Generalized Phase Change Model for Melting and Solidification with Internal Heat Generation

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Melting and solidification of materials with internal heat generation are investigated. Solutions to several problems by an enthalpy method have been obtained and presented. The solutions reveal the existence of a mushy zone in which liquid and solid coexist. This distinct mushy zone, which is not allowed for in the classical phase change model, is located between the pure liquid zone on one side and the pure solid zone on the other. It exhibits unique characteristics and plays a significant role in phase change analysis. Results confirm that a generalized phase change model should consist of three possible zones: the liquid, mushy, and solid.

Nomenclature

b	= arbitrary length
c	= specific heat
i	= enthalpy
k	= conductivity
n	= unit vector
r	= mass melting rate per unit mixture volume
q	= internal heat generation rate per unit mixture volume
s_1, s_2	= first and second interfaces
t	= time
$\bar{t}$	= dimensionless time
T	= temperature
V	= volume
x	= physical coordinate normal to wall
α	= thermal diffusivity
ϵ	= liquid volume fraction
θ	= dimensionless enthalpy
λ	= latent heat of fusion per unit mass
ρ	= density
τ	= dimensionless distance
τ_p	= dimensionless interface location
ρ	= density
ϕ	= dimensionless temperature

Subscripts

i	= nodal location
l	= liquid

Superscripts

m	= time level
x	= saturated state

Introduction

HEAT transfer associated with phase change, either melting or solidification, has long been a subject of considerable importance in various engineering applications, such as ice making, welding, casting, and nuclear reactor safety analysis. To analyze a material undergoing a phase change, the prevailing mathematical model is often based on the classical two-zone concept that assumes a pure liquid zone adjacent to a pure solid zone, separated by an interface, with one zone growing and the other receding.

When the melting is induced by an internal heating, a third zone may appear that has not been accounted for in the classical phase change model. This third zone is located between the pure liquid and solid zones mentioned above. It is a mushy zone in which liquid and solid coexist; the liquid or solid fraction may vary throughout the mushy zone. There are a few papers dealing with problems of this nature. Two mathematical papers[1,2] examined the phase change induced by an internal heat source (sink), with one[1] emphasizing the convergency of a finite-difference technique and the other[2] emphazing the existence and stability of superheated (supercooled) regions. Three other recent articles[3-5] are concerned with the phase change induced by the internal radiation absorption or emission due to internal or external radiation. Other applications include the melting of nuclear reactor materials by neutron heating or melting by electrical resistance heating. In these instances, the internal heat generation is relatively uniform throughout if the materials are not too large in physical size.

In the absence of an internal heat source or sink, it should be mentioned in passing that the mushy zone can also exist, although of very small width, at the interface when dendritic structures formed in a supercooled liquid.[6-8]

The purpose of this paper is to present dimensionless solutions of several simple phase change problems with uniform internal heat generation for the exposition of the mushy zone behavior. Solutions are obtained by an enthalpy method that can greatly simplify the mathematical complexity of moving interfaces in three possible zones and can illustrate how the mushy zone is evolved naturally during the phase change process.

The Generalized Phase Change Model

To describe the generalized three-zone model, consider the melting of a semi-infinite solid material with a uniform internal heat source, initially at a temperature lower than its melting temperature, with a sudden change of its surface temperature, say, to a temperature T_w above the melting temperature. For simplicity, in the following formulation, thermal physical properties of both phases are taken as constant and identical and the phase change is assumed to take place at a unique temperature. A typical temperature profile is shown in Fig. 1, which illustrates a mushy zone situated between the liquid and solid zones. In the absence of the heat source, the mushy zone is expected to vanish and the generalized three-zone model is reduced to the classical two-zone model.

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It is assumed that the solid/liquid mixture in the mushy zone maintains its identity so that the solid in the mushy zone, for example, would not be floated away and convected into the purely liquid zone. The assumption is reasonable if the density change after phase change is small or the liquid in the mushy zone is in the dispersed phase. Under such conditions, a definite boundary is maintained even at the $x=s_1$ boundary that is marked by a sudden jump in solid volume fraction, as will be seen later.

Following Ref. 4, the energy equation can generally be written as

$$\rho c\frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = q - \lambda r \tag{1}$$

The last term in this equation designates the latent heat contribution due to the phase change. In the liquid and solid zones, the latent heat term should be omitted since there is no internal phase change. In the mushy zone, however, both terms on the left-hand side are set to zero. If the resulting equation in the mushy zone is combined with the continuity (or species) equation of the liquid phase, they yield

$$\frac{\partial \epsilon}{\partial t} = \frac{q}{\rho_s \lambda} \tag{2}$$

The above equations are to be solved, subjected to the corresponding initial and boundary conditions in each region, as well as the two moving interface conditions at $x=s_1$ and s_2.

The interface condition at $x=s_1$, for example, is[4]

$$-k_l\frac{\partial T_l}{\partial x}\bigg|_{s_1^-} = (1-\epsilon\bigg|_{s_1^+})\rho_s\lambda\frac{\mathrm{d}s_1}{\mathrm{d}t} \tag{3}$$

which contains an additional term, $\epsilon(s_1^+)$, not found in the classical model. It is noted that the liquid volume fraction on the mushy side adjacent to the interface is not necessarily unity or zero; it is a time-dependent unknown to be solved from Eq. (2).

In the following, instead of solving the above equations in each region and matching them through the interfacial conditions, a much simpler technique, namely, the enthalpy method,[9] is employed. This method can eliminate both interfaces from consideration in the solution procedure and can consolidate the differential equations in the three regions into one.

By making an energy balance of a control volume fixed in space, one finds that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho i \mathrm{d}V = \int_A k \nabla T\cdot\hat{n}\mathrm{d}A + \int_V q\mathrm{d}V \tag{4}$$

As shown in Ref. 9, the differential equation for the liquid and solid zones [i.e. Eq. (1) with no latent heat term] can be recovered when Eq. (4) is applied to a control volume in those regions. Similarly, it can be easily shown that the equation in the mushy region can be recovered from the above if the latter is applied to the mushy region. Furthermore, if it is applied to a control volume across an interface, the appropriate interfacial condition, as in Eq. (3), can be derived.[4] For one-dimensional problems, Eq. (4) reduces to

$$\rho\lambda\Delta x\frac{\partial \theta}{\partial t} = \left(k\frac{\partial T}{\partial x}\right)\bigg|_{x+\Delta x} - \left(k\frac{\partial T}{\partial x}\right)\bigg|_{x} + q\Delta x$$

where

$$\theta = \frac{1}{\rho\Delta x}\int_x^{x+\Delta x} \rho\frac{i-i_l^*}{\lambda}\mathrm{d}x$$

As $\Delta x \to 0$, it can be further simplified and cast into a dimensionless form

$$\frac{\partial \theta}{\partial \bar{t}} = \frac{\partial^2 \phi}{\partial \tau^2} + 1 \tag{5a}$$

where

$$\phi = \frac{c(T-T_{\rm sat})}{\lambda}, \quad \bar{t} = \frac{qt}{\rho\lambda}, \quad \tau = \left(\frac{q}{\alpha\rho\lambda}\right)^{1/2} x \tag{5b}$$

The dimensionless enthalpy θ is treated as the dependent variable and the dimensionless temperature ϕ has to be expressed in terms of θ. From the definitions of θ and ϕ, we find the necessary relationships:

$$\phi = \theta \quad \text{when } \theta \geq 0 \quad \text{(liquid region)} \tag{6a}$$

$$= 0 \quad \text{when } 0 \geq \theta \geq -1 \quad \text{(mushy region)} \tag{6b}$$

$$= \theta + 1 \quad \text{when } \theta \leq -1 \quad \text{(solid region)} \tag{6c}$$

Solutions will be presented in the next section for a given initial condition $\theta(0,\tau)$ and the boundary conditions $\theta(\bar{t},\tau_i)$, $i=1$ and 2.

It is noted that without an internal heat source, the corresponding equation is

$$\frac{\partial \theta}{\partial \bar{t}} = \frac{\partial^2 \phi}{\partial \tau^2} \tag{7a}$$

provided $\bar{t}$ and τ are defined as

$$\bar{t} = \alpha t/b^2, \quad \tau = x/b \tag{7b}$$

Solutions and Discussion

It is unlikely that Eq. (5) together with Eq. (6) can be solved analytically. An implicit finite-difference technique is used here. The finite-difference representation of Eq. (5) for an interior node i can be written as

$$\theta_i^{m+1} = \theta_i^m + [\phi_{i-1}^{m+1} + \phi_{i-1}^{m+1} - 2\phi_i^{m+1}]\frac{\Delta\bar{t}}{(\Delta\tau)^2} + \Delta\bar{t} \tag{8}$$

The solution procedure is to employ θ values at time m to evaluate all ϕ by Eq. (6). These ϕ values are substituted into the right-hand side of Eq. (8) to calculate θ^{m+1} values, which in turn are used to evaluate ϕ and the new θ^{m+1} values. The iteration process continues until the desired accuracy is achieved. The process is found to converge rapidly.

To confirm the accuracy of the method, the method is applied to solve Eq. (7a) [which is equivalent to Eq. (8) without the last term $\Delta\bar{t}$] for the melting of a semi-infinite solid with no internal heat generations, initially at its melting temperature $\theta(0,\tau) = -1.0$ and subjected to the boundary conditions $\theta(\bar{t},0) = 0.3$ and $\theta(\bar{t},\infty) = -1.0$. Excellent agreement was found when the dimensionless temperature profiles and

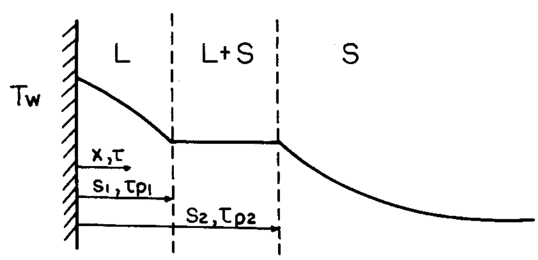

Fig. 1 Generalized three-zone phase change model.

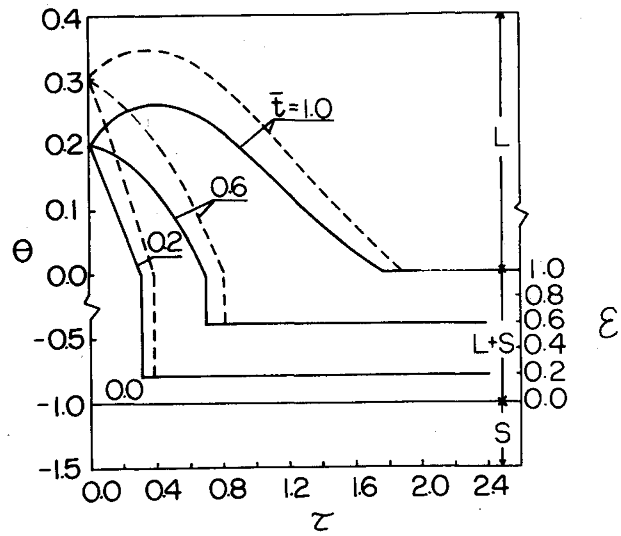

Fig. 2 Enthalpy and liquid fraction profiles: S = solid, L = liquid, $\theta(\tau=0)=0.2$ for solid line, 0.3 for dotted line, $\theta(\tau=\infty)=-1.0+\bar{t}$, $\theta(\bar{t}=0)=-1.0$.

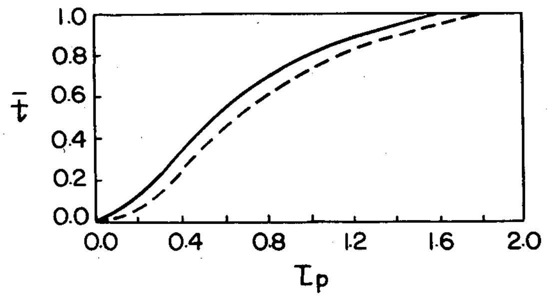

Fig. 3 Interfacial location: S = solid, L = liquid, $\theta(\tau=0)=0.2$ for solid line, 0.3 for dotted line, $\theta(\tau=\infty)=-1.0+\bar{t}$, $\theta(\bar{t}=0)=-1.0$.

thicknesses of the melt layers are compared with those of the existing exact solutions.

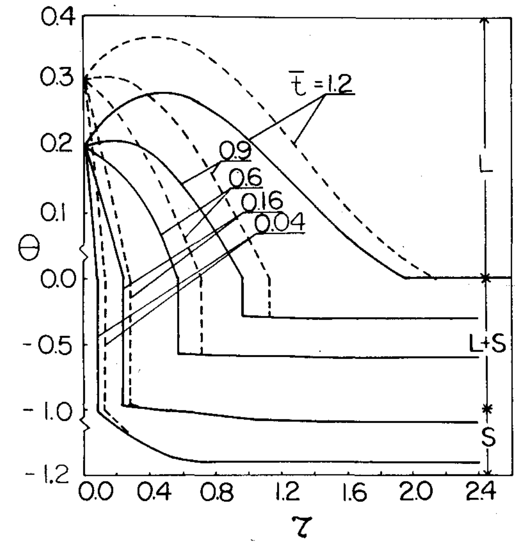

Fig. 4 Enthalpy and liquid fraction profiles: $\theta(\tau=0)=0.2$ for solid line, 0.3 for dotted line, $\theta(\tau=\infty)=-1.2+\bar{t}$, $\theta(\bar{t}=0)=-1.2$.

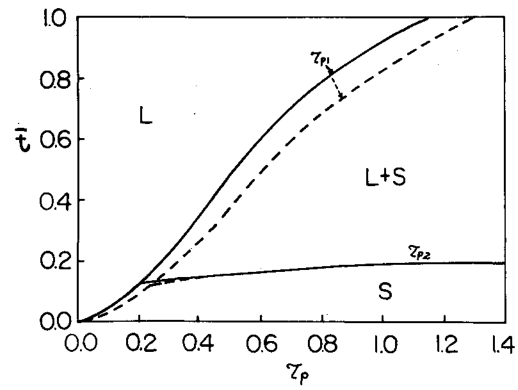

Fig. 5 Interfacial location and the liquid, mushy, and solid regions: $\theta(\tau=0)=0.2$ for solid line, 0.3 for dotted line, $\theta(\tau=\infty)=-1.2+\bar{t}$, $\theta(\bar{t}=0)=-1.2$.

Melting of a Semi-infinite Solid Initially at Its Melting Temperature with an Internal Heat Generation

Equation (8) is solved, subjected to $\theta(0,\tau)=-1.0$, $\theta(\bar{t},0)=0.2$ or 0.3, and $\theta(\bar{t},\infty)=-1.0+\bar{t}$. To better illustrate the mushy zone, the dimensionless enthalpy profiles $\phi(\bar{t},\tau)$ are plotted in Fig. 2 vs τ for various $\bar{t}$. It is noted that the liquid zone lies in the $\theta\geq 0$ region, the mushy zone in $0\geq\theta\geq -1.0$, and the solid zone in $\theta\leq -1.0$. In the liquid zone, the enthalpy (or temperature) profile develops a peak away from the surface boundary at a later time. The peak shifts away from the surface as the melt layer grows. Physically what happens is that, when the melt layer gets thicker, the gradient of the temperature profile becomes smaller. The conduction heat-transfer mechanism becomes incapable of removing all the heat generated, resulting in a net rise of temperature internally. In the mushy zone, the liquid fraction ϵ is shown to increase from 0 to 1 when the dimensionless time proceeds from 0 to 1. The interface between the melt layer and the mushy layer is located at the intersection of a θ profile and $\theta=0$ line. It is interesting to note that the enthalpy has a jump at the interface before the material turns completely into liquid (i.e., $\bar{t}<1.0$). This unique behavior is attributed to the existence of the mushy zone. Such a jump could not be detected in the temperature ϕ vs τ plot. Finally, the thickness of the melt layer vs time is given in Fig. 3. As it approaches the end of the duration to complete the phase transformation (i.e., $\bar{t}\rightarrow 1$), the remaining solid fraction $(1-\epsilon)$ in the mushy zone becomes smaller and smaller. Since the heat is continuously generated at the same rate coupled with the heat conduction to the interface from the liquid side, the remaining solid melts into liquid at the end. This explains the rapid growth of the melt layer in Fig. 3 as $\bar{t}\rightarrow 1$.

Melting of a Semi-infinite Solid Initially at a Temperature Lower than Its Melting Point with an Internal Heat Generation

The conditions under consideration are $\theta(0,\tau)=-1.2$, $\theta(\bar{t},0)=0.2$ or 0.3, and $\theta(\bar{t},\infty)=-1.2+\bar{t}$; the solutions are presented in Fig. 4. While all the observations made above are equally applicable here, attention is directed to a time period of $\bar{t}<1.2$ in the solid and mushy zones. Contrary to the above case, the liquid fraction (= $|\theta|$ value) profile in the mushy zone is no longer constant. Furthermore, a period of short duration exists when all three zones coexist. The latter can be clearly seen by referring to Fig. 5, which plots both interface fronts τ_{p1} and τ_{p2} vs time (see also Fig. 1). It is seen that as time increases, the original solid material splits into two zones (liquid and solid), then into three zones (liquid, mushy, and solid) and finally into two zones (mushy and liquid). Naturally, they eventually all transform into the liquid phase after $\bar{t}>1.2$.

Melting and Solidification of a Semi-infinite Solid with an Internal Heat Generation

Consider the case of a semi-infinite solid initially at a uniform temperature, $\theta(0,\tau)=-1.2$, below the melting point, which is heated by internal heating such that $\theta(\bar{t},\infty)=-1.2+\bar{t}$. The boundary is maintained at its initial

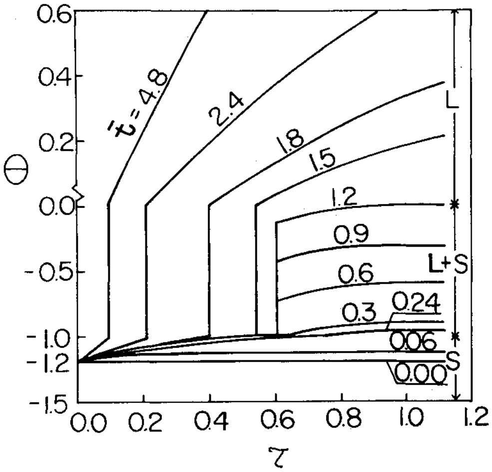

Fig. 6 Enthalpy and liquid fraction profiles: $\theta(\tau=0)=-1.2$, $\theta(\tau=\infty)=-1.2+\bar{t}$, $\theta(\bar{t}=0)=-1.2$.

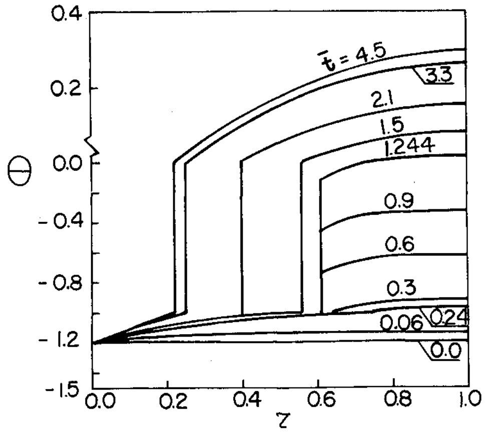

Fig. 7 Enthalpy and liquid fraction profiles: $\theta(\tau=0)=-1.2$, $\theta(\tau=2)=-1.2$, $\theta(\bar{t}=0)=-1.2$.

temperature of $\theta(\bar{t},0)=-1.2$. Figure 6 shows that as the solid is being heated by the internal heat generation, part of it becomes mushy. The mushy zone widens as the solid zone is shrinking. However, it is interesting to point out that, at some later time (see $\bar{t}=0.6$, 0.9, and 1.2 curves in the figure), the mushy zone fails to advance further until the mushy zone vanishes by transforming itself into the liquid phase. Such a quasisteady-state phenomenon occurs because, as time proceeds, the conduction heat transfer away from the interface to the solid eventually catches up with and exceeds the internal heat generation rate. The solid zone resists receding until the mushy zone is melted away. After the liquid zone appears on the right-hand side of the interface, additional heat is conducted to the interface from the liquid side (see, for example, $\bar{t}=1.5$ curve) to override the heat loss to the solid, resulting in further erosion of the remaining solid layer.

Melting and Solidification of a Slab with an Internal Heat Generation

Finally, the phase change in a finite slab is considered. The conditions chosen are $\theta(0,\tau)=\theta(\bar{t},0)=\theta(\bar{t},2)=-1.2$ with the

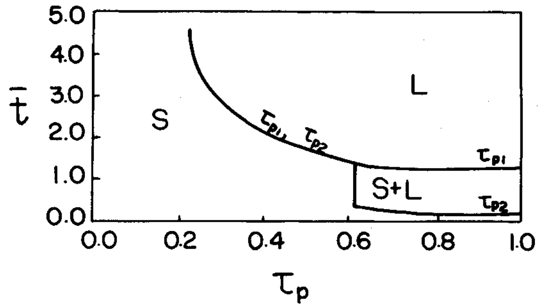

Fig. 8 Interfacial location-time: $\theta(\tau=0)=-1.2$, $\theta(\tau=2)=-1.2$, $\theta(\bar{t}=0)=-1.2$.

results presented in Figs. 7 and 8. Due to the symmetry of the problem, only solutions for a half-region are given. Many features exhibited in the previous case also prevail here, including the quasisteady-state phenomenon.

Conclusions

Solutions of several phase change problems with internal heat generations have been obtained and presented. The existence and characteristics of a mushy zone have been illustrated and discussed. This mushy zone is in addition to the liquid and solid zones in the classical phase change model. This confirms that a generalized model to allow for internal heat generation should constitute three zones: the liquid, solid, and mushy. The latter plays a significant role in phase change and should not be ignored.

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