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A Mushy-Zone Model with an Exact Solution

A. D. SolomonD. G. WilsonV. Alexiades

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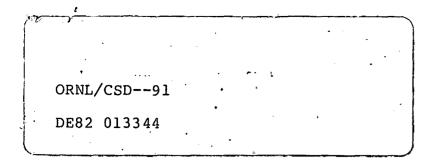
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A. D. Solomon D. G. Wilson V. Alexiades

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A MUSHY ZONE MODEL WITH AN EXACT SOLUTION

A. D. Solomon D. G. Wilson V. Alexiades

ABSTRACT

In this paper we propose a very simple model of a mushy zone which admits of an explicit solution. To our knowledge, it is the only instance where an actual observation of the mushy zone width and structure is used as a partial basis for the model definition. The model rests upon two unknown parameters. The first determines the relation between the equilibrium temperature gradient and the mushy zone width. The second depends upon the dendritic structure in the mushy zone, and is related to the solid fraction. Both can be estimated from experiments. We will limit ourselves to defining the model, presenting its closed form solution, and giving tables from which the solution can be found explicitly. It is shown that in most cases the predicted mushy zone is of very negligible importance.

1. INTRODUCTION

The term "mushy" zone appears in the literature on metal castings and solidification of other materials [2], [5], [6]. It refers to a zone where solid and liquid coexist and it appears to arise from the complex way in which liquid material solidifies, namely, by locally forming dendrites that leap into the liquid and entrap some of it. The zone of coexistence of liquid and solid may be very long or very short depending on the material and the conditions under which solidification takes place. Assuming that the dendrite comes into being because of some local supercooling and instability, one would believe that the greater the temperature gradient in the material the shorter will the width of the zone be. Indeed, this is one of the key results obtained from microscopic studies of the phase change front by Thomas and Westwater [5]. Roughly speaking, they found that the temperature gradient and the width of the zone obey the relation

width X temperature gradient = .031 degrees°C (1.1) for N-Octadecane paraffin wax under steady state conditions.

We are aware of very few attempts at modeling mushy zones of this type in phase change processes. A reasonable model was proposed by Tien and Geiger [6], who consider the mushy zone as the region between two isotherms (at the solidus and liquidus temperatures), in which the time rate of change of the solid fraction provides a heat generation effect. At the solidus front, the freezing of the remaining liquid provides the latent heat needed for the movement of the front whereas there is no latent heat effect at the liquidus front. Under a variety of assumptions the model for a semi-infinite body with constant

surface temperature admits a similarity solution. The case of timedependent surface temperature is treated in [3] by Goodman's heat balance integral method. Cho and Sunderland [4] obtained a similarity solution for the problem with initial temperature not at the liquidus temperature. The same basic mathematical model was generalized to the semilinear heat equation in any number of dimensions with the solid fraction being any function of temperature by Alexiades and Cannon [1] and its well-posedness was established.

In this paper we propose a very simple model of a mushy zone which is based on the observation (1.1) and admits of an explicit solution. The attraction of this model is that it is, to our knowledge, the only instance where an actual observation of the mushy zone width and structure is used as a partial basis for the model definition. The model rests upon two unknown parameters. The first determines the relation between the equilibrium temperature gradient and the mushy zone width, and based on [5] is taken as .031°C for N-Octadecane Paraffin wax. The second depends upon the dendritic structure in the mushy zone, and is related to the solid fraction. Both can be estimated from the kind of experiments described in [5]. We will limit ourselves to defining the model, presenting its closed form solution, and giving tables from which the solution can be found explicitly. As we will see, in most cases the predicted mushy zone is of very negligible importance; it is hoped that the present work can shed some light on the kind of material and experimental setup that can be used to study the mushy zone growth more thoroughly for situations where it might be of importance.

2. THE MODEL AND ITS SOLUTION

Consider a slab of material occupying the region $x \ge 0$. Initially the material is assumed to be in its liquid state at its solidification temperature T_{cr} . Beginning at time t = 0 a constant temperature $T_s < T_{cr}$ is imposed at x = 0. A solidification process ensues, in which three distinct regions can be distinguished.

- 1. Liquid, at temperature T_{cr} , occupying the region $x \ge Y(t)$;
- 2. Solid, at temperature $T(x,t) < T_{cr}$, occupying the region $0 \le x < X(t)$ where $X(t) \le Y(t)$;
- 3. "Mushy zone", at temperature $T(x,t) \equiv T_{cr}$ occupying the region $x(t) \leq x \leq Y(t)$.

Thus, the mushy zone is taken to be isothermal, and we make the following two assumptions on its structure:

- a) the material in the mushy zone contains a fixed fraction $\theta H(0 \le 0 \le 1)$ of the total latent heat H;
- b) its width is inversely proportional to the temperature gradient, that is,

$$T_{i}(X(t),t) [Y(t) - X(t)] = \gamma.$$
 (2.1)

The constants θ and γ are characteristics of the material. The solid fraction θ expresses the degree of "packing" of the mushy zone by crystals. Taking θ = constant, as we have done, amounts to assuming "uniform packing" throughout the mushy zone. On the other hand, (2.1) is suggested by the experimentally observed relation (1.1), and for the paraffin wax of [5],

 $\gamma = .031^{\circ}C$

Assumptions a), b) are of course simplifications of the actual physical process. In particular, a) is based on the assumption of "uniform" packing throughout the mushy zone, while b) is suggested by the observation (1.1) which was seen for the steady state.

From assumption a) and considerations of energy conservation we are led to the boundary condition

$$KT_{v}(X(t),t) = \rho H\{\theta X'(t) + (1-\theta) Y'(t)\}$$
(2.2)

In addition to (2.1), (2.2), the temperature T(x,t) obeys the conditions

$$T_{t}(x,t) = \alpha T_{xx}(x,t), \quad 0 < x < X(t)$$
 (2.3)

$$T(x,t) \equiv T_{cr}, \qquad x \ge X(t) \qquad (2.4)$$

$$T(0,t) = T_0, t > 0$$
 (2.5)

$$T(x,0) = T_{cr}, \qquad 0 < x < \infty$$
 (2.6)

Functions X(t), Y(t), T(x,t) satisfying (2.1) - (2.6) can easily be found in the form

$$\Gamma(x,t) = T_s + \Delta T \operatorname{erf}(x/2\sqrt{\alpha}t)/\operatorname{erf} \lambda, 0 < x < X(t), \quad (2.7a)$$

$$x(t) = 2\lambda \sqrt{at}$$
 (2.7b)

$$f(t) = 2\mu/\alpha t,$$
 (2.7c)

with

$$\mu = \lambda + [\gamma / \pi e^{\lambda^2} erf \lambda] / 2\Delta T \qquad (2.7d)$$

while λ is the unique root of the transcendental equation

$$\frac{\mathrm{St}}{\sqrt{\pi}} = \lambda \mathrm{e}^{\lambda^2} \mathrm{erf}\lambda + \frac{\gamma(1-\theta)}{\Delta T} \frac{\sqrt{\pi}}{2} (\mathrm{e}^{\lambda^2} \mathrm{erf}\lambda)^2 \qquad (2.7\mathrm{e})$$

where

$$\Delta T = T_{cr} - T_{s}$$

and

St =
$$c\Delta T/H$$

is the Stefan number for the process.

Note that for $\theta = 1$, (2.7e) reduces to the transcendental equation for the ordinary one-phase freezing problem. [2]

If St \approx 0, then (2.7e) implies

$$\lambda \approx [St/2(1 + \gamma(1-\theta)/\Delta T)]^{1/2},$$
 (2.8)

$$\mu \approx \lambda (1 + \gamma/\Delta T). \tag{2.9}$$

For each value of the dimensionless parameter

$$\omega = \frac{\gamma(1-\theta)}{\Delta T},$$

equation (2.7e) relates λ and the Stefan number St. Its graph and some values for various values of ω when $\theta = 0$ are given in Figure 1 and Table 1 (we have stopped arbitrarily at St \approx 25; in phase change processes involving metals, the Stefan number is generally of the order of 10).

The dimensionless relative mushy zone width

$$\Gamma = \frac{\Delta T}{\gamma} \frac{\mu - \lambda}{\lambda} = \frac{\sqrt{\pi}}{2} \frac{e^{\lambda^2} erf\lambda}{\lambda}$$
(2.10)

versus λ is pictured in Figure 2.

Thus, for a given material and imposed temperature T_s (i.e. for given ω and St), equation (2.7e) determines λ from which the temperature, interfaces and zone width can be found via (2.7) and (2.9). Example. For freezing N-Octadecane Paraffin wax in a thermal storage process we would anticipate St to be about .25, while with $\Delta T = 20^{\circ}C$, $\gamma/\Delta T \approx .0015$. Hence for all intents and purposes we will estimate λ to be approximately .1 (from table 1) and so, from Figure 2,

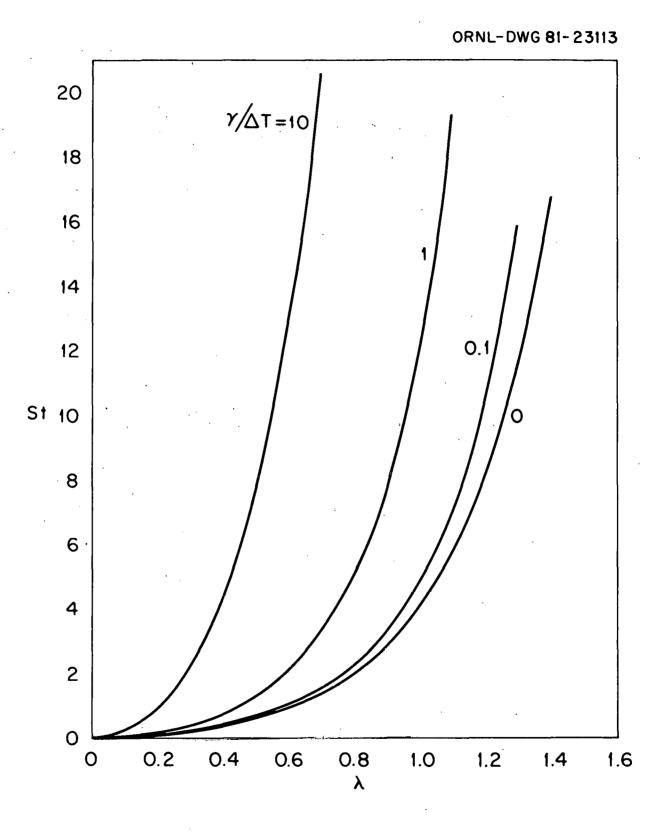


Figure 1. St as a Function of λ for 0 = 0.

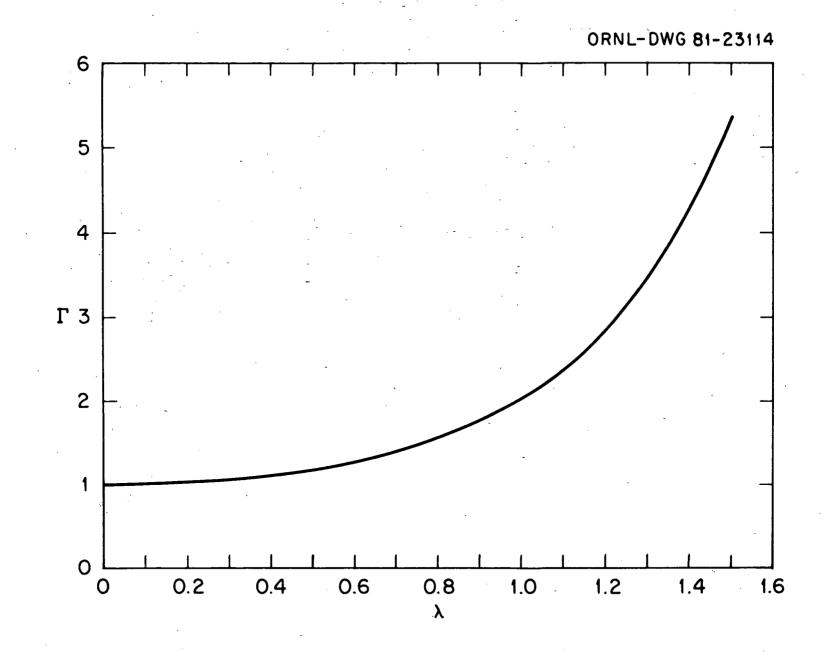
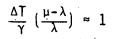


Figure 2. Γ as a Function of λ_{*}

ω



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 $\frac{\mu-\lambda}{\lambda} \approx .0015$

which provides an estimate of the mushy zone width, $Y(t) - X(t) \approx .0015 X(t)$.

Table 1	'
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St for $\theta = 0$

^Y /∆T		. 1	1.0	10.0
λ	0	.1	1.0	10.0
			•	,
0	0	. 0	0	. 0
.1	.020	.022	.040	.223
.2	.082	.091	.167	.926
.3	.191	.212	.394	2.222
.4	.356	.396	.753	4.326
.5	.592	.662	1.294	7.609
.6	.920	1.038	2.097	12.688
.7	1.373	1.565	3.296	20.601
.8	1.996	2.307	5.107	*
.9	2.858	3.362	7.898	*
1.0	4.060	4.884	12.303	*
1.1	5.755	7.124	19.441	*
1.2	8.172	10.491	*	*
1.3	11.663	15.688	*	*
1.4	16.776	*	*	*
1.5	24.370	*	*	*

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Nomenclature

С	specific heat	(KJ/Kg-°C)
Н	latent heat	(KJ/Kg)
K	thermal conductivity	(KJ/m-s-°C)
t	time	(s)
T	temperature	(°C)
Tcr	solidification temperature	(°C)
T _s	imposed surface temperature	(°C)
x	position variable	(m)
X	"solidus" front	(m)
Y .	"liquidus" front	(m)

Greek letters

α	K/co thermal diffusivity	(m²/s)
ρ	density	(KG/m ²)
θ	"packing" constant	
Y	zone width vs gradient constant	(°C)

REFERENCES

- V. Alexiades and J. Cannon, Free boundary problems in solidification of alloys, SIAM Journal of Mathematical Analysis 11 (1980), 254-264.
- [2] H. Carslaw and J. Jaeger, Conduction of Heat in Solids, 2nd ed., Oxford University Press, Oxford, 1959.
- [3] B. Chalmers, Principles of Solidification, John Wiley and Sons, New York, 1964.
- [4] S. Cho and J. Sunderland, Heat conduction problems with melting or freezing, Journal of Heat Transfer 910 (1969), 421-426.
- [5] L. Thomas and J. Westwater, Microscopic study of solid-liquid interfaces during melting and freezing, Heat Transfer-Houston, Chemical Engineering Progress Symposium Series 41 (1963), 155-164.
- [6] R. Tien and G. Geiger, A heat-transfer analysis of the solidification of a binary cutectic system, Journal of Heat Transfer 895 (1967), 230-234.

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