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The analytical solution of the one alloy solidification problem

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ABSTRACT

In this paper we obtain the analytical solution for a semi-infinite solidifying alloy. Thus, a three-phase problem including solid, solid–liquid, and liquid phases is analytically solved. Linearization of the heat conduction equation for an alloy is based on the method proposed in our recent papers.

Note that the method does not allow one to solve the problem of solidification of an alloy with the given function $\lambda(T)$ (liquid fraction). The dependence $\lambda(T)$ is determined from the condition of linearization of the heat conduction equation within the mush zone.

The analytical solution presented is an important test example for analysis of the numerical schemes used for systems with moving boundaries, e.g., for programs simulating vacuum arc remelting.

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1. Introduction

The general methodology of obtaining the analytical solution for an alloy with a finite crystallization range used in this paper is described in recent works [1,2], and we will consider it below in detail. Some solutions see in [3].

In order to obtain an analytical solution, we reformulate the equation of energy conservation in the mush zone in terms of the total enthalpy $H(T)$. The key idea of papers [1,2] consists of the requirement of constancy of the temperature conductivity in the mush zone. From this condition, we can find the volume fraction of the liquid phase $\lambda(T)$, which allows one to linearize the initial heat conduction equation. Thus, the method of obtaining the analytical solution for the heat conduction equation with a mush zone consists of the following:

1. We write the heat conduction equation for the total enthalpy of the system, including the evolution of the phase transition heat.
2. We demand that the temperature conductivity in the solid, solid–liquid (mush), and liquid phases is constant.
3. We write the condition of the constancy of the temperature conductivity in the mush zone $\alpha(T) = \alpha_{sl} = const$ in the form of a differential equation to obtain the temperature dependence of the liquid phase quantity $\lambda = \lambda(T)$ with the condition $\lambda(T_l) = 1$ (T_l is liquidus temperature).
4. We solve the differential equation obtained and find the explicit form of the function $\lambda = \lambda(T, \alpha_{sl})$.
5. We impose an additional condition $\lambda(T_s, \alpha_{sl}) = \lambda_0$ (T_s is the solidus temperature) on the function $\lambda = \lambda(T, \alpha_{sl})$. For $\lambda_0 = 0$, we have a noneutectic alloy, while, for $\lambda_0 \neq 0$, it is eutectic. From this condition, we find the value of the temperature conductivity in the mush zone α_{sl}.
6. After that, we obtain a parabolic equation of the heat conduction equation type with piecewise constant coefficient of heat conductivity, which are performed by temperature conductivity α. The solution of such an equation can be obtained in a closed analytical form.

Note that the method does not allow one to solve the problem of solidification of an alloy with the given function $\lambda(T)$. The dependence $\lambda(T)$ is determined from the condition of linearization of the heat conduction equation within the mush zone.

2. Linearization of the equation for enthalpy

In this paper, we consider the general method for linearization of the equation for the total enthalpy described briefly in the Introduction and in papers [1,2]. In this case, the total enthalpy of the system can be in the form [3]

$$H(T) = [1 - \lambda(T)]\rho_s C_s T + \lambda(T)\rho_l [C_l T + L] \quad (1)$$

where C_s and C_l are the specific heat capacities in the solid and liquid phases, respectively; L is the latent heat; ρ_s and ρ_l are the

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Nomenclature

C	heat capacity (J kg^{-1} K^{-1})	λ	liquid fraction
H	enthalpy (J m^{-3})	$\bar{\lambda}$	averaged liquid fraction
k	solidification constant (m s$^{-1/2}$)	ρ	density (kg m^{-3})
L	latent heat (J kg^{-1})	ξ	self-similar variable (m^2 s^{-1})
T	temperature (K)		
t	time (s)	*Subscripts*	
v	velocity (m s^{-1})	L	liquidus
X	isotherm position (m)	l	liquid phase
x	coordinate (m)	S	solidus
		s	solid phase
Greeks		sl	solid–liquid (mushy) zone
α	temperature conductivity (m^2 s^{-1})	*out*	outer boundary
γ	coefficient (m s$^{-1/2}$)	*init*	initial
κ	heat conductivity (W m^{-1} K^{-1})	0	eutectic alloy

densities in the solid and liquid phases, respectively; and T is the temperature. Since we consider effects related to the difference of the densities in the solid and liquid phases, the equation of balance for the enthalpy can include a convective term taking into account the relative movement of the phases; therefore, we write in the general form [4]

$$\frac{\partial H}{\partial t} + v(t)\frac{\partial H}{\partial x} = \frac{\partial}{\partial x}\left(\alpha(H)\frac{\partial H}{\partial x}\right) \tag{2}$$

where v is the velocity, t is the time, x is the coordinate along the ingot, and α is the temperature conductivity. In the following, we will assume [5] that only the liquid moves; i.e. the velocity of the solid phase $v_s = 0$, while the velocity of the liquid phase $v_l = v$. There are two cases:

When $\rho_s > \rho_l$, the solid metal shrinks and the liquid moves toward the solidification front to eliminate the shrinkage; i.e. $v < 0$ (we choose the beginning of the coordinates at the bottom of ingot $x = 0$).
When $\rho_s < \rho_l$, the solid phase expands and the liquid moves away from the solidification front; i.e. $v > 0$.

We will find the velocity of the liquid phase movement from the law of mass conservation. Let the point $x = \xi(t)$ be the location of a fixed material point far from the liquidus isotherm (solidification front) in the liquid phase. The total mass per unit of the transverse section area inside the interval $0 \leqslant x \leqslant \xi(t)$ is given by the expression

$$M_\xi(t) = \rho_s X_s(t) + \bar{\rho}_{sl}[X_l(t) - X_s(t)] + \rho_l[\xi(t) - X_l(t)] \tag{3}$$

where $X_{s,l}(t)$ is the location of the solidus/liquidus fronts, and $\bar{\rho}_{sl}$ is the average density of the metal in the mush zone, which is defined by the expression

$$\bar{\rho}_{sl} = \rho_s + (\rho_l - \rho_s)\bar{\lambda} = \rho_s + \frac{\rho_l - \rho_s}{T_L - T_S}\int_{T_S}^{T_L} \lambda(T)\,\mathrm{d}T \tag{4}$$

In what follows, we will determine the explicit form of the function $\lambda(T)$ and calculate the integral $\bar{\lambda}$. Since $v(t) = \mathrm{d}\xi(t)/\mathrm{d}t$, from Eq. (3) and the law of mass conservation $\mathrm{d}M_\xi(t)/\mathrm{d}t = 0$, one can easily obtain the expression for the velocity of the liquid phase in the form

$$v(t) = \left(1 - \frac{\rho_s}{\rho_l}\right)\left[\bar{\lambda}\frac{\mathrm{d}X_S(t)}{\mathrm{d}t} - (1 - \bar{\lambda})\frac{\mathrm{d}X_L(t)}{\mathrm{d}t}\right] \tag{5}$$

We will present the heat conductivity in the mush zone in the form

$$\kappa(T) = [1 - \lambda(T)]\kappa_s + \lambda(T)\kappa_l \tag{6}$$

where $\kappa_{s,l}$ are the heat conductivity in solid/liquid phase. The heat conduction equations linearized by the requirement that the thermal diffusion (temperature conductivity) in the mush zone is constant, i.e. by the following condition:

$$\alpha = \frac{\kappa}{\frac{\mathrm{d}H}{\mathrm{d}T}} = \alpha_{sl} = const \tag{7}$$

With trivial conversions we obtain the equation for $\lambda(T)$

$$[1 + pT]\frac{\mathrm{d}\lambda(T)}{\mathrm{d}T} + a\lambda(T) + b = 0 \tag{8}$$

where we introduced the notations (and the ratio of densities in the liquid and solid phases $\mu = \rho_l/\rho_s$ [5]):

$$a = \frac{\alpha_{sl}\rho_l(C_l - C_s/\mu) - (\kappa_l - \kappa_s)}{\alpha_{sl}\rho_l L}, \tag{9}$$

$$b = \frac{\alpha_{sl}\rho_l C_s/\mu - \kappa_s}{\alpha_{sl}\rho_l L}, \tag{10}$$

$$p = \frac{C_l - C_s/\mu}{L}. \tag{11}$$

Furthermore, we require satisfaction of the condition in the liquidus point

$$\lambda(T_l) = 1. \tag{12}$$

The solution of Eqs. (8) and (12) is given by the expression

$$\lambda(T) = -\frac{b}{a} + \frac{a+b}{a}\left(\frac{1 + pT_l}{1 + pT}\right)^{\frac{a}{p}}. \tag{13}$$

Now, it is necessary to define the additional condition for the function $\lambda(T)$ at the solidus (or eutectic) temperature

$$\lambda(T_s) = \begin{cases} 0 \\ \lambda_0 \neq 0 \end{cases} \tag{14}$$

From this additional equation, we obtain the constant α_{sl}. Now, knowing the explicit form of the function $\lambda(T)$, we can calculate $\bar{\lambda}$:

$$\bar{\lambda} = \frac{\Lambda(T_L) - \Lambda(T_S)}{T_L - T_S}, \tag{15}$$

where

$$\Lambda(x) = -\frac{a}{b}x - \frac{(a+b)(1+px)}{a(a-p)}\left(\frac{1 + pT_L}{1 + px}\right)^{\frac{a}{p}}. \tag{16}$$

3. An example of the analytical solution

When we have linearized the equation for enthalpy, we can investigate particular systems and obtain analytical solutions. In paper [2], the problem of the solidification of a finite one-dimensional array with the upper boundary (intake) moving according to the rule $X_t(t) = k_t\sqrt{t}$ was considered (where k_t is a known constant). In this paper, we consider a half-infinite system. Solidifying of a semi-infinite slab ($0 \leqslant x < \infty$), initially liquid at a uniform temperature $T_{init} > T_L$, by imposing a constant temperature $T_{out} < T_S$ on the face $x = 0$. The problem for the total enthalpy can be formulated in the following way:

$$\frac{\partial H}{\partial t} + v(t)\frac{\partial H}{\partial x} = \frac{\partial}{\partial x}\left(\alpha(H)\frac{\partial H}{\partial x}\right), \tag{17}$$

$$H(x > 0, t = 0) = H_{init} = H(T_{init}), \tag{18}$$

$$H|_{x=0} = H_{out} = H(T_{out}), \quad t \geqslant 0, \tag{19}$$

$$H|_{x\to\infty} = H_{init} = H(T_{init}). \tag{20}$$

Solution of these equations with piecewise constant function $\alpha(H)$ can be easy obtained [6]. For this, we divide the whole domain $[0,\infty)$ into the intervals $[0,X_S)$, $[X_S,X_L]$ and (X_L,∞). Furthermore, we assume that (the so called self-similar solution):

$$X_S(t) = k_S\sqrt{t}, \quad X_L(t) = k_L\sqrt{t}, \tag{21}$$

where k_S and k_L are constants. Let us introduce the following notation:

$$\gamma = \frac{\mu - 1}{\mu}[\bar{\lambda}k_S + (1 - \bar{\lambda})k_L], \quad v(t) = \frac{\gamma}{2\sqrt{t}}. \tag{22}$$

Then, after introduction of the new variable $\xi = x^2/t$, Eq. (17) can be rewritten in the form of ordinary differential equation

$$\frac{d^2H}{d\xi^2} = -\frac{1}{4}\left[\frac{1}{\alpha(H)} + \frac{2}{\xi} - \frac{\gamma}{\alpha(H)\sqrt{\xi}}\right]\frac{dH}{d\xi}. \tag{23}$$

Solutions of this equation on the intervals have the form [7]

$$H(x,t) = H_{out} + (H_s - H_{out})\frac{\mathrm{erf}\left(\frac{x}{2\sqrt{\alpha_s t}}\right)}{\mathrm{erf}\left(\frac{k_S}{2\sqrt{\alpha_s}}\right)}, \quad x \in [0, X_S), \tag{24}$$

$$H(x,t) = \frac{(H_l - H_s)\mathrm{erf}\left(\frac{x-\gamma\sqrt{t}}{2\sqrt{\alpha_{sl}t}}\right) + H_s\mathrm{erf}\left(\frac{k_L-\gamma}{2\sqrt{\alpha_{sl}}}\right) - H_l\mathrm{erf}\left(\frac{k_S-\gamma}{2\sqrt{\alpha_{sl}}}\right)}{\mathrm{erf}\left(\frac{k_L-\gamma}{2\sqrt{\alpha_{sl}}}\right) - \mathrm{erf}\left(\frac{k_S-\gamma}{2\sqrt{\alpha_{sl}}}\right)},$$
$$x \in [X_S, X_L] \tag{25}$$

$$H(x,t) = H_{init} - (H_{init} - H_l)\frac{erfc\left(\frac{x-\gamma\sqrt{t}}{2\sqrt{\alpha_l t}}\right)}{erfc\left(\frac{k_L-\gamma}{2\sqrt{\alpha_l}}\right)}, \quad x \in (X_L, \infty) \tag{26}$$

Using two conditions (note that, in the case $\rho_s \neq \rho_l$, these conditions are approximate [5]) on the interval's boundaries

$$\alpha_s\frac{\partial H}{\partial x}\bigg|_{x=X_S-0} = \alpha_{sl}\frac{\partial H}{\partial x}\bigg|_{x=X_S+0} + \rho_s\lambda_0 L\frac{dX_S(t)}{dt}, \tag{27}$$

$$\alpha_{sl}\frac{\partial H}{\partial x}\bigg|_{x=X_L-0} = \alpha_l\frac{\partial H}{\partial x}\bigg|_{x=X_L+0}, \tag{28}$$

we obtain two equations to determine k_S and k_L:

$$\frac{\sqrt{\alpha_s}(H_s - H_{out})\exp\left(-\frac{(k_S-\gamma)^2}{4\alpha_s}\right)}{\mathrm{erf}\left(\frac{k_S-\gamma}{2\sqrt{\alpha_s}}\right)} - \frac{\sqrt{\alpha_{sl}}(H_l - H_s)\exp\left(-\frac{(k_S-\gamma)^2}{4\alpha_{sl}}\right)}{\mathrm{erf}\left(\frac{k_L-\gamma}{2\sqrt{\alpha_{sl}}}\right) - \mathrm{erf}\left(\frac{k_S-\gamma}{2\sqrt{\alpha_{sl}}}\right)}$$
$$= \frac{\sqrt{\pi}}{2}\rho_s\lambda_0 L k_S, \tag{29}$$

$$\frac{\sqrt{\alpha_{sl}}(H_l - H_s)\exp\left(-\frac{(k_L-\gamma)^2}{4\alpha_{sl}}\right)}{\mathrm{erf}\left(\frac{k_L-\gamma}{2\sqrt{\alpha_{sl}}}\right) - \mathrm{erf}\left(\frac{k_S-\gamma}{2\sqrt{\alpha_{sl}}}\right)} - \frac{\sqrt{\alpha_l}(H_{init} - H_l)\exp\left(-\frac{(k_L-\gamma)^2}{4\alpha_l}\right)}{\mathrm{erfc}\left(\frac{k_L-\gamma}{2\sqrt{\alpha_l}}\right)}$$
$$= 0. \tag{30}$$

These equations could be solved numerically.

4. Conclusion

In this paper, we obtained the analytical solution for a semi-infinite volume of binary alloy. That is, the analytical solution for the three-phase problem including solid, solid–liquid, and liquid phases has been obtained. Linearization of the heat conduction equation for the alloy is based on the method proposed in papers [1,2].

The presented analytical solution of the problem is an important test example for analysis of numerical schemes used for system with moveable boundaries, e.g., for programs modeling vacuum arc remelting [8].

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