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The Apparent Mass Capacity Method for Transient Diffusion Problems with Change of Phase

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Abstract

A numerical method for treating transient diffusion involving change of phase is presented. In other methods of dealing with this class of problems, the mass flux balance at the moving phase boundary requires explicit treatment of two distinct phases. The technique, originating from the apparent heat capacity method in transient heat conduction with the phase change, avoids the difficulty by transferring the concentration discontinuity at the boundary to smoothed physical property variations near the moving front. This technique accomodates the nonlinearities which preclude use of analytical solutions. It was tested against known analytical solutions for simple cases and turned out to be quite accurate.

I. Introduction

Solutions of problems involving transient heat conduction accompanied by a solId-liquid transformation present difficulties not encountered in single-medium situations because of the moving phase-change boundary and the production or removal of heat at this location. Analytical solutions are available only for simple boundary conditions and for temperature-independent thermal properties[1-9]. Some practically-important processes, such as pulse surface heating by laser or electron beam irradiation, or welding in complex geometries are not amenable to analytic solution and must be dealt with numerically. Precluding the use of commercial partial differential equation solvers, the presence of the moving phase boundary requires that the user must develope and implement the numerical method[10-14].

Metal oxidation problems that involve a change of phase from metal to oxide within the material represent a moving-front situation which is formally identical to that associated with progression of a melt layer in a heated solid. The analog of the heat of fusion is the difference in the oxygen concentrations on the two sides of the phase boundary. This difference is a thermodynamic quantity determined by the phase diagram of the metal-oxygen system. By identifying common dimensionless parameters in the two processes, the oxide-metal transition can be treated in the same way as the solid-liquid transformation.

Recently several authors [15-18] have published new schemes, so-called 'apparent' heat capacity method, which enable the users to deal with the transient heat conduction with change of phase as pseudo single-phase problem. In the medium undergoing phase change 'equivalent' heat capacity can be written as $C_p + L\delta(T\text{-}T_f)$, where L is latent heat of fusion. In the apparent heat capacity $L\delta(T\text{-}T_f)$ of the 'equivalent' heat capacity is replaced by $L/\Delta T$ around T_f in a manner that correctly accounts for the heat of fusion contains. That is, melting is spread over a nonzero temperature interval ΔT, instead of occurring discontinuously at a unique temperature at a unique plane. It is incorporated into the transient heat conduction equation in the method joining two different phase media in one medium.

In the present work $L/\Delta T$ in the apparent heat capacity is substituted again by Gaussian distribution, $\frac{L}{\sqrt{\pi}\Delta T_f}\exp\left[-\left\{\left(T-T_f\right)/\Delta T_f\right\}^2\right]$, to avoid the discontinuity of heat capacity near ΔT. Thus, firstly, this new version of apparent heat capacity method is tested against the analytical solutions of transient heat conduction problems with two simple boundary conditions, constant surface temperature and constant surface heat flux. Secondly, apparent mass capacity method is developed based on the apparent heat capacity technique and compared to the analytical solution for parabolic metal oxidation case (i.e., the oxide layer thickness is proportional to $t^{1/2}$). Last it was tested for a three-phase scaling problem, zirconium steam oxidation taken as an example, in which two layers grow parabolically in time.

II. Formulation of Transient Heat and Mass Transfer Problems with Change of Phase

II.1 Formulation of the Problem in Semi-infinite Medium

Transient Heat Transfer problems	Domain	Transient Mass Transfer problems
$\rho C_{pI}\frac{\partial T_I}{\partial t}=k_I\frac{\partial^2 T_I}{\partial x^2}$	$0\le x\le x_f$	$\frac{\partial C_I}{\partial t}=D_I\frac{\partial^2 C_I}{\partial x^2}$
$\rho C_{pII}\frac{\partial T_{II}}{\partial t}=k_{II}\frac{\partial^2 T_{II}}{\partial x^2}$	$x_f\le x\le\infty$	$\frac{\partial C_{II}}{\partial t}=D_{II}\frac{\partial^2 C_{II}}{\partial x^2}$
$-k_I\left(\frac{\partial T_I}{\partial x}\right)_{x_f}+k_{II}\left(\frac{\partial T_{II}}{\partial x}\right)_{x_f}=\rho L\frac{dx_f}{dt}$	Heat or Mass Balance at Interface	$-D_I\left(\frac{\partial C_I}{\partial x}\right)_{x_f}+D_{II}\left(\frac{\partial C_{II}}{\partial x}\right)_{x_f}=\left(C_A-C_B\right)\frac{dx_f}{dt}$
$T_I(x,0)=T_{II}(x,0)=T_i$	Initial Condition	$C_I(x,0)=C_{II}(x,0)=C_i$
$T_I(0,t)=T_s$ or $\frac{\partial T_I(0,t)}{\partial x}=const$ $T_{II}(\infty,t)=T_i$	Boundary Conditions	$C_I(0,t)=C_s$ $C_{II}(\infty,t)=C_i$

II.2 Apparent Capacity Formulation

$$\tilde{C}_p=C_p+\frac{L}{\sqrt{\pi}\Delta T_f}\exp\left[-\left\{\left(T-T_f\right)/\Delta T_f\right\}^2\right]$$

Transient Heat Transfer problems	Domain	Transient Mass Transfer problems
$\rho \tilde{C}_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right)$	$0 \le x \le \infty$	$\tilde{E}\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(E \frac{D}{D_l}\frac{\partial C}{\partial x}\right)$
$T(x,0) = T_i$ $T(0,t) = T_s$ or $\frac{\partial T(0,t)}{\partial x} = const$ $T(\infty,t) = T_i$	Initial and Boundary Condition	$C(x,0) = C_i$ $C(0,t) = C_s$ $C(\infty,t) = C_i$

III. Solutions for Transient Heat Conductions with Change of Phase

III.1 Constant Surface Temperature Condition

Analytical Solution: Neumann's Solution

$$\theta = 1 - (1 - A)\frac{\text{erfc}\eta}{\text{erfc}\lambda} \qquad 0 \le \eta \le \lambda \text{ (liquid)}$$

$$\theta = A\frac{\text{erfc}\eta}{\text{erfc}\lambda} \qquad \lambda \le \eta \le \infty \text{ (solid)}$$

where $\theta = \frac{T - T_i}{T_s - T_i}$, $A = \frac{T_f - T_i}{T_s - T_i}$, $\eta = \frac{x}{2\sqrt{\alpha t}}$, and $\lambda = \frac{x_f}{2\sqrt{\alpha t}}$.

λ is determined by: $\frac{\sqrt{\pi}\lambda}{\text{Ste}}\exp\left(\lambda^2\right) = \frac{1-A}{\text{erf}\lambda} - \frac{A}{\text{erfc}\lambda}$ where $\text{Ste} = \frac{C_p\left(T_s - T_i\right)}{L}$.

Numerical Solution

Figure 2.a)

III.2 Constant Surface Heat Flux Condition

Analytical Solution: Goodman's Solution

$$\theta = \frac{1}{\text{Ste}}\left(-\frac{1}{4} + \frac{1}{4}\sqrt{1 + 4\eta_f} + \eta_f\right) \text{ where } \text{Ste} = \frac{C_p T_f}{L},\ \eta_f = \frac{x_f}{\beta}, \text{ and } \beta = \frac{\alpha\rho L}{q}.$$

Goodman's position of the melt front is: $\tau = \frac{\eta_f}{6}\left(\eta_f + 5 + \sqrt{1 + 4\eta_f}\right)$ where $\tau = \frac{\alpha t}{\beta^2}$.

Numerical Solution

Figure 2.b)

IV. Solutions for Transient Diffusion Problems with Change of Phase

IV.1 Parabolic Scaling Problem in Two Phases

Neumann's Solution *vs*. Numerical Solution

Figure 3.a)

IV.2 Application to Zircaloy Corrosion: Parabolic Scaling Problem in Three Phases

Pawel's Solution *vs*. Numerical Solution

Figure 3.b)

V. Conclusions

The apparent capacity method offers a computational tool intermediate between analytical solutions, which are useful only in restricted cases, and detailed numerical solutions, which are generally complex, require development of numerical methods and are applicable only for particular situations.

Comparison of the apparent capacity technique with available analytical solutions of simple moving boundary problems shows the accuracy to be satisfactory. In fact, the computation errors in the location of the phase change interface and the total energy or mass absorbed turned out to be within a few percent over a wide range of parameters.

The application of the apparent capacity method can be extended to any geometry, multiple media case, temperature-dependent material property problems, and non-linear boundary conditions. The technique can use readily-available commercial partial differential equation solvers.

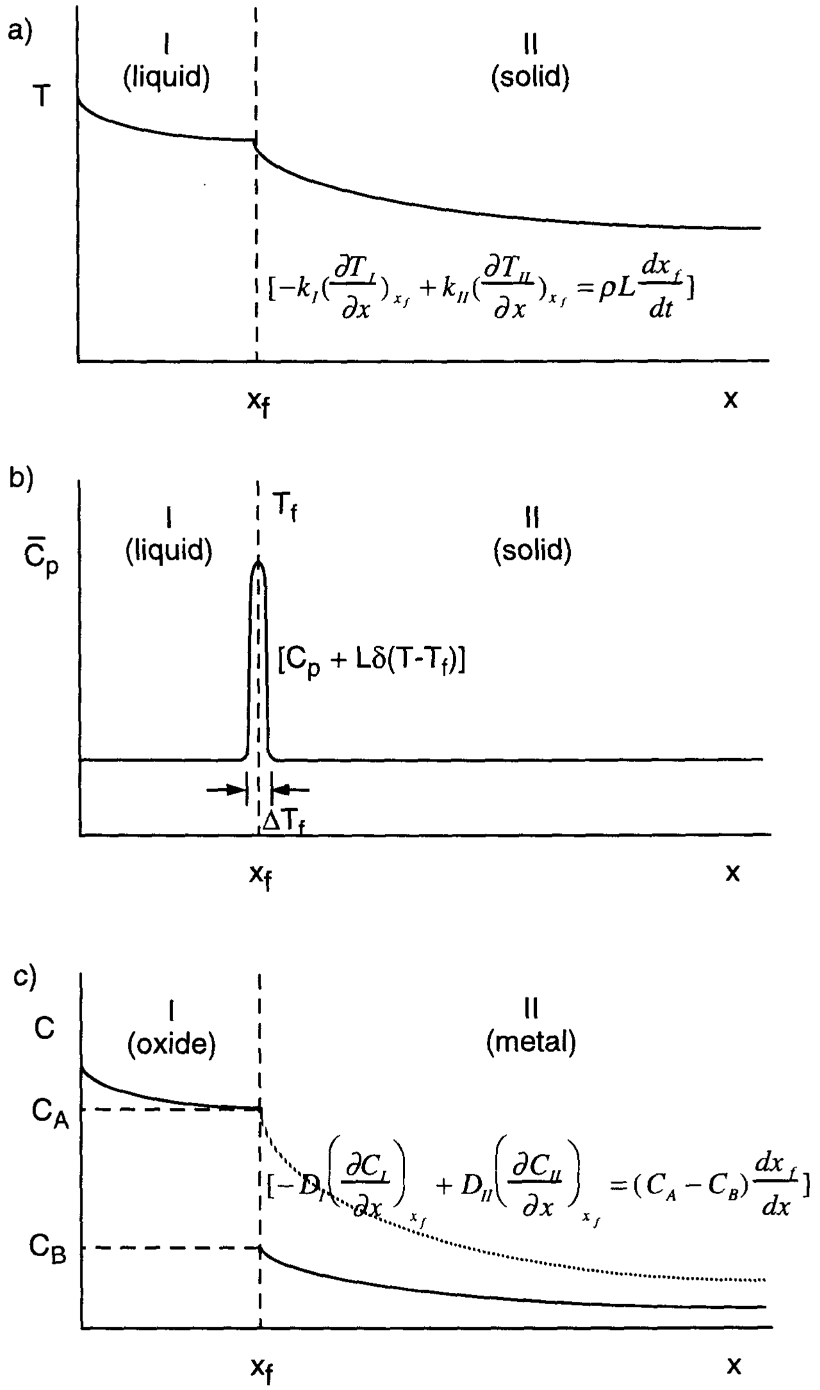

Figure 1 a) temperature profile in medium undergoing change of phase b) apparent heat capacity c) oxygen concentration profile in oxidizing medium

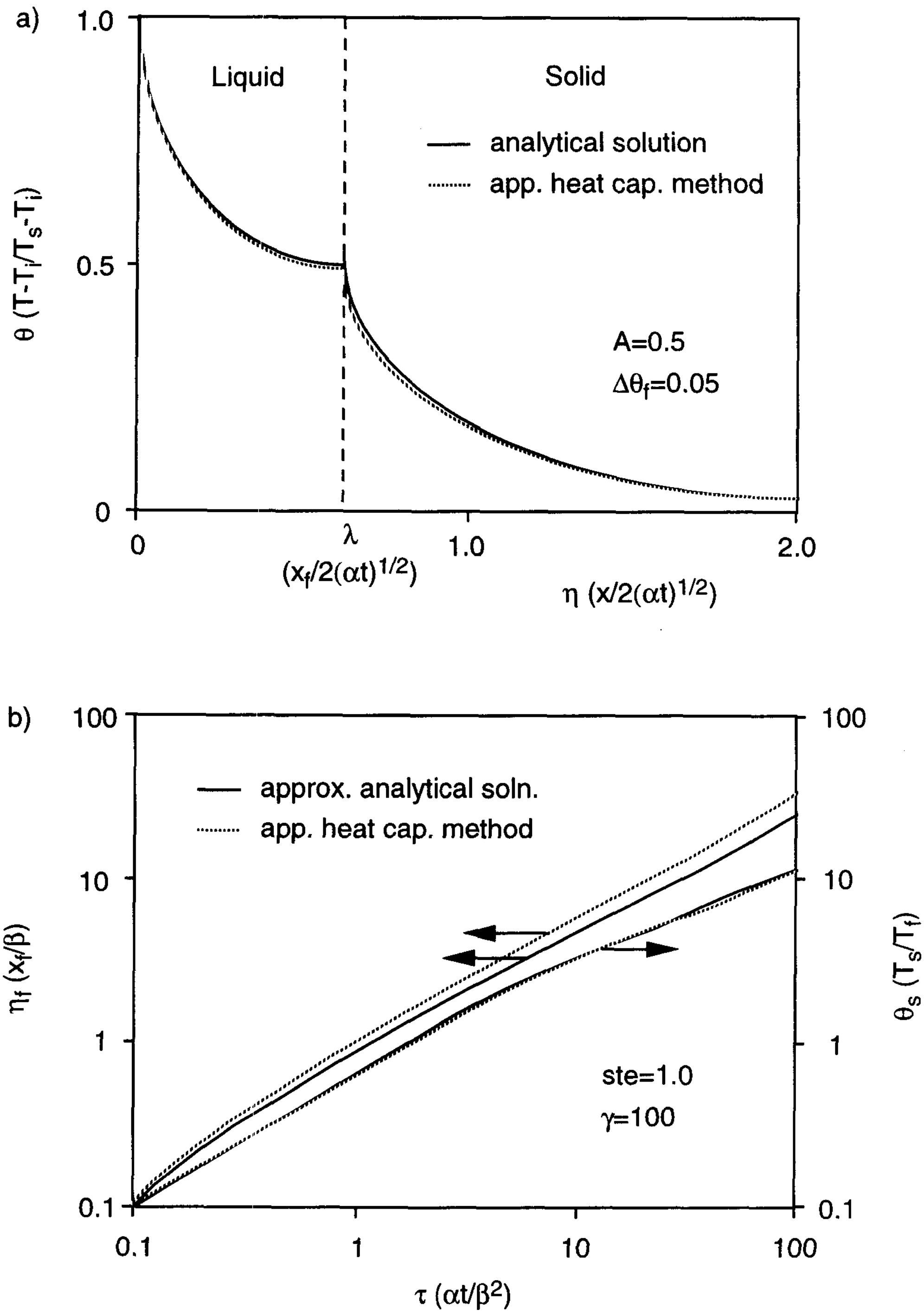

Figure 2 Comparison of numerical solution by apparent heat capacity method with analytical solutions in a) constant surface temperature and b) constant surface heat flux cases

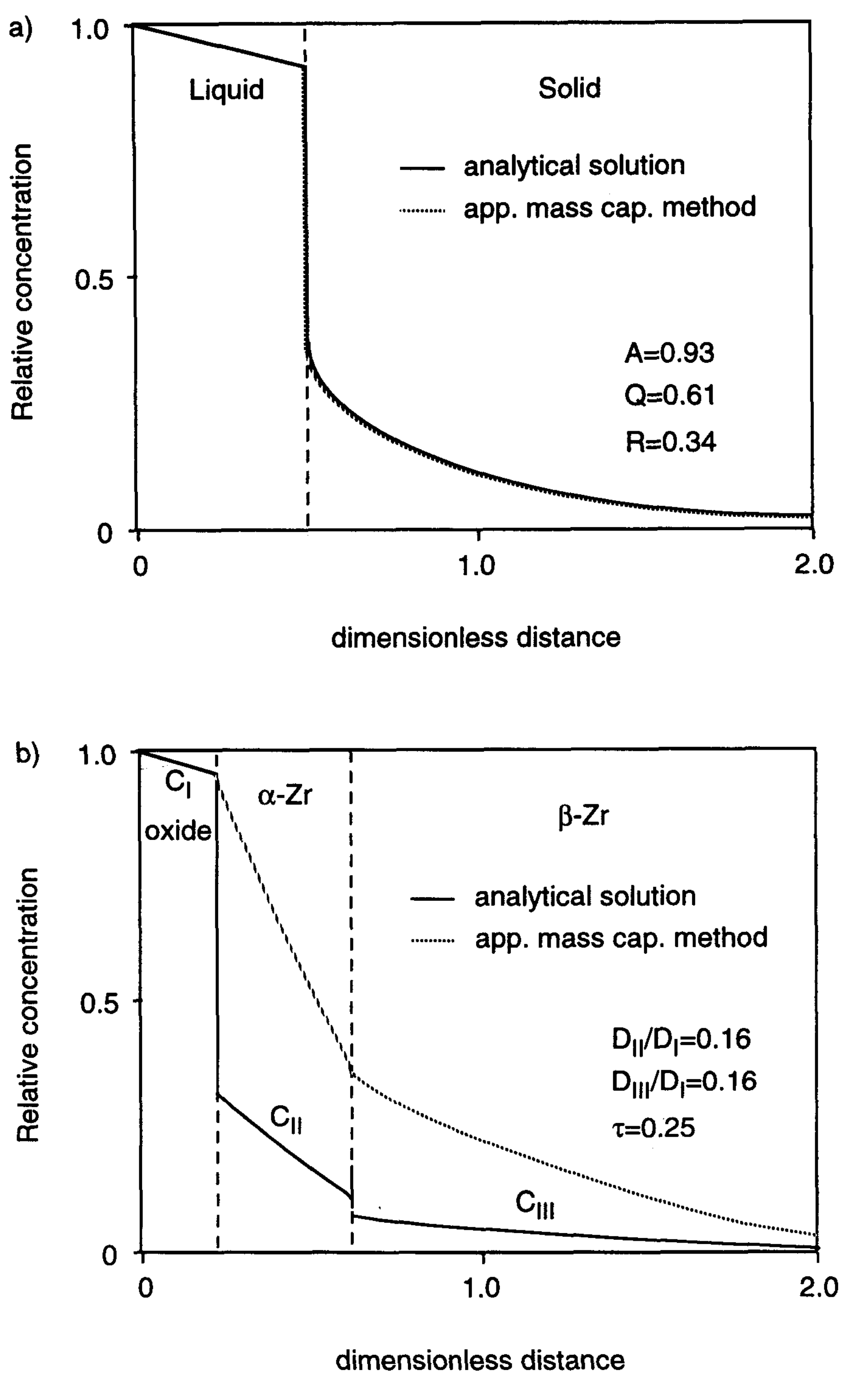

Figure 3 a) oxygen concentration profile during scaling of a metal b) oxygen concentration profile in oxidized zircaloy (both analytical and numerical solution by apparent mass capacity method fall on the solid curves)