Adaptation of the Method Of Lines (MOL) to the MATLAB Code for the Analysis of the Stefan Problem

ANTONIO CAMPO*
ULISES LACOA
Department of Mechanical Engineering
The University of Texas at San Antonio
San Antonio, TX 78249, USA
* antonio.campo@utsa.edu

Abstract – This paper describes the application of the potent Method Of Lines (MOL) to the classical one-dimensional Stefan problem. The mathematical model of the Stefan problem experiences unique features, such as structural changes in the ordinary differential equation that describes the solid-liquid interface of a half-space region. To overcome these obstacles, MOL was implemented with the ordinary differential equation solver of the MATLAB code, using the unique event location property. The feasibility of MOL for treating the Stefan problem was validated upon comparing the obtained semi-numerical results against the exact analytical results available in the archival literature. Using a wide variety of Stefan numbers for engineering applications, it was realized that the Method Of Lines (MOL) coupled with the event location property tracked the temperature-time history and the moving liquid-solid interface in the half-space region admirably.

Keywords: Stefan problem, Moving solid-liquid boundary, Method Of Lines (MOL), MATLAB code, Event location property.

Nomenclature

c specific heat
k thermal conductivity
l characteristic length
N number of lines
L latent heat
x space variable
x^* dimensionless x, eq. (6)
$S(t)$ position of moving front
S^* dimensionless S, eq. (7)
Ste Stefan number, eq. (9)
t time
t^* dimensionless t, eq. (6)
T temperature
T^* dimensionless T, eq. (5)
T_o high temperature
T_m fusion temperature

Greek letters
α thermal diffusivity
λ eigenvalues of eq. (8)
ρ density

Subscripts
l liquid

1 Introduction

Heat conduction problems involving change of phase in materials due to melting or freezing (solidification) are very important in engineering and science. Referred as moving boundary problems, these problems occur in industrial applications, such as casting of metals and plastics, melting and solidification of alloys, crystal growth, ice production, freezing/thawing of foods, thermal energy storage, aerodynamic ablation, etc.

In complex problems on phase-change heat conduction, the bounding surface separating the frozen and unfrozen regions of the material changes with time. Herewith, this aspect revolves around the mathematical determination of the interface

location as a function of time. In order to solve these problems, two objectives need to be pursued: one is the solution of the heat conduction equation and the other is the position of the unknown solid-liquid boundary, which has to be tracked as part of the solution. The existence of a moving boundary generally means that the phase-change heat conduction problem does not admit a closed form, exact analytical solution and consequently much research has focused on approximate solution techniques, both analytical and numerical.

The study of heat conduction in a medium with solid-liquid phase changes was initiated by Jožef Stefan [1,2], the Slovene physicist who published six treatises on deciphering the ice formation in the polar seas between 1889 and 1891. Stefan considered first the problem of a semi-infinite half-space $0 \leq x < \infty$ containing a pure material, which can exist in either liquid or solid phase. A detailed biography of J. Stefan was provided by Crepeau [3].

In applied mathematics, the Stefan problem literally relates to moving boundary value problems; a special type of a boundary value problem highlighting a phase boundary that moves with time (Cannon and Hill [4]). The two phases (solid and liquid) are merely regions in which the coefficients of the heat conduction equation are continuous and differentiable up to the order of the PDE. In thermal physics, such coefficients represent thermal properties of the medium for each phase. The moving boundaries (or interfaces) are infinitesimally thin surfaces that separate the two adjacent phases. In view of this, the coefficients of the heat conduction equation and its derivatives may suffer discontinuities across the interfaces. Issues related to the existence, uniqueness, and stability in the Stefan problem have been discussed in [4].In addition, there is a book written by Gupta [5] and a state-of-the art review article assembled by Tarzia [6]. There are several solution procedures for the Stefan problem that are not included in Refs. [5,6]. A peculiar numerical method based on an integro-differential formulation of the one-dimensional Stefan problem was proposed by Ang [7]. The numerical results indicated that accurate solutions are obtainable offering a viable alternative method. Javierre et al. [8] presented a critical comparison on the suitability of several numerical methods, level set, moving grid and phase field model to address the Stefan problem in phase transformation studies. The comparison showed that the type of phase transformation determines the convenience of the numerical technique.

The main goal in this work is to address the classical one-dimensional Stefan problem with a potent analytical-numerical method, the so-called Method Of Lines (MOL), which is conveniently framed in the platform of the MATLAB code with event location property. As evidenced in the detailed literature review, the combined computational procedure to be implemented in the present work has never been explored before.

2 Problem Description

Consider a semi-infinite, half-space region $0 \leq x < \infty$ made with a homogeneous solid. The initial temperature of the solid coincident with the fusion temperature, T_m, was scaled to be zero for convenience. At time $t = 0$, the temperature at the exposed surface of the solid $x = 0$ was suddenly raised to the scaled value of $T_o = 1$, and maintained subsequently for all time $t > 0$. Consequently, the solid starts to melt at x = 0 and the solid-liquid interface moves in the positive x-direction. After a certain time *t*, the problem boils down to determining the temperature distribution and the thickness *s(t)* of the solid layer. The sketch of the Stefan problem in the proper Cartesian coordinates is illustrated in Figure 1.

Under the assumption of constant thermal properties, the mathematical formulation of the Stefan problem begins with the 1-D heat conduction equation (Luikov [9], Özişik [10], Poulikakos [11]):

$$\frac{\partial T}{\partial t} = \alpha_l \frac{\partial^2 T}{\partial x^2}, \quad 0 < x < s(t), \quad t > 0 \tag{1}$$

subject to the initial condition

$$T(x, t = 0) = T_m \tag{2}$$

and the two boundary conditions

$$T(x = 0, t) = 1, \quad T(x = s(t), t) = 0 \tag{3}$$

In the preceding equations (1)-(3), T is the temperature, α_l is the thermal diffusivity of the liquid and $s(t)$ is the position of the moving front.

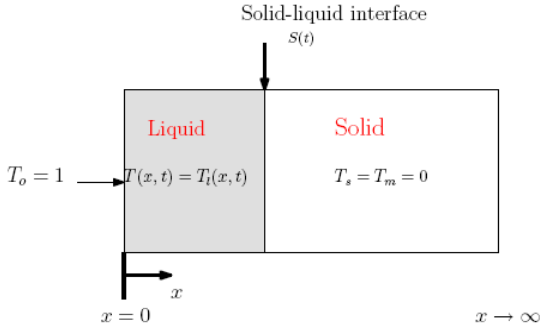

Figure 1. Sketch of the Stefan problem and coordinate system

After the first boundary condition is applied at $x = 0$, melting of the solid begins at this location. Immediately thereafter, the liquid-solid interface penetrates into the solid and moves in the positive x-direction, $x > 0$ to reach the moving second boundary condition at $x = s(t)$.

Owing that the underlying heat conduction equation (1) is not valid at the phase change interface and $s(t)$ is an unknown variable, an additional equation is required for its determination. The new equation for closure is known as the *Stefan condition*. Fundamentally, the *Stefan condition* states that the freezing front moves in a special way, such that the front velocity is proportional to the jump in heat flux across the front.

In general, pure substances change phases isothermally and there is a latent heat associated with the phase change. In general, the latent heat of a given phase change is the quantity of heat liberated when a unit mass undergoes that phase change completely and isothermally. In particular, the latent heat of fusion is the quantity of heat liberated when a unit mass of pure liquid completely freezes at its fusion temperature. Conversely, the latent heat of fusion is the quantity of heat, which must be added to melt a unit mass of pure solid at its fusion temperature. The latent heat has dimensions of [energy]/[mass] and is usually given in units of Joule/gram. Essentially, the *Stefan condition* is derived from a physical constraint, which comes from the conservation of energy at the liquid-solid interface, so that the local interface velocity depends on the heat flux discontinuity there. Accordingly, the *Stefan condition* is expressed by the nonlinear boundary condition

$$\rho L \frac{ds}{dt} = -k_l \frac{\partial T}{\partial x} \tag{4}$$

along with the initial condition $s(0) = 0$. The participating properties are: ρ the density of the liquid, k_l the thermal diffusivity of the liquid and L the latent heat of the phase change material.

3 Exact Analytical Solution

Exact analytical solutions of equations (1)-(4) are usually found in Refs. [9-11]. From here, the dimensionless temperature distribution T^* has the form

$$T^* = \frac{T - T_m}{T_o - T_m} = 1 - \frac{erf\left(x^*/2\sqrt{t^*}\right)}{erf(\lambda)} \tag{5}$$

where *erf* is the Gaussian error function. In addition, the dimensionless coordinate $x*$ and the dimensionless time t^* are written as

$$x^* = \frac{x}{l}, \quad t^* = \frac{t}{l^2/\alpha_l} \tag{6}$$

where l is the characteristic length.

The dimensionless displacement of the melt interface S^* is expressed by

$$S^* = 2\lambda\sqrt{t^*} \tag{7}$$

In the pair of eqs. (5) and (7), λ stands for the positive roots of the transcendental equation

$$\lambda \exp(\lambda^2)\, erfc(\lambda) = Ste/\sqrt{\pi} \tag{8}$$

Herein, the Stefan number (or the phase change parameter), *Ste*, defines the ratio of the sensible heat of the solidifying phase to the latent heat L as

$$Ste = \rho c(T_O - T_m)/L \tag{9}$$

Named after J. Stefan, the Stefan number, *Ste*, is an important dimensionless group in solid-liquid phase change phenomena [9-11].

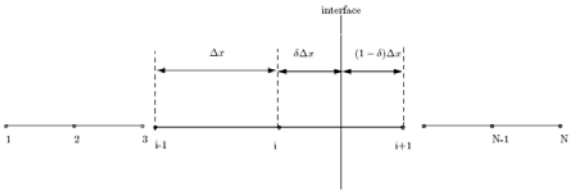

Figure 2. Discretization mesh

4 Approximate Analytical/Numerical Solution: The Method Of Lines (MOL)

Unquestionably, the two most commonly used approximate methods for the solution of phase-change heat conduction problems are the integral method (Goodman [12]) and the numerical method cited by Tarzia [6]. In this work, the heat conduction equation (1) with the boundary conditions in eqs. (2) and (3) is analyzed with the potent Method Of Lines (MOL), a general procedure for solving time-dependent partial differential equations of parabolic type (Liskovets [13]). When applied to the 1-D heat conduction equation (1), MOL discretizes the second order space derivative with a second-order centered formulation, while leaving the first order time derivative continuous. In essence, the MOL procedure transforms the partial differential equation (1) into a system of ordinary differential equations of first order. The pioneering work on MOL for solving the heat conduction equation was carried out by Ivanov [14]. Depending on the size, the resulting systems of ordinary differential equations of first order may be integrated analytically or numerically. For analytical techniques, several papers by Sarmin and Chudov [15], Zafarullah [16] and Verwer and Sanz-Serna [17] have dealt with the stability, convergence and accuracy of MOL. For the numerical treatment of MOL, the fourth/fifth order Runge-Kutta method is considered the most popular (Wouwer et al. [18]). There is a book written by Schiesser and Griffiths [19] linking MOL with the MATLAB code Deviating from the direct heat conduction problems (DHCP), Campo and Ho [20] combined MOL with numerical differentiation for solving an inverse heat conduction problem (IHCP) in a plane wall receiving variable surface heat flux.

In the present work, the discretization procedure follows the footsteps of the one suggested by Chun and Park [21] and Furenes and Lie [22] in which the spatial domain is divided into $N-1$ uniform step size Δx. With the interface located between lines i and $i+1$ as shown in Fig. 2, the line temperatures T_k are determined from the following system of first order differential equations:

$$\frac{dT_k}{dt} = \alpha_l \frac{T_{k+1} - 2T_k + T_{k-1}}{(\Delta x)^2}, \quad for \quad k = 2,...i-1 \tag{10}$$

and

$$\frac{dT_i}{dt} = \alpha_l \frac{T_m - 2T_i + T_{i-1}}{(\Delta x)^2} + \frac{\alpha_l}{k_l} \frac{(1-\delta)\rho L}{\Delta x} \frac{ds}{dt} \tag{11}$$

where the subscript *i* indicates

$$i = max(T_k \geq T_m), k = 1,..., N-1. \tag{12}$$

Turning the attention to eq. (11), the symbol

$$\delta = (s - i\Delta x)/\Delta x$$

represents the dimensionless distance from the line i to the interface. In this regard, the location for i can be found by comparing the line temperature T_k against the melting temperature T_m implicating that

$$\frac{ds}{dt} = -\frac{k_l}{\rho L} \frac{\partial T}{\partial x}\bigg|_{x=s(t)} \tag{13}$$

To contend with the singularity that arises when the solid/fluid interface gets very close to the grid line, Verma [23] recommended to calculate the temperature gradient at the interface *x = s(t)* with a truncated Taylor series. Adopting this simple approach, and retaining two terms, the temperature gradient can be written as

$$\frac{\partial T}{\partial x}\bigg|_{x=s(t)} = \frac{T_i - T_{i-2}}{2\Delta x} + (1+\delta)\frac{T_{i-2} - 2T_{i-1} + T_i}{\Delta x} \tag{14}$$

Next, merging eqs. (13) and (14) gives rise to the differential equation for the prediction of the interface velocity

$$\frac{ds}{dt} = -\frac{k_l}{\rho L}\left(\frac{T_i - T_{i-2}}{2\Delta x} + (1+\delta)\frac{T_{i-2} - 2T_{i-1} + T_i}{\Delta x}\right) \tag{15}$$

To summarize, the system of ordinary differential heat equations of first-order composed by eqs. (10), (11) and (15) will be solved numerically with an appropriate ODE solver algorithm, like the fourth/fifth order Runge-Kutta [19].

5 Event Location Property in MATLAB

In certain engineering problems modeled with ODEs, the times of specific events are important, such as the times at which the ODE solution reaches certain target values. While solving a certain problem, the MATLAB ODE solvers can locate transitions to, from, or through zeros of a vector of user-defined functions. The mathematical model experiences structural changes in the definition of the ordinary differential equations as indicated in equations (10) and (11). To overcome these difficulties, the model was implemented in the MATLAB platform [24] and right away the event-function in the ODE solver was activated. The event location strategy to be employed was taken from Refs. [21,22].

The changes are examples of events, and two types of events exist. Time events are events, which occur at a given time, whereas state events are events, which occur when the subsystem reaches some pre-set conditions. Because most ODE solvers are structured on a hypothesis of smoothness in the continuous subsystem, integration along discontinuities without event location may cause severe inefficiency, simulation failures. As a consequence, incorrect event sequences can be generated. The points we need to find are given when event functions vanish, where *y (t)* is the state vector at a given time. The process of finding these points is called event location. Sometimes, the integration needs to be terminated at the time of the event, and possibly restart integrating the states with initial values and state definition depending on the termination time.

Most continuous simulation languages have capabilities of locating events. If an ODE solver has the capability of locating events, the step size may be adapted to hit the instants of time when the discontinuities occur. A specification of what kind of events need to be located, and what the solver must do when an event occurs, and the only additional program lines necessary. Numerical results have demonstrated that ODEs with event location has been solved accurately at a cost scarcely greater than when no events occur.

During a certain numerical integration step, it is important to ensure that the model not allowed to switch from one definition to another. Thus, we need to have the capability of terminating the integration temporarily each time the interface crosses a grid line. The syntax of the ODE solver in a MATLAB platform is expressed by

```
[t, y] = solver (@odefun, tspan, y0)
```

where the solver is one of ode45, ode23, ode113, ode 15s, ode23s,ode23t.The solvers are based on different recurrence algorithms and have different orders of comparable accuracy, for example ‘odefun’ is a function that evaluates the right-hand side of the differential equation, tspan is a vector specifying the time interval of integration, and y0 is the vector of initial conditions. The ODE solver returns a column vector of time points (t), and a solution array (y) in which each arrow corresponds to the solution at the time points in t.

In some cases, the ODE solver performance can be improved by overriding these defaults. This improvement can be done by supplying the solvers with one or more property values in an options structure. The available integration properties depend on the ODE solver used. The argument is created with the ‘odeset function’ named ‘process_events’. The events property is created with

```
options = odeset (‘ Évents’, @process_events)
```

The ODE solver solves for the default case while also finding where the events functions of (t, y) are zero. The ODE solver has the syntax

```
[t, y, te, ie] = solver (@solid_process, tspan, y0, options)
```

where ‘solid_process’ is the name of the ode function. If an events function is specified and events are detected, the ODE solver delivers three additional outputs. If an events function is specified and events are detected, the ODE solver delivers three additional outputs: a column vector of times at which events occurred (te), solution values corresponding to these times (ye), and the indices of the event that the solver detected (ie). For each event function, it is mandatory to specify whether the integration is to terminate at a zero and whether the direction of the zero crossing matters.

6 Presentation of Results

The assessment of MOL for solving the one-dimensional Stefan problem with the MATLAB code is carried out by employing substances with Stefan numbers covering three different orders of magnitude, i.e., *Ste* = 0.1, 1 and 10 in Table 1. The first five substances possess *Ste* values that range between 0.37 and 0.65, which fall inside the interval $0.1 < Ste < 1$. For instance, tin with a Ste = 1.26 is slightly greater than 1 and water with a Ste value nearly 8 is close to 10.

Table 1. Properties of selected substances

Substance	Latent heat L (J/g)	Fusion temperature T_f (K)	Specific heat c(J/g.K)	Stefan number Ste
Aluminum	370	933	0.90	0.65
Copper	204	1356	0.39	0.49
Iron	251	1813	0.45	0.37
Lead	23	600	0.13	0.59
Nickel	307	1723	0.44	0.49
Tin	60	505	0.23	1.26
Water	333	273	4.20	7.93

For simplicity, the discretized system of first order heat equations was deduced for uniform grid spacings Δx. The accuracy of the numerical results is sensitive to the choice of the number of lines N in the computational domain. In this regard, a sensitivity analysis of the grid revealed that a reasonable number of lines is N = 51.

The comparison between the analytical and numerical solutions for the dimensionless position of the liquid-solid interface S^* changing with the dimensionless time t^* is showed in Fig. 3 for three Stefan numbers: *Ste* = 0.1, 1 and 10 under study here. It is observable in the figure that the agreement for the three curves is perfect.

Shown in Figs. 4 and 5 are the numerical and the analytical dimensionless temperature fields $T^* = f(x^*, t^*)$ for two limiting St values, the smallest *Ste* = 0.1 and the largest *Ste* = 10. Fig. 4 corresponds to *Ste* = 0.1 for two pre-selected locations $x^* = 0.1$ and 0.5, whereas Fig. 5 contains *Ste* = 1 for two pre-selected locations $x^* = 1$ and 5. The four curves in the pair of figures exhibited excellent parity when compared against the analytical results obtained originally by Stefan [1, 9-11]. In view of this, it may be inferred that the comparison for $T^* = f(x^*, t^*)$ involving an intermediate *Ste* value should have precision of equal quality.

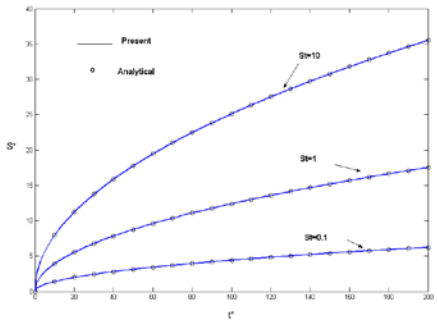

Figure 3. Variation of the dimensionless interfacial position S^* with the dimensionless time t^* parameterized by three Stefan numbers: *Ste* = 0.1, 1, 10. The exact, analytical temperatures are taken from Ref. [11].

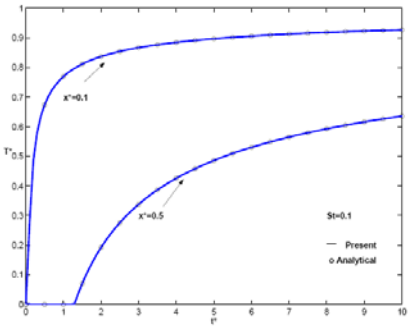

Figure 4. Variation of the dimensionless temperature T^* with the dimensionless time t^* parameterized by the dimensionless coordinate x* = 0.1 and 0.5 for Stefan number, *Ste* = 0.1. The exact analytical temperatures are taken from Ref. [11].

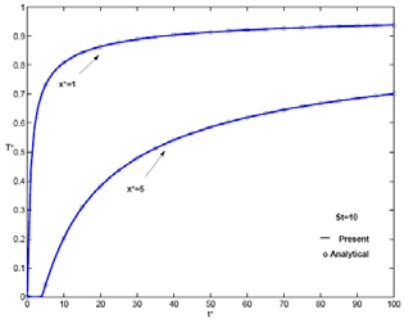

Figure 5. Variation of the dimensionless temperature T^* with the dimensionless time t^*. parameterized by the dimensionless coordinate x* = 1 and 5 for a fixed Stefan number, *Ste* = 10. The exact, analytical temperatures are taken from Ref. [11].

7 Conclusions

A hybrid analytical/numerical study based on the Method Of Lines (MOL) for solving the classical 1-D Stefan problem has been developed for the first time in this study. The systematic implementation of MOL in a MATLAB platform with event location property has proven to be efficient, accurate and economical. The MOL outcome produces an oscillation-free solution, because the phase boundary is treated as a line rather than a control volume. With a reasonable number of lines N, MOL is able to accurately track: 1) the temperature-time history in the solid as well and 2) the moving liquid-solid interface. All numerical temperatures and numerical interfacial locations agree extremely well with the exact, analytical results across a wide spectrum of Stefan numbers for substances of interest in heat engineering applications. Extensions to more involved 1-D Stefan problems accounting for variable thermal properties seem to be straightforward.

References

[1] J. Stefan, Über die Theorie der Eisbildung, Insbesondere über die Eisbildung im Polarmeere, Annalen der Physik und Chemie, Vol. 42, 1891, pp. 269-286.

[2] B. Šarler, Stefan's Work on Solid-Liquid Phase Changes, Engineering Analysis with Boundary Elements, vol. 16, n. 2, 1995, pp. 83-92.

[3] J. C. Crepeau, Josef Stefan: His life and Legacy in the Thermal Sciences, Experimental Thermal Fluid Science, Vol. 31, 2007, pp. 795-803.

[4] J. R. Cannon and C. D. Hill, Existence, Uniqueness, Stability, and Monotone Dependence in a Stefan Problem for the Heat Equation, Journal of Mathematics and Mechanics, Vol. 17, 1967, pp. 1-19.

[5] S. C. Gupta, The Classical Stefan Problem, Elsevier Press, 2003.

[6] D. A. Tarzia, A Bibliography on Moving-Free Boundary Problems for the Heat Diffusion Equation: The Stefan Problem and Related Problems, MAT-Serie A #2, 2000 (with 5869 titles and 300 pages). Also in www.austral.edu.ar/MAT-SerieA/2, 2000.

[7] W.-T. Ang, A Numerical Method Based on Integro-Differential Formulation for Solving a One-Dimensional Stefan Problem, Numerical Methods for Partial Differential Equations, Vol. 24, 2008, pp. 939-949.

[8] E. Javierre, C. Vuik, F. J. Vermolen and S. van der Zwaag, A Comparison of Numerical Models for One-Dimensional Stefan Problems, Journal of Computational and Applied Mathematics, Vol. 192, 2006, pp. 445-459.

[9] A. V. Luikov, Analytical Heat Diffusion Theory, Academic Press, 1968.

[10] M. Özişik, Heat Conduction, John Wiley, 1980.

[11] D. Poulikakos, Conduction Heat Transfer, Prentice Hall, 1993.

[12] T. R. Goodman, Application of Integral Methods to Transient Nonlinear Heat Transfer, In Advances in Heat Transfer, Vol. 1, pp. 51-122, Academic Press, 1964.

[13] O. A. Liskovets, The Method of Lines, Journal of Differential Equations, Vol. 1, 1965, pp. 1662-1678.

[14] V. T. Ivanov, Solving Heat Conduction Problems by the Straight-Lines Method, Journal of Engineering Physics, Vol. 17, No. 4, 1969, pp. 1287-1290, DOI:10.1007/ BF00832111, (Translated from Inzhenerno Fizicheskii Zhurnal, Vol. 17, No. 4, 1969, pp. 709-713).

[15] E. N. Sarmin, L. A. Chudov, On the Stability of the Numerical Integration of Systems of Ordinary Differential Equations Arising in the use of the Straight Line Method, USSR Computational Mathematics and Mathematical Physics, Vol. 3, 1963, pp. 1537-1543.

[16] A. Zafarullah, Application of the Method of Lines to Parabolic Partial Differential Equations with Error Estimates, Journal of the Association for Computing Machinery, Vol. 17, 1970, pp. 294-302.

[17] J. G. Verwer, and J. M. Sanz-Serna, Convergence of the Method of Lines Approximations to Partial Differential Equations, Computing, Vol. 33, 1984, pp. 297-313.

[18] A. V. Wouwer, P. Saucez and E. Schiesser, Adaptive Method of Lines, Chapman & Hall/CRC Press, 2001.

[19] W. E. Schiesser and G. W. Griffiths, A Compendium of Partial Differential Equation Models: Method of Lines Analysis with MATLAB, Cambridge University Press, 2009.

[20] A. Campo and J. Ho, Effortless Application of the Method of Lines for the Inverse Estimation of Temperatures in a Large Slab with Two Surface Heating Wavefronts, Journal of Heat Transfer, Vol. 131, 2009, Paper number 024501, (5 pages).

[21] C. Chun and S. Park, A Fixed-Grid Finite-Difference Method for Phase-Change Problems, Numerical Heat Transfer, Part B: Fundamentals, Vol. 38, 2000, pp. 59-73.

[22] B. Furenes and B. Lie, Using Event Location in Finite-Difference Methods for Phase Change Problems, Numerical Heat Transfer, Part B: Fundamentals, Vol. 50, 2006, pp. 143-155.

[23] A. Verma, S. Chandra and B. Dhindaw, An Alternative Fixed Grid Method for the Solution of the Classical One-Phase Stefan Problem, Applied Mathematics and Computation, Vol. 158, 2004, pp. 573-584.

[24] MATLAB 7, The MathWorks, Inc., 3 Apple Hill Drive, Natick, MA 01760, USA.