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ระเบียบวิธีไฟไนท์ดิฟเฟอเรนซ์แบบกริดอยู่นิ่งในการแก้ปัญหาการแข็งตัว *

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บทคัดย่อ

ระเบียบวิธีไฟไนท์ดิฟเฟอเรนซ์แบบกริดอยู่นิ่งเป็นระเบียบวิธีที่นิยมใช้ในการคำนวณเชิงตัวเลขของปัญหาการแข็งตัว เนื่องจากมีความง่ายในการควบคุมและรวดเร็วในการคำนวณ อย่างไรก็ตามดีสครีไทเซชันของระเบียบวิธีกริดอยู่นิ่งมีแนวโน้มทำให้เกิดความผิดพลาดในการคำนวณอุณหภูมิและตำแหน่งของขอบเขตระหว่างของแข็งและของเหลว ความผิดพลาดของการคำนวณเชิงตัวเลขนี้เกิดจากการจำลองการคายความร้อนแฝงของการเปลี่ยนสถานะของของเหลวที่ขอบเขตระหว่าง ของแข็ง และของเหลวไม่เหมาะสม ในงานวิจัยนี้ระเบียบวิธีดีสครีไทเซชันถูกปรับปรุงเพื่อแก้ไขความผิดพลาดในการคำนวณและได้นำมาใช้ เพื่อแก้ปัญหาการแข็งตัวหนึ่งมิติที่ทราบผลเฉลย โดยวิธีเชิงวิเคราะห์แล้วเพื่อสาธิตประสิทธิภาพ ของระเบียบวิธีที่นำเสนอ

คำสำคัญ: ระเบียบวิธีไฟไนท์ดิฟเฟอร์เรนท์, กริดอยู่นิ่ง, การแข็งตัว, การเปลี่ยนสถานะ

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A Fixed-Grid Finite-Difference Method for Solidification Problems *

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Abstract

For a numerical solution of solidification problems, a fixed-grid finite-difference method is a popular approach due to the ease of its implementation and less computational effort than the moving-grid system. However, the simple discretisation of the fixed-grid method has a tendency to oscillate numerically in temperature and solid-liquid interface position. The numerical oscillations arise from improper handling of the evolution of the latent heat at the solid-liquid interface. In this work, a modified discretisation is described such that the numerical error could be overcome. A one-dimensional solidification problem with known analytical solution is applied to demonstrate the efficiency of the method.

Keywords: finite difference method, fixed grid, solidification, phase change

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Introduction

Solidification is a heat transfer controlled process by which a liquid changes to solid. Thermal effects during solidification are of great interest in many engineering applications such as in the making of ice, the freezing of food, thermal energy storage, growth of crystals, casting and welding of metals, *etc.* The effect of solidification is most evident when casting is the final operation. Since a solidification structure and its associated defects are difficult to eliminate once they are created, good control of the solidification at the starting point is therefore most important [Flemings, M. C. 1974.].

Solidification is governed by nonlinear equations and the complexity is that the solid-liquid interface is moving as the latent heat is released at the interface; as a result, the location of the interface is *a priori* unknown and must follow as a part of solution. The numerical technique is difficult due to the presence of this highly nonlinear moving boundary condition. To overcome this numerical difficulty, a great many methods have been developed [Muehlbauer, J. C. and Sunderland, J. 1965. , Voller, V. R., Cross, M. and Markatos, N. C. 1987. , Schneider, G. E. 1987. and Lee, S. L., Tzong, R. Y. 1991.]. However, most of the finite-difference methods predicted oscillatory temperature and interface due to improper handling of the evolution of the latent heat at the interface. The oscillation would give an incorrect solution and prevent the numerical solution from converging.

The objective of this work is to develop a fixed-grid finite-difference method which removes numerical oscillation in temperature and solid-liquid interface position. An interfacial energy-balance equation was used to track the solid-liquid interface in combination with a modified discretisation of heat fluxes crossing control surfaces. A one-dimensional solidification problem which known analytical solution is applied as a numerical example.

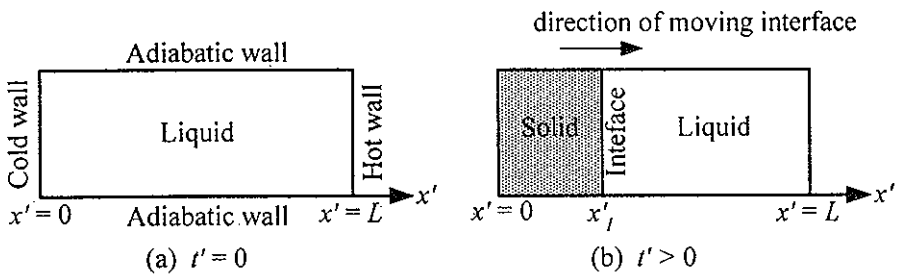


Figure 1 *Physical model*

Mathematical Model

Solidification due to temperature change at one end of pure material in an enclosure (Figure 1) has been studied; the wall at $x' = 0$ and $x' = L$ are isothermal while the others are adiabatic. Initially, the cavity is filled with an isothermal liquid ($T_i' > T_m'$). At $t' > 0$, the temperature is lowered below the melting temperature ($T_0' < T_m'$) at the left wall, and solidification is initiated thereafter. The interface propagates into the liquid and the thickness of the solid increases with the passage of time.

The energy equation is expressed in term of temperature, with a source term (in square bracket) representing an amount of latent heat liberated at the solid-liquid interface:

$$\rho' c_p' \frac{\partial T'}{\partial t'} = \frac{\partial}{\partial x'}\left(k' \frac{\partial T'}{\partial x'} \right) - \left[\rho' h_f \frac{\partial f_l}{\partial t'} \right] \quad (1)$$

where ρ, c_p, k, t represent density, specific heat, thermal conductivity and time. h_f is the latent heat and f_l is the liquid fraction which is unity in the liquid phase and zero in the solid phase. Thus, f_l falls from unity to zero after a liquid is completely solidified. Primes denote dimensional quantities.

The solid-liquid interface is tracked with the use of an interfacial energy equation:

$$\rho' h_f \frac{\partial x_l'}{\partial t'} = \left(k_s' \frac{\partial T_s'}{\partial x'} - k_l' \frac{\partial T_l'}{\partial x'} \right) \quad (2)$$

where the solid-liquid interface is given by $x' = x_l'(t')$. s and l denote solid and liquid, respectively. After introducing a non-dimensional transformation, defined by

$$T = (T' - T_0')/\Delta T'; \quad \rho = \rho'/\rho_s'; \quad c_p = c_p'/c_{p,s}'; \quad x = x'/L;$$
$$\mathrm{Ste} = c_p'(T_m' - T_0')/h_f; \quad t = t' k_s'/(\rho' c_p' L^2); \quad k = k'/k_s'; \quad x_l = x_l'/L. \quad (3)$$

$\Delta T'$ can be either $T_m' - T_0'$ or $T_i' - T_0'$. Assuming constant properties, equations (1) and (2) become

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x} \right) - \left[\frac{1}{\mathrm{Ste}} \frac{\partial f_l}{\partial t} \right], \quad (4)$$

$$\frac{\partial x_l}{\partial t} = \mathrm{Ste}\left(k_s \frac{\partial T_s}{\partial x} - k_l \frac{\partial T_l}{\partial x} \right). \quad (5)$$

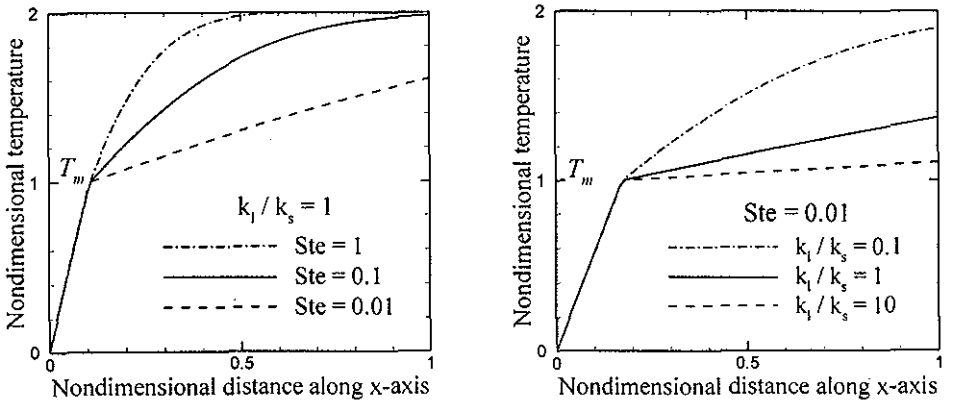
One-Dimensional Finite-difference Discretisation

The energy equation is discretised by a direct substitution of backward difference approximations in time and central difference approximations in space, together with an application of semi-implicit scheme:

$$\frac{T_i^k - T_i^{k-1}}{\Delta t} = \left(k_{i+\frac{1}{2}} \frac{\frac{1}{2}(T_{i+1}^k + T_{i+1}^{k-1}) - \frac{1}{2}(T_i^k + T_i^{k-1})}{(\Delta x)^2} - k_{i-\frac{1}{2}} \frac{\frac{1}{2}(T_i^k + T_i^{k-1}) - \frac{1}{2}(T_{i-1}^k + T_{i-1}^{k-1})}{(\Delta x)^2} \right) - \frac{1}{\mathrm{Ste}}\left(\frac{f_{l,i}^k - f_{l,i}^{k-1}}{\Delta t} \right). \quad (6)$$

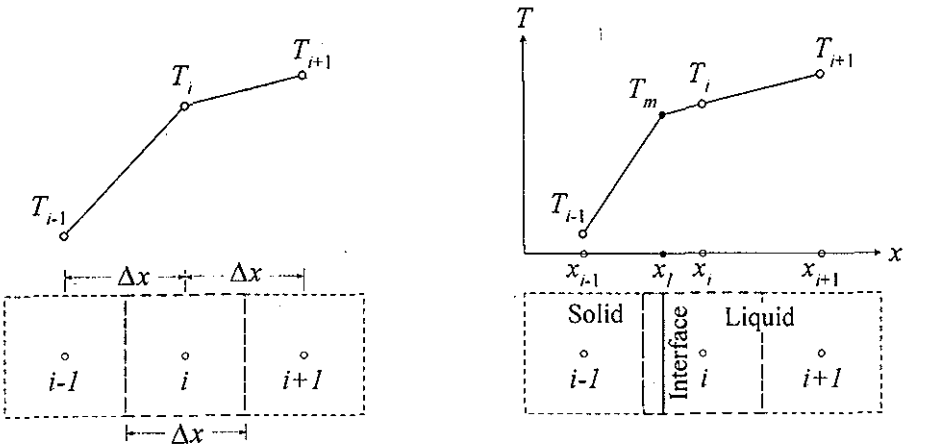
where i and k are notation indexes for a control volume and time, respectively. $k_{i-\frac{1}{2}}$ and $k_{i+\frac{1}{2}}$ are thermal conductivities at boundaries of the control volume i.

In solidification problems, temperature gradient may be discontinuous across the solid-liquid interface due to the latent heat liberated at the interface. The discontinuous temperature gradient is controlled by a Stefan number and a liquid-solid thermal conductivity ratio as shown in Figure 2. The discontinuous temperature gradient becomes large with decreasing Stefan number or increasing values of k_l / k_s.



(a) various Stefan number (b) various k_l / k_s

Figure 2 *Temperature profiles*



(a) Piecewise-linear profile (b) Linearlised profile

Figure 3 *Temperature profiles for discretisation method*

In a simple discretisation, a piecewise-linear profile of temperature (Figure 3a) is assumed between mesh points [Patankar, S. V. 1980.]. This simple profile assumption cannot handle the discontinuity and produces some spatial oscillations. A linearised profile (Figure 3b) is proposed in order to represent the interface by a surface rather than a control volume. To account for the discontinuity of temperature gradient, thermal conductivities at boundaries of the solidifying control-volume are calculated by equation (7).

$$k_{i-\frac{1}{2}}=\begin{cases} k_l \ \text{ for } x_l < x_{i-1} \\ k_l\left(\dfrac{\Delta x}{T_i-T_{i-1}}\right)\dfrac{T_i-T_m}{x_i-x_l} \ \text{ for } x_{i-1} < x_l < x_{i-\frac{1}{2}} \\ k_s\left(\dfrac{\Delta x}{T_i-T_{i-1}}\right)\dfrac{T_m-T_{i-1}}{x_l-x_{i-1}} \ \text{ for } x_{i-\frac{1}{2}} < x_l < x_i \\ k_s \ \text{ for } x_l > x_i \end{cases}, \quad k_{i+\frac{1}{2}}=\begin{cases} k_l \ \text{ for } x_l < x_i \\ k_l\left(\dfrac{\Delta x}{T_{i+1}-T_i}\right)\dfrac{T_{i+1}-T_m}{x_{i+1}-x_l} \ \text{ for } x_i < x_l < x_{i+\frac{1}{2}} \\ k_s\left(\dfrac{\Delta x}{T_{i+1}-T_i}\right)\dfrac{T_m-T_i}{x_l-x_i} \ \text{ for } x_{i+\frac{1}{2}} < x_l < x_{i+1} \\ k_s \ \text{ for } x_l > x_{i+1} \end{cases} \tag{7}$$

The interface is tracked with the use of the interfacial energy-balance equation, discretised as

$$\frac{x_l^k - x_l^{k-1}}{\Delta t} = \mathrm{Ste}\left(k_s\frac{T_m-T_{i-1}}{x_l-x_{i-1}} - k_l\frac{T_{i+1}-T_m}{x_{i+1}-x_l}\right) \tag{8}$$

Once the interface position is found, the liquid fraction is calculated by

$$f_{l,i}=\begin{cases} 1 & \text{for } x_l < x_{i-\frac{1}{2}} \\ \dfrac{x_{i+\frac{1}{2}}-x_l}{\Delta x} & \text{for } x_{i-\frac{1}{2}} < x_l < x_{i+\frac{1}{2}} \\ 0 & \text{for } x_l > x_{i+\frac{1}{2}} \end{cases}. \tag{9}$$

Numerical Solutions

The finite-difference equations obtained in the previous section are solved following the procedures described below.

Step 1. Specify the initial and boundary conditions. Specify time step (Δt) such that the initial movement of the interface is less than a half of grid size ($x_l < 0.5\Delta x$). Initially using a small time step could overcome difficulties caused by a sudden change in boundary condition in the initial stage.
Step 2. Compute thermal conductivities at control-volume boundaries by equation (7).
Step 3. Compute interface location and liquid fraction by equation (8) and (9).
Step 4. Compute temperature from equation (6) using the tri-diagonal matrix algorithm.
Step 5. Repeat steps 2 through 4 until the temperature values are converged. Convergence criterion was $\varepsilon_T = 10^{-8}$, where $\varepsilon_T = \dfrac{1}{\mathrm{NX}(\max\left|T^{n,k}\right|)}\sum_{i=1}^{\mathrm{NX}}\left|T_i^{n,k} - T_i^{n-1,k}\right|$.

Here, the subscript n is the iteration index and NX is the number of nodes.

Step 6. For the next time step, repeat steps 2 through 5 with the data at the previous time step.

Numerical Example

One-dimensional solidification (Stefan problems) in a half space ($x \geq 0$) was used as a test problem. The analytical solution of the Stefan problem is known as Neumann's solution [2] and is given by

$$x_l(t) = 2\lambda\sqrt{\alpha_s t} \tag{10}$$

$$T(x,t) = \begin{cases} \left(\dfrac{T_m - T_0}{\operatorname{erf}(\lambda)}\right)\operatorname{erfc}\left(\dfrac{x}{2\sqrt{\alpha_s t}}\right) + T_0 & ; x < x_l \\ T_m & ; x = x_l \\ T_i - \left(\dfrac{T_i - T_m}{\operatorname{erfc}(\lambda\sqrt{\alpha_s/\alpha_l})}\right)\operatorname{erfc}\left(\dfrac{x}{2\sqrt{\alpha_l t}}\right) & ; x > x_l \end{cases} \tag{11}$$

where λ is obtained from

$$\frac{e^{-\lambda^2}}{\operatorname{erf}(\lambda)} + \frac{k_l}{k_s}\sqrt{\frac{\alpha_s}{\alpha_l}}\left(\frac{T_m - T_i}{T_m - T_0}\right)\frac{e^{-\lambda^2(\alpha_s/\alpha_l)}}{\operatorname{erfc}(\lambda\sqrt{\alpha_s/\alpha_l})} = \frac{\lambda\sqrt{\pi}}{\mathrm{Ste}}. \tag{12}$$

α is thermal diffusivity, defined as $\alpha = k/(\rho c_p)$.

For comparison purposes, the parameters were assigned the same values as Lee and Tzong[6]: Ste = 1.2 and $[T_i, T_m, T_0] = [1.667, 1, 0]$. The properties for both the liquid and the solid were the same.

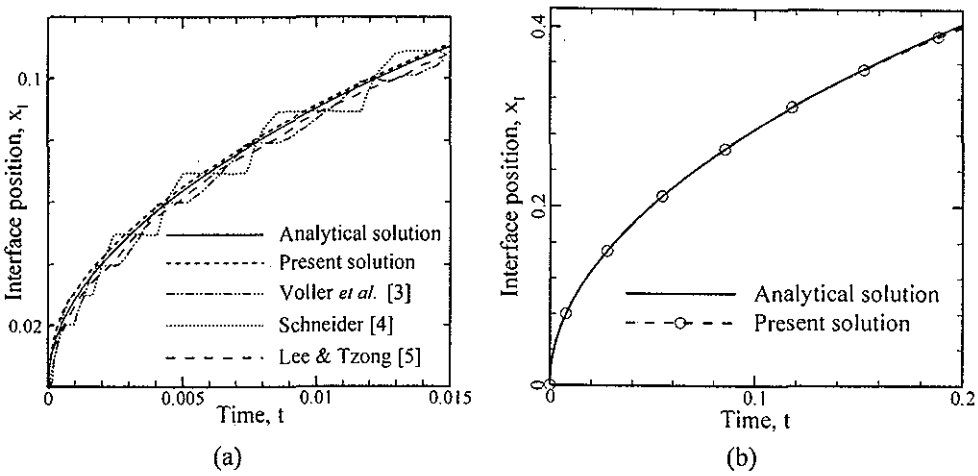
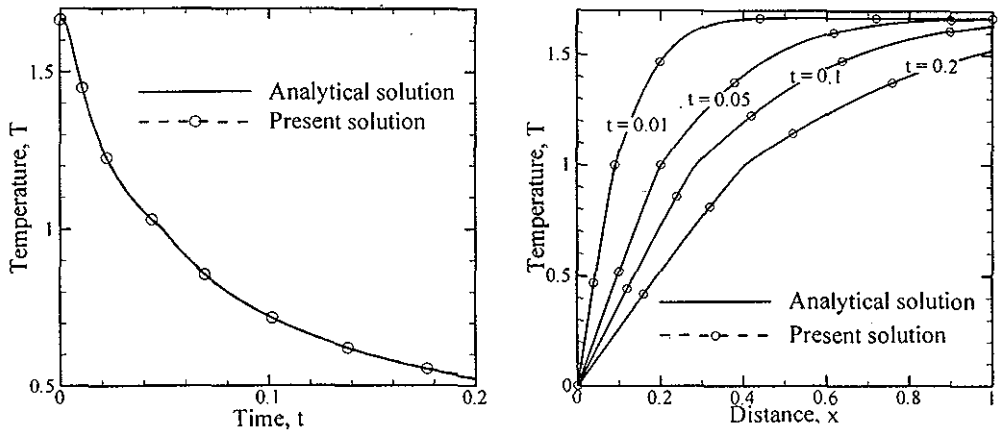


Figure 4 *Interface position*

Figure 4a shows the interface position from the present method and analytical solution for solidification period up to $t = 0.015$. The numerical results by Voller *et al.* [Voller, V. R., Cross, M. and Markatos, N. C. 1987.], Schneider [Schneider, G. E. 1987.], and Lee and Tzong [Lee, S. L., Tzong, R. Y. 1991.] were also plotted for comparisons. All numerical solutions used the same grid spacing ($\Delta x = 0.02$) and time step ($\Delta t = 0.0001$). The interface positions produced by Voller and Schneider are seen to produce zigzag variations. Voller and Schneider have simulated the enthalpy change at a grid point as the latent heat released from the corresponding control volume. The control volume will suddenly release its entire latent heat at the instant while the solid-liquid interface is sweeping through its grid point. Hence, the interface positions were approximated from the ratio of the volumetric latent heat and total enthalpy. This would result in a zigzag function with jumps having the size of grid spacing.

The present solution and Lee and Tzong's solution are smooth and close to the analytical solution. This is because the latent heat is represented by the liquid fraction (f_l) for each control volume such that the latent heat can be released evenly. However, the relative error of 2% is observed from Lee and Tzong's solution since the interface position was calculated by using the simplified interfacial energy-balance equation in which the transient term was neglected. The transient term was included in the present method and hence the predicted solution is very close to the analytical solution with a relative error of order 0.2%. Good agreements with the analytical solution were also observed for calculation up to $t = 0.2$ by; interface position (Figure 4b), temperature history at $x = 0.1$ (Figure5a) and temperature profiles (Figure5b).



(a) temperature history at $x = 0.1$ (b) temperature profiles

Figure 5 *Temperature history and profiles*

Conclusion

This paper has described an efficient fixed-grid finite-difference method for solidification problems. The solid-liquid interface was tracked with the use of the interfacial energy-balance equation. The modified discretization was obtained in terms of the thermal conductivities at the control volume boundaries, to account for the discontinuity of temperature gradient in the vicinity of the solid-liquid interface. A one-dimensional half-space solidification problem was computed to validate the present method. This strategy has been proved to have an excellent performance as it can removes numerical oscillation when compared with other numerical solutions of the fixed-grid method. The present method can also be extended to two-dimensional problems without much difficulty for directional solidification whereas the analytical solution is applicable only to a simpler one-dimensional problem.

References

Flemings, M. C. 1974. **Solidification Processing**. New York, McGraw Hill.

Lee, S. L., Tzong, R. Y. 1991. An Enthalpy Formulation for Phase Change Problems with a Large Thermal Diffusivity Jump Across the Interface. **Int. J. Heat and Mass Transfer**.(34, 6): 1491-1502.

Muehlbauer, J. C. and Sunderland, J. 1965. Heat Conduction with Freezing or Melting.**Applied Mechanics Reviews**. (18, 12): 951-959.

Patankar, S. V. 1980. **Numerical Heat Transfer and Fluid Flow**. Hemisphere: Washington. D. C.

Schneider, G. E. 1987. Computational of Heat Transfer with Solid/Liquid Phase Change including Convection. **AIAA J. Thermophys. Heat Transfer**. 4 : 136-145.

Voller, V. R., Cross, M. and Markatos, N. C. 1987. An Enthalpy Method for Convection/Diffusion Phase Change. **Int. J. Numerical Methods in Engineering**. 24:271-284.