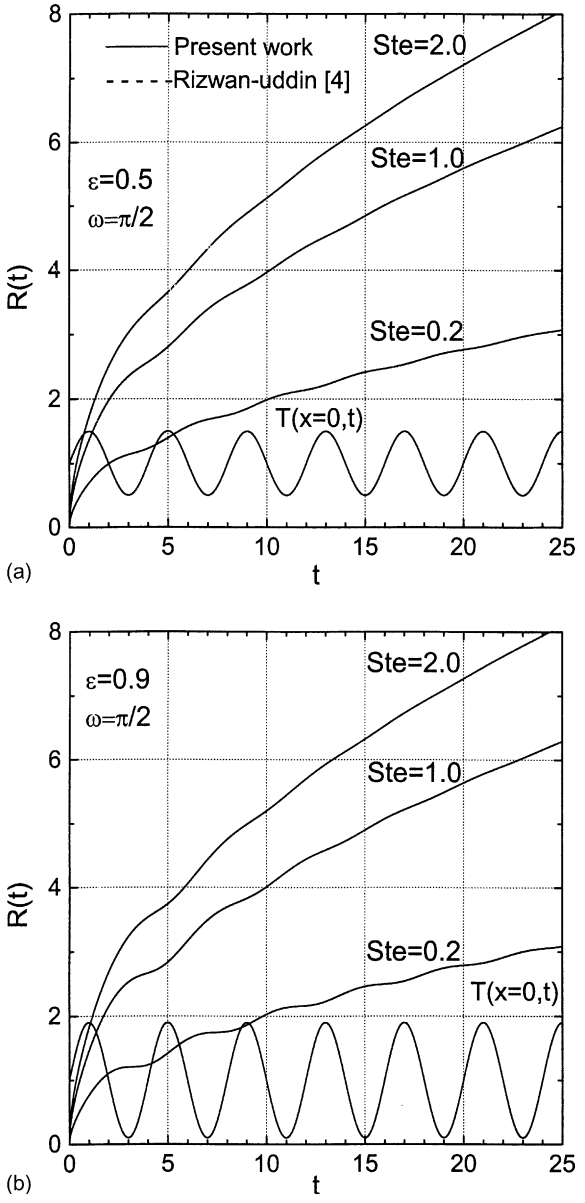


Fig. 1. Evolution of the moving boundary for different Stefan numbers for oscillation amplitude (a) $\varepsilon = 0.5$ and (b) $\varepsilon = 0.9$. Also shown are the temperature oscillations at the $x = 0$ surface for $\omega = \pi/2$.

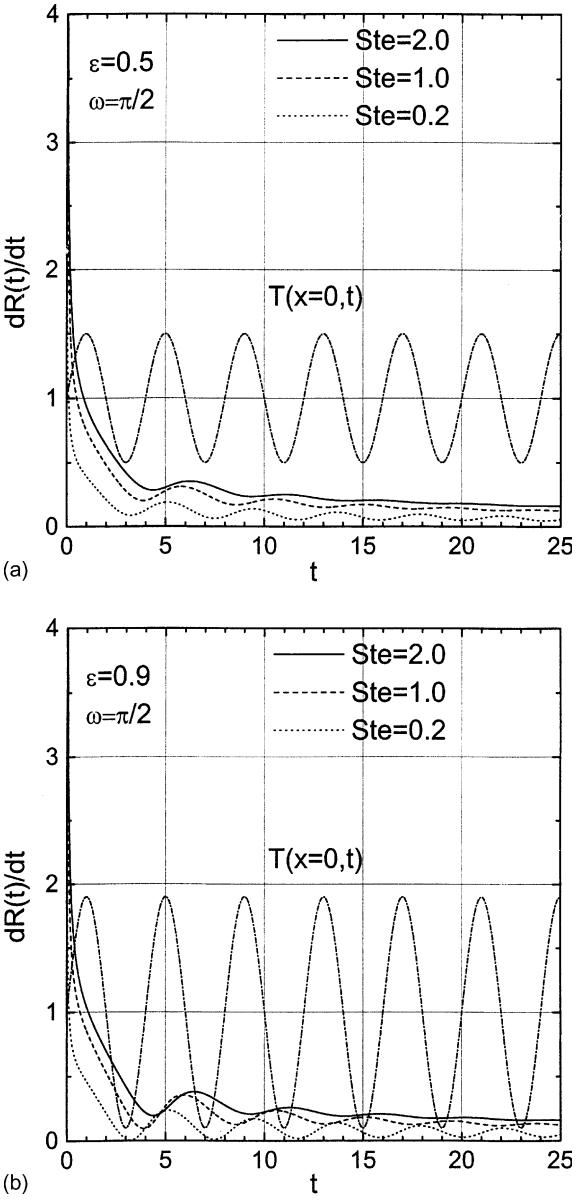
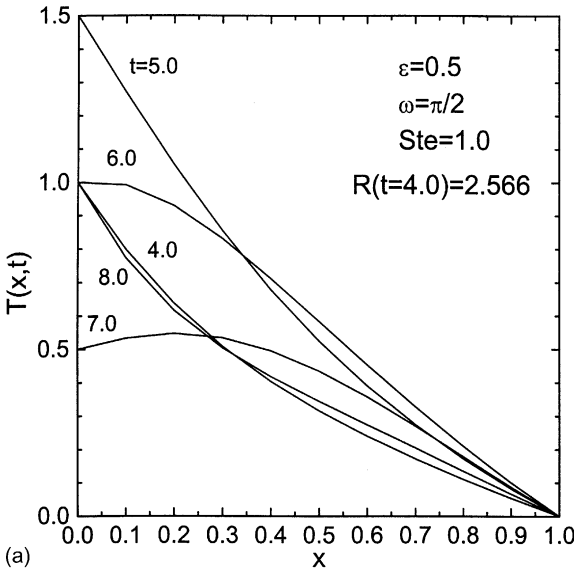


Fig. 2. Velocity of the moving boundary as a function of time for different Stefan numbers for oscillation amplitude (a) $\varepsilon = 0.5$ and (b) $\varepsilon = 0.9$. Also shown are the temperature oscillations at the $x = 0$ surface for $\omega = \pi/2$.

that it is not only the size of the domain but also the oscillation parameters, particularly the oscillation amplitude of the temperature distribution at the left boundary, that strongly influence the characteristics of the boundary movement.

In Figs. 3 and 4, the impact of the oscillation boundary temperature at $x = 0$ with different oscillation amplitudes on the temperature distribution for material with Ste = 1.0 is shown. For smaller oscillation amplitude, $\varepsilon = 0.5$, and smaller domain size, $R(t = 4.0) = 2.566$, the temperature is changing in the whole domain $0 \leqslant x \leqslant 1$ (Fig. 3a), while for larger domain size, $R(t = 20.0) = 5.595$, the temperature is changing in only about the left half of the domain (Fig. 3b). Increasing the oscillation amplitude to $\varepsilon = 0.9$ leads to a more pronounced change in the temperature distribution in the whole domain both for the smaller domain size ($R(t = 4.0) = 2.644$) and the larger one ($R(t = 20.0) = 5.632$) (Fig. 4).



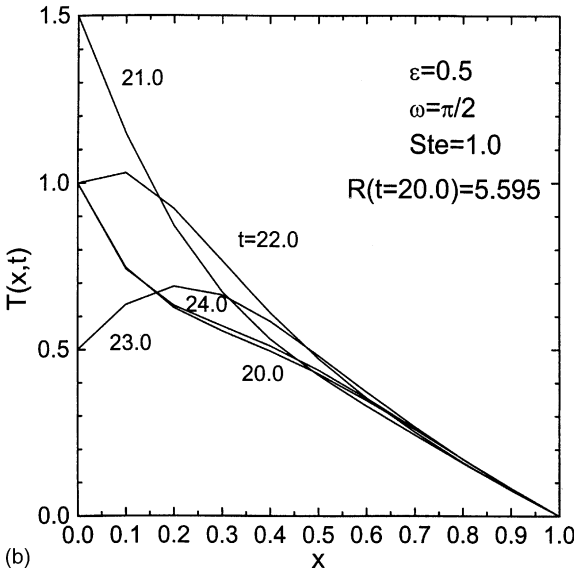
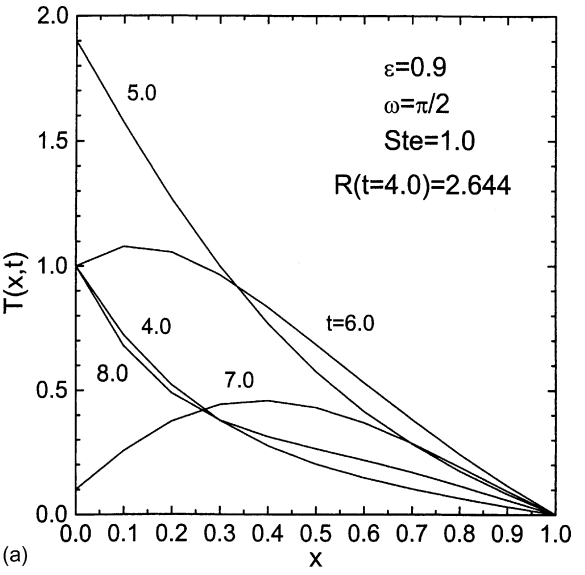


Fig. 3. Temperature distributions over a forcing period for Ste = 1.0, oscillation frequency $\omega = \pi/2$ and oscillation amplitude $\varepsilon = 0.5$, when the domain size is (a) 2.566 and (b) 5.595.



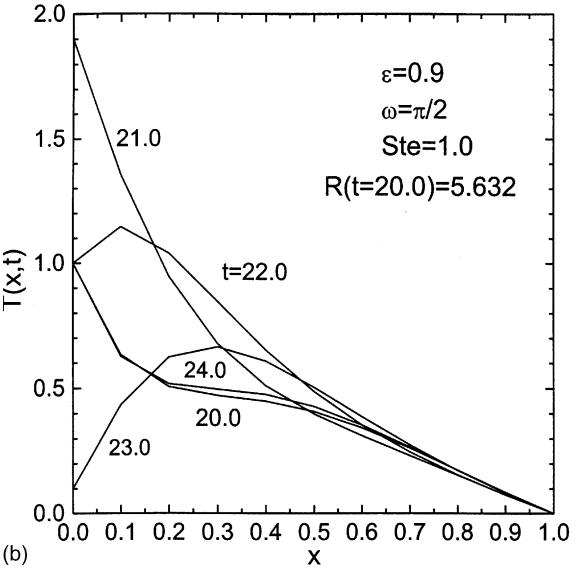


Fig. 4. Temperature distributions over a forcing period for Ste = 1.0, oscillation frequency $\omega = \pi/2$ and oscillation amplitude $\varepsilon = 0.9$, when the domain size is (a) 2.644 and (b) 5.632.

Thus one can conclude that, for given oscillation frequency, both the size of the domain and the oscillation amplitude of the temperature distribution at the left boundary, strongly influence the temperature distribution, as has been shown for the boundary movement.

It should be mentioned here that the finite difference approach used in the present work has been successfully applied earlier to the Stefan problem with Neumann boundary condition at $x = 0$ by Caldwell and Savović [17] in describing the evaporation of droplets. We have successfully applied the method to even more complicated Stefan problems with time-dependent boundary conditions at $x = 0$ (with exponentially varying and linearly ramped temperature at the left boundary) by the same authors [18,22] in describing the one-dimensional single-phase melting process. Hence, the finite difference approach may be considered as sufficiently accurate and efficient for a wide class of Stefan problems which include both problems with time-independent, as well as more complicated ones with time-dependent, boundary conditions.

5. Conclusion

We report on the finite difference solution of the Stefan problem with periodic boundary conditions describing the melting process of a solid. The position of the moving boundary and its velocity are evaluated for different materials with finite different Stefan number. We obtain that it is not only the size of the domain but also the oscillation parameters, particularly the oscillation amplitude of the temperature distribution at the left boundary, that strongly influence both the boundary movement (boundary position and its velocity) and temperature distribution. We further obtain that the effect of periodically varying boundary condition at $x = 0$ on the boundary movement and the temperature distribution is most pronounced when the domain is small and diminishes as the domain grows. This diminishing can be slowed down by increasing the oscillation amplitudes applied. In the case of sufficiently large oscillation amplitude applied to materials with small Stefan number, the velocity of the moving boundary periodically may become zero, i.e. the periodical termination of the melting process may occur.

The present computational results for the moving boundary position agree well with the results obtained previously using the nodal integral method [4]. Although the nodal integral method permits the use of relatively large time steps, the finite difference approach which needs smaller time steps is shown to provide sufficiently accurate solutions of the Stefan problem with periodically oscillating (in time) boundary conditions.

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