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A phase change problem with temperature-dependent thermal conductivity and specific heat

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Abstract—A semi-analytic solution is obtained to model conduction heat transfer with phase change into a semi-infinite slab, where the thermal conductivities and specific heats of both phases are a linear function of the temperature. This model extends the model of a previous work to include temperature-dependent specific heats.

INTRODUCTION

HEAT CONDUCTION problems with a concomitant change of phase have received a great deal of study in recent years. Due to the non-linear nature of phase change problems, only a few analytic solutions to such problems have been proposed. Perhaps the best known of these analytic solutions is the Newmann solution presented in Carslaw and Jaeger [1], which presents a solution for heat transfer in a semi-infinite slab with a phase change. More recent analytic analyses of phase change problems include Tao [2], and Fredrick and Greif [3].

The preceding solutions assumed that the thermal properties of each phase were constant. When large temperature differences are associated with heat transfer, large variations may occur in the thermal properties of each phase. Imber and Huang [4] used an integral method to predict heat transfer with phase change and variable thermal properties to a semi-infinite slab. Due to the limited accuracy of integral methods, the solution of Imber and Huang is not accurate enough for purposes such a computer code verification.

Cho and Sunderland [5] used a modified error function to more accurately predict heat transfer to a semi-infinite slab with variable thermal conductivity. However, their solution procedure assumed that the specific heat of each phase was constant and not a function of the temperature. It is often the case that the temperature induced variation in specific heats is as large as the temperature induced variations in the thermal conductivities. It is the intent of this work to extend the work of Cho and Sunderland to include the effects of variable specific heats.

PROBLEM STATEMENT

The present problem is identical to that proposed in Cho and Sunderland with the single exception that both the thermal conductivity and the specific heat of each phase is assumed to vary linearly with temperature. The reader is referred to Cho and Sunderland for more details of the assumptions used in this work.

The basic equations for phase 1 and phase 2 are respectively

$$(\rho_1 c_1)\frac{\partial T_1}{\partial t} = \frac{\partial}{\partial x}\left(k_1\frac{\partial T_1}{\partial x}\right), \quad 0 < x < S(t) \quad (1)$$

$$(\rho_2 c_2)\frac{\partial T_2}{\partial t} + (\rho_1 - \rho_2)c_2\frac{\mathrm{d}S}{\mathrm{d}t}\frac{\partial T_2}{\partial x} = \frac{\partial}{\partial x}\left(k_2\frac{\partial T_2}{\partial x}\right), \quad x > S(t). \quad (2)$$

The boundary and initial conditions are

$$T_0 = T_1 \quad \text{at } x = 0 \quad (3)$$

$$k_1\frac{\partial T_1}{\partial x} - k_2\frac{\partial T_2}{\partial x} = \pm\rho_1 H\frac{\mathrm{d}S}{\mathrm{d}t} \quad \text{at } x = S(t) \quad (4)$$

$$T_1 = T_2 = T_f \quad \text{at } x = S(t) \quad (5)$$

$$\lim_{x\to\infty} T_2 = T_i \quad (6)$$

$$T_2 = T_i \quad \text{and} \quad S(t) = 0 \quad \text{at } t = 0 \quad (7)$$

where T_0 is the imposed temperature at the left-hand boundary, T_1 and T_2 are the temperatures of phase 1 and phase 2, respectively, T_f is the fusion temperature, and $S(t)$ is the phase change front location (see Fig. 1). The sign on the right-hand side of equation (4) is positive for freezing and negative for melting.

Equation (1) may be transformed to the following dimensionless ordinary non-linear differential equation:

$$\frac{\mathrm{d}}{\mathrm{d}\eta}(1+\beta_1\theta_1)\frac{\mathrm{d}\theta_1}{\mathrm{d}\eta} + 2\eta(1+\alpha_1\theta_1)\frac{\mathrm{d}\theta_1}{\mathrm{d}\eta} = 0 \quad (8)$$

where α_1 and β_1 are such that

NOMENCLATURE

a	thermal diffusivity
c	specific heat
H	latent heat of fusion
k	thermal conductivity
$S(t)$	phase change front coordinate
Ste	Stefan number, equation (19)
T	temperature
t	time
x	spatial coordinate.

Greek symbols

α	specific heat coefficient, equations (9) and (14)
β	thermal conductivity coefficient, equations (10) and (15)
ε	dummy variable
η	dimensionless coordinate, equation (12)
θ	dimensionless temperature, equation (11)
λ	dimensionless phase change front coordinate
ρ	density
$\phi_{\gamma\delta}$	modified error function (Appendix).

Subscripts

0	at $x = 0$
1 and 2	phases 1 and 2, respectively
i	initial
f	at the fusion (or melting) temperature.

$$c_1 = c_{01}(1+\alpha_1\theta_1) \tag{9}$$

$$k_1 = k_{01}(1+\beta_1\theta_1) \tag{10}$$

and

$$\theta = (T-T_0)/(T_i-T_0) \tag{11}$$

$$\eta = \frac{x}{2\sqrt{(a_{01}t)}}, \quad a_{01} = \frac{k_{01}}{c_{01}\rho_1}. \tag{12}$$

Equation (2) may also be transformed into a similar form

$$a_{12}\frac{\mathrm{d}}{\mathrm{d}\eta}(1+\beta_2\theta_2)\frac{\mathrm{d}\theta_2}{\mathrm{d}\eta}+2\left[\eta+\left(\frac{1}{\rho_{12}}-1\right)\lambda\right] \times (1+\alpha_2\theta_2)\frac{\mathrm{d}\theta_2}{\mathrm{d}\eta} = 0 \tag{13}$$

where

$$a_{12} = \frac{a_{02}}{a_{01}}, \quad \rho_{12} = \frac{\rho_2}{\rho_1} \tag{14}$$

$$c_2 = c_{02}(1+\alpha_2\theta_2)$$

$$k_2 = k_{02}(1+\beta_2\theta_2) \tag{15}$$

$$\lambda = S(t)/(2\sqrt{(a_{01}t)}) \quad (\lambda \text{ is a calculated parameter}). \tag{16}$$

The boundary conditions on equations (8) and (13) are

$$\theta_1(0) = 0 \tag{17}$$

$$\theta_1(\lambda) = \theta_2(\lambda) = \theta_f \tag{18}$$

$$\frac{\mathrm{d}\theta_1}{\mathrm{d}\eta} - k_{12}\frac{1+\beta_2\theta_f}{1+\beta_1\theta_f}\frac{\mathrm{d}\theta_2}{\mathrm{d}\eta} = 2\lambda/Ste \quad \text{at } \eta = \lambda \tag{19}$$

where Ste is the Stefan number

$$Ste = \frac{(1+\beta_1\theta_f)c_{01}|T_i-T_0|}{H}$$

$$k_{12} = \frac{k_{02}}{k_{01}}$$

and

$$\lim_{\eta\to\infty}\theta_2(\eta) = 1. \tag{20}$$

Equations (8) and (13), with the above boundary conditions may be shown (by direct substitution) to be satisfied by

$$\theta_1(\eta) = \theta_f\frac{\phi_{\gamma_1\delta_1}(\eta)}{\phi_{\gamma_1\delta_1}(\lambda)} \tag{21}$$

$$\theta_2(\eta) = 1-(1+\theta_f) \times \frac{1-\phi_{\gamma_2\delta_2}\left[\dfrac{(\eta+(1/\rho_{12})\lambda)}{\sqrt{\left(a_{12}\dfrac{(1+\beta_2\varepsilon)}{(1+\alpha_2\varepsilon)}\right)}}\right]}{1-\phi_{\gamma_2\delta_2}\left[\dfrac{1}{\rho_{12}}\sqrt{\left(\dfrac{(1+\alpha_2\varepsilon)}{a_{12}(1+\beta_2\varepsilon)}\right)}\right]} \tag{22}$$

where $\phi_{\gamma\delta}(\eta)$ is the modified error function (see the appendix) and the six unspecified coefficients (γ_1, γ_2, δ_1, δ_2, λ, and ε) are specified by the following relations:

$$\gamma_2 = \frac{\alpha_2(1-\varepsilon)}{1+\alpha_2\varepsilon} \tag{23}$$

$$\delta_2 = \frac{\beta_2(1-\varepsilon)}{1+\beta_2\varepsilon} \tag{24}$$

$$\gamma_1\phi_{\gamma_1\delta_1}(\lambda) = \alpha_1\theta_f \tag{25}$$

$$\delta_1\phi_{\gamma_1\delta_1}(\lambda) = \beta_1\theta_f \tag{26}$$

$$\frac{\phi'_{\gamma_1\delta_1}(\lambda)}{\lambda\phi_{\gamma_1\delta_1}(\lambda)} - c_{12}\frac{1-\theta_f}{\theta_f}\frac{1+\beta_2\theta_f}{1+\beta_1\theta_f} \times \frac{1+\alpha_2\varepsilon}{1+\beta_2\varepsilon}\frac{\phi'_{\gamma_2\delta_2}(\zeta)}{\zeta[1-\phi_{\gamma_2\delta_2}(\zeta)]} = 2/(Ste\,\theta_f) \tag{27}$$

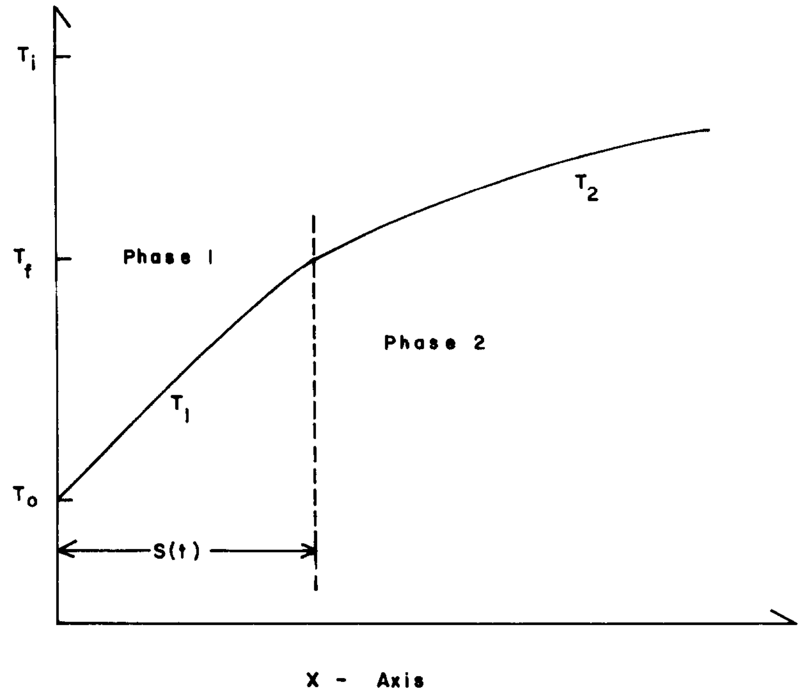

FIG. 1. Schematic of solution domain.

where

$$\zeta = \frac{\lambda \rho_1}{\rho_2} \sqrt{\left(\frac{(1+\alpha_2 \varepsilon)}{a_{12}(1+\beta_2 \varepsilon)}\right)}.$$

The solution to the above equations is found iteratively. First a value of ε is assumed in equation (23). Then equations (24)–(27) are solved. The value of ε is iterated upon until equation (27) is satisfied. A Runge–Kutta scheme was used to evaluate the modified error functions (hence the use of the term 'semi-analytic').

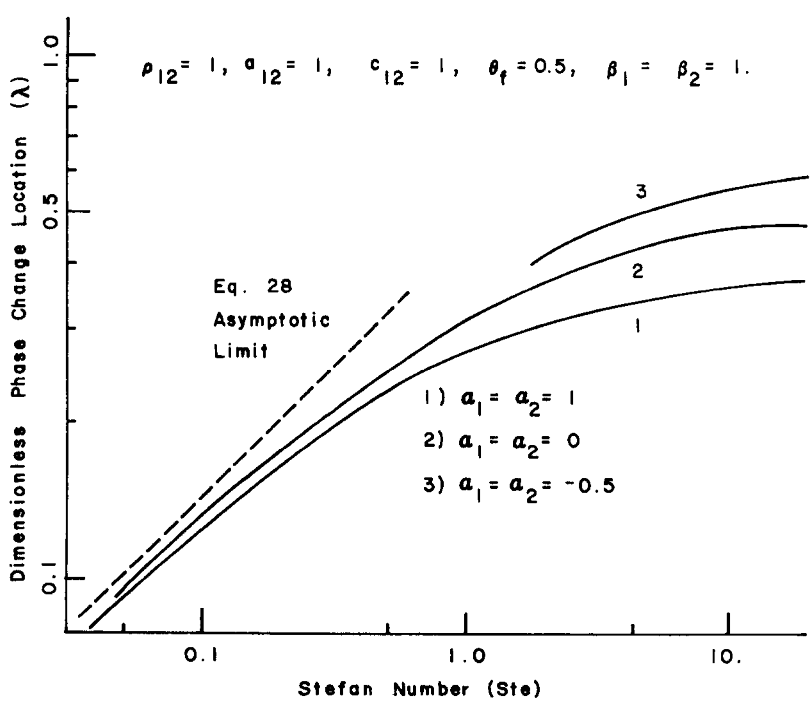

FIG. 2. Dimensionless phase change location vs Stefan number.

An error was found in equation (43) of Cho and Sunderland (which corresponds to equation (27) of the present work). Equation (43) of Cho and Sunderland was missing a single term which was required for equation (43) to be in conformity with equation (24) of Cho and Sunderland. With this change, equation (27) reduces to equation (43) of Cho and Sunderland if the specific heats are not a function of temperature (α_1 and α_2 are zero).

The present solution procedure has been confirmed by comparing special cases with the Newmann solution (constant thermal properties for each phase), and with an unpublished numerical code which uses finite differences to solve equations (1) and (2) directly.

RESULTS AND DISCUSSION

Perhaps the most interesting calculated parameter related to phase change problems is the location of the phase change front. The location of the phase change front is given by

$$S(t) = 2\lambda\sqrt{(a_{01}t)}.$$

On Fig. 2 the dimensionless phase change location, λ, is plotted as a function of the Stefan number (*Ste*), for three special cases of α_1 and α_2. For large Stefan numbers, the dimensionless phase change location approaches a constant value. As the Stefan number decreases, the dimensionless phase change location asymptotically approaches a value which may be derived assuming a quasi-steady state temperature profile

$$\lambda \simeq \left[\frac{(2+\beta_1\theta_f)}{(1+\beta_1\theta_f)}\frac{\theta_f\, Ste}{4}\right]^{1/2}, \quad Ste \ll 1. \tag{28}$$

From the above analysis it is clear that including the effects of temperature dependence of the specific heat are most important at low values of the dimensionless heat of fusion. At higher values of the heat of fusion (low values of *Ste*), the variations in the thermal conductivity are important, but the effects of variable specific heats diminishes.

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APPENDIX: MODIFIED ERROR FUNCTION

Consider the second-order non-linear ordinary differential equation

$$\frac{d}{d\eta}(1+\delta\phi_{\gamma\delta})\frac{d\phi_{\gamma\delta}}{d\eta}+2\eta(1+\gamma\phi_{\gamma\delta})\frac{d\phi_{\gamma\delta}}{d\eta}=0 \tag{A1}$$

with boundary conditions

$$\phi_{\gamma\delta}(0) = 0 \tag{A2}$$

$$\lim_{\eta\to\infty}\phi_{\gamma\delta}(\eta) = 1. \tag{A3}$$

The solution (approximated in this work by a Runge–Kutta scheme) to equations (A1)–(A3) is defined as the modified error function. The following theorem presents a result that is useful in the solution of the phase change problem presented in the main body of this work.

The following function:

$$\phi = \theta_0+(\theta_\infty-\theta_0)\phi_{\gamma\delta\eta}\sqrt{\left(\frac{1+\alpha\theta_0}{1+\beta\theta_0}\right)} \tag{A4}$$

where

$$\gamma = \frac{\alpha(\theta_\infty-\theta_0)}{1+\alpha\theta_0} > -1, \quad 1+\alpha\theta_0 > 0 \tag{A5}$$

$$\delta = \frac{\beta(\theta_\infty-\theta_0)}{1+\beta\theta_0} > -1, \quad 1+\beta\theta_0 > 0 \tag{A6}$$

satisfies the following equation:

$$\frac{d}{d\eta}(1+\beta\theta)\frac{d\theta}{d\eta}+2\eta(1+\alpha\theta)\frac{d\theta}{d\eta}=0 \tag{A7}$$

with boundary conditions

$$\theta(0) = \theta_0 \tag{A8}$$

$$\lim_{\eta\to\infty}\theta(\eta) = \theta_\infty. \tag{A9}$$

UN PROBLEME DE CHANGEMENT DE PHASE AVEC CONDUCTIVITE ET CAPACITE THERMIQUE DEPENDANT DE LA TEMPERATURE

Résumé—On obtient une solution semi-analytique pour représenter la conduction thermique avec changement de phase dans un milieu semi-infini pour lequel les conductivités et les capacités thermiques des deux phases sont des fonctions linéaires de la température. Ce modèle élargit celui d'un travail antérieur pour inclure la dépendance des capacités thermiques vis-à-vis de la température.

EIN PHASENWECHSEL-PROBLEM MIT TEMPERATURABHÄNGIGER WÄRMELEITFÄHIGKEIT UND SPEZIFISCHER WÄRMEKAPAZITÄT

Zusammenfassung—Es wird eine halbanalytische Lösung zur Modellierung des Wärmetransports durch Wärmeleitung mit Phasenwechsel in einem halbunendlichen Spalt vorgestellt, in dem Wärmeleitfähigkeit und Wärmekapazität beider Phasen linear von der Temperatur abhängen. Dieses Modell erweitert ein früheres Modell durch Berücksichtigung der Temperaturabhängigkeit der spezifischen Wärmekapazität.

ЗАДАЧА ТЕПЛОПРОВОДНОСТИ ПРИ НАЛИЧИИ ФАЗОВОГО ПЕРЕХОДА С УЧЕТОМ ТЕМПЕРАТУРНОЙ ЗАВИСИМОСТИ ТЕПЛОЕМКОСТИ И КОЭФФИЦИЕНТА ТЕПЛОПРОВОДНОСТИ

Аннотация—Получено полуаналитическое решение модельной задачи теплопроводности при фазовом переходе в полубесконечной пластине в случае, когда теплопроводность и теплоемкость обеих фаз являются линейными функциями температуры. Данная модель является более полной, чем рассмотренная в предыдущей работе, поскольку учитывает температурную зависимость теплоемкости.