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Boundary integral approach for elliptical dendritic paraboloid as a form of growing crystals

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Abstract. A method based on the boundary integral approach to the phase interface propagation is used to obtain the Horvay and Cahn solutions. An elliptical paraboloid as one of the crystal (dendritic) shapes growing under the steady state conditions is derived from the boundary integral.

1. Introduction

The dynamics of phase interfaces plays a very important role in different phase and structural transformations and leads to various types of pattern formation in materials [1–7]. The Stefan-like problems occurring in the presence of moving boundary problems [8–28] may be mentioned as an important class of such evolutionary tasks.

The boundary integral method represents one of the useful approaches to describe the time-dependent moving boundary problems. This technique was developed for the first time by Nash [29] and Nash and Glicksman [30] in their pioneering papers. This method leans upon a single integral equation for the interface function, which is derived on the basis of the Green's function technique. Langer and Turski [31,32] developed the boundary integral method to describe a chemical diffusion problem in two-phase solid/liquid, solid/solid and fluid/fluid systems. Recently, their theory was extended for the description of binary non-isothermal mixtures by Alexandrov and Galenko in [33]. Note that the integral equation for the interface function represents the basis for stability and selection problems [34–40].

It is well-known that in many cases the growing dendrites are non-symmetrical in their shapes and cannot be described by means of the Ivantsov solutions [39,41]. In this case, one can use the Horvay and Cahn solutions describing the non-symmetrical shape of a dendritic tip [42–44]. The present paper connects the Horvay and Cahn solutions with the boundary integral theory [33]. Namely, we discuss below how to derive the Horvay and Cahn solutions describing the elliptical paraboloid from the boundary integral method [33].

2. Equation of the interface motion and its analysis for elliptical paraboloid

Horvay and Cahn [42] obtained a form of an isothermal dendrite that has an elliptical cross section. The surface of the dendrite in dimensionless coordinates is given by

$$\frac{x^2}{\omega - b} + \frac{y^2}{\omega + b} = \omega - 2z, \tag{1}$$

where $2D_T/V = \rho/P_T$ is the length scale and $P_T = \rho v/2D_T$ is the growth Péclet number (V and ρ represent the dendrite tip velocity and diameter of its any cross section (or the average value of dendritic tip curvature radii), and D_T is the thermal diffusivity). The interface corresponds to $\omega = P_T$. Here b determines the aspect ratio of the elliptical cross-section of dendrite. For $b = 0$ the cross-section is circular; we will assume $|b| < P_T$. Eq. (1) is actually a symmetrized version of the corresponding expression given by Horvay and Cahn, with dimensionless radii of curvature $P_T - b$ in the $x-z$ plane and $P_T + b$ in the $y-z$ plane. Thus, the average dimensionless radius of curvature is P_T [44]. In dimensional form this equations transforms to

$$\frac{x_d^2}{\omega_d - b_d} + \frac{y_d^2}{\omega_d + b_d} = \omega_d - 2z_d, \tag{2}$$

where $\omega_d = \omega\rho/P_T$ and $b_d = b\rho/P_T$ and subscript d designates the dimensional variables and parameters. An arbitrary deformed solid-liquid interface then propagates in the z-direction and is defined by the function $z_{\text{interface}} = \zeta(x,t)$, where t stands for the time. The dimensionless undercooling as a function of P_T in the three-dimensional case can be written out as [33]

$$\Delta - \frac{d_c}{\rho}K - \beta V\left(1 + \frac{\partial\zeta(x,t)}{\partial t}\right) = I_\zeta^T, \tag{3}$$

where (in dimensionless variables)

$$\begin{aligned} I_\zeta^T &= P_T^{3/2}\int\limits_0^\infty \frac{\mathrm{d}\tau}{(2\pi\tau)^{3/2}} \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} \mathrm{d}^2x_1 \left[1 + \frac{\partial\zeta(x_1, t-\tau)}{\partial t}\right] \\ &\times \exp\left\{-\frac{P_T}{2\tau}\left[|x - x_1|^2 + (\zeta(x,t) - \zeta(x_1, t-\tau) + \tau)^2\right]\right\}. \end{aligned} \tag{4}$$

Here $\Delta = (T_M - T_\infty)c_p/Q$ is the dimensionless undercooling, T_M is the freezing temperature of the planar front, T_∞ is the liquid phase temperature far from the moving interface, Q is the latent heat released per unit volume of the solid phase, c_p is the specific heat β is the kinetic coefficient, variables x, x_1 and ζ are measured in units of ρ whereas variables t and τ are measured in units of ρ/V. In dimensional coordinates, when the elliptical paraboloid does not change its shape and moves with the constant velocity V (i.e. $\partial\zeta(x,t)/\partial t = 0$), Eq. (4) takes the following form

$$\begin{aligned} I_{\zeta d}^T &= \left(\frac{P_T}{2\pi\rho}\right)^{3/2}\frac{1}{\sqrt{V}} \\ &\times \int\limits_0^\infty \frac{\mathrm{d}\tau}{\tau^{3/2}} \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} \mathrm{d}^2x_1 \exp\left\{-\frac{P_T}{2\tau}\frac{1}{\rho V}\left[|x - x_1|^2 + (\zeta(x,t) - \zeta(x_1, t-\tau) + \tau V)^2\right]\right\}. \end{aligned} \tag{5}$$

Here $I_{\zeta d}^T$ denotes the integration over dimensional coordinates. Taking into account expressions (2) and (5) one can get

$$I_{\zeta d}^T = \left(\frac{P_T}{2\pi\rho}\right)^{3/2}\frac{1}{\sqrt{V}}$$

$$\times \int_0^\infty \frac{\mathrm{d}\tau}{\tau^{3/2}} \int_{-\infty}^\infty \int_{-\infty}^\infty \exp\left\{-\frac{P_T}{2\tau}\frac{1}{\rho V}\left[(x-x_1)^2+(y-y_1)^2 \right.\right.$$
$$\left.\left. + \left(\frac{x_1^2-x^2}{2(\omega_d-b_d)}+\frac{y_1^2-y^2}{2(\omega_d+b_d)}+\tau V\right)^2\right]\right\}\mathrm{d}x_1\mathrm{d}y_1. \quad (6)$$

Replacing two integration variables τ and y_1 by ω_1 and z_1 as

$$\tau = \frac{(x-x_1)^2}{2\omega_1}, \quad y-y_1=(x-x_1)z_1, \quad (7)$$

we get

$$I_{\zeta d}^T = \left(\frac{P_T}{\pi\rho}\right)^{3/2}\frac{1}{2\sqrt{V}}\int_0^\infty \frac{\mathrm{d}\omega_1}{\sqrt{\omega_1}}\int_{-\infty}^\infty \exp(-\frac{P_T\omega_1}{\rho V}(1+z_1^2))\mathrm{d}z_1$$
$$\times \int_{-\infty}^\infty \exp\left\{-\frac{P_T\omega_1}{\rho V}\left(-\frac{x_1+x}{2(\omega_d-b_d)}-\frac{z_1(2y-z_1(x-x_1))}{2(\omega_d+b_d)}+\frac{V(x-x_1)}{2\omega_1}\right)^2\right\}\mathrm{d}x_1. \quad (8)$$

Integration of the right-hand side of Eq. (8) over x_1 leads to

$$I_{\zeta d}^T = \frac{P_T(\omega_d+b_d)}{\pi\rho}\int_0^\infty \frac{\exp(-\frac{P_T\omega_1}{\rho V})\mathrm{d}\omega_1}{\omega_1}\int_{-\infty}^\infty \frac{\exp(-\frac{P_T\omega_1 z_1^2}{\rho V})\mathrm{d}z_1}{z_1^2+(\omega_d+b_d)(\frac{V}{\omega_1}+\frac{1}{\omega_d-b_d})}. \quad (9)$$

Now it is possible to integrate the right-hand side of the Eq. (9) over z_1

$$I_{\zeta d}^T = \frac{P_T\sqrt{\omega_d+b_d}}{\rho}\int_0^\infty \frac{\exp\left(\frac{P_T}{V\rho}(\omega_d+b_d)\left(V+\frac{\omega_1}{(\omega_d-b_d)}\right)-\frac{P_T\omega_1}{V\rho}\right)}{\sqrt{\omega_1}\sqrt{V+\frac{\omega_1}{(\omega_d-b_d)}}}$$
$$\times \operatorname{erfc}\left(\sqrt{\frac{P_T}{V\rho}(\omega_d+b_d)\left(V+\frac{\omega_1}{\omega_d-b_d}\right)}\right)\mathrm{d}\omega_1. \quad (10)$$

Here it has been taken into consideration that [45]

$$\int_0^\infty \frac{\exp(-\mu^2u^2)\mathrm{d}u}{u^2+\beta^2} = \frac{\pi}{2\beta}\operatorname{erfc}(\beta\mu). \quad (11)$$

Replacing the variable ω_1 by $u=\frac{1}{\sqrt{V}}\sqrt{V+\frac{\omega_1}{\omega_d-b_d}}$, we obtain

$$I_{\zeta d}^T = \frac{2P_T}{\rho}\sqrt{\omega_d^2-b_d^2}\exp(\frac{P_T}{\rho}(\omega_d-b_d))J(\omega_d), \quad (12)$$

where

$$J(\omega_d) = \int_1^\infty \frac{\exp\left(\frac{P_T}{\rho}2b_du^2\right)\operatorname{erfc}\left(u\sqrt{\frac{P_T}{\rho}(\omega_d+b_d)}\right)\mathrm{d}u}{\sqrt{u^2-1}}. \quad (13)$$

Further, applying the method of differentiation and integration of $J(\omega_d)$ and keeping in mind that

$$\int_1^\infty \frac{\exp(-\mu u)\mathrm{d}u}{\sqrt{u-1}} = \sqrt{\frac{\pi}{\mu}}\exp(-\mu), \tag{14}$$

we get

$$I^T_{\zeta d} = \frac{P_T}{\rho}\sqrt{\omega_d^2 - b_d^2}\exp\left(\frac{P_T\omega_d}{\rho}\right)\int_{\omega_d}^\infty \frac{\exp\left(-\frac{P_T}{\rho}t\right)\mathrm{d}t}{\sqrt{t^2 - b_d^2}}. \tag{15}$$

At the interface, $\omega_d = \rho$, one obtains

$$I^T_{\zeta d} = \sqrt{P_T^2 - b_d^2\frac{P_T^2}{\rho^2}}\exp(P_T)G(P_T), \tag{16}$$

where

$$G(P_T) = \int_{P_T}^\infty \frac{\exp(-y)\mathrm{d}y}{\sqrt{y^2 - b_d^2\frac{P_T^2}{\rho^2}}}, \tag{17}$$

and

$$\frac{c_p(T_M - T_\infty)}{Q} = I^T_{\zeta d}. \tag{18}$$

This relation shows that the undercooling $\Delta T = T_M - T_\infty$ connects two unknown dendrite parameters: ρ and V of the paraboloid. Our solution (16) transforms to the Horvay-Cahn two-fold solution [44] after returning to the dimensionless value $b = b_d P_T/\rho$

$$I^T_\zeta = I^T_{\zeta d} = \sqrt{P_T^2 - b^2}\exp(P_T)\int_{P_T}^\infty \frac{\exp(-y)dy}{\sqrt{y^2 - b^2}}. \tag{19}$$

For $b = 0$, the cross-section is circular and one recovers the Ivantsov's solution [39, 41].

The thermal field can be expressed as [41, 44]

$$T_d(\omega) = (T_M - T_\infty)\frac{G(\omega) - G(P_T)}{G(P_T)}. \tag{20}$$

The function $\omega = \omega(x, y, z)$ is given by Eq. (1). This equation has three roots, but only one of them is positive at all possible values of parameters. It can be found from the Cardano's formula

$$\omega(x, y, z) = \frac{2z}{3} + \sqrt[3]{\frac{-q + \sqrt{q^2 + \frac{4p^3}{27}}}{2}} + \sqrt[3]{\frac{-q - \sqrt{q^2 + \frac{4p^3}{27}}}{2}}, \tag{21}$$

where

$$q(x, y, z) = \frac{4}{3}zb^2 - bx^2 + by^2 - \frac{16}{27}z^3 - \frac{2}{3}z(x^2 + y^2), \tag{22}$$

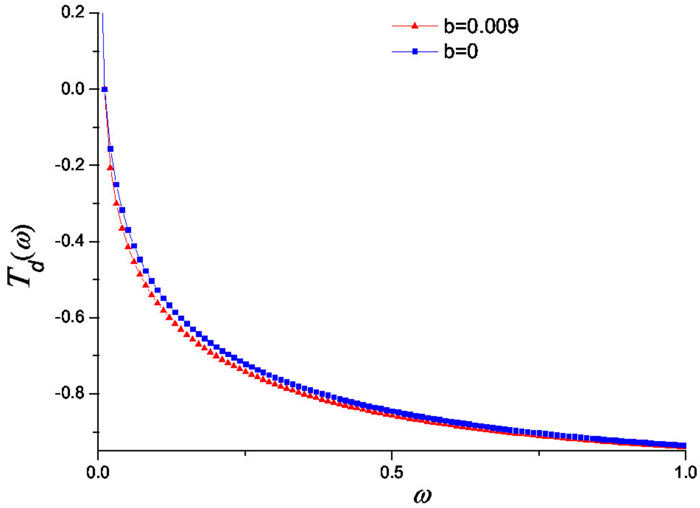

Figure 1. The temperature as a function of dimensionless variable ω at different values of parameter b.

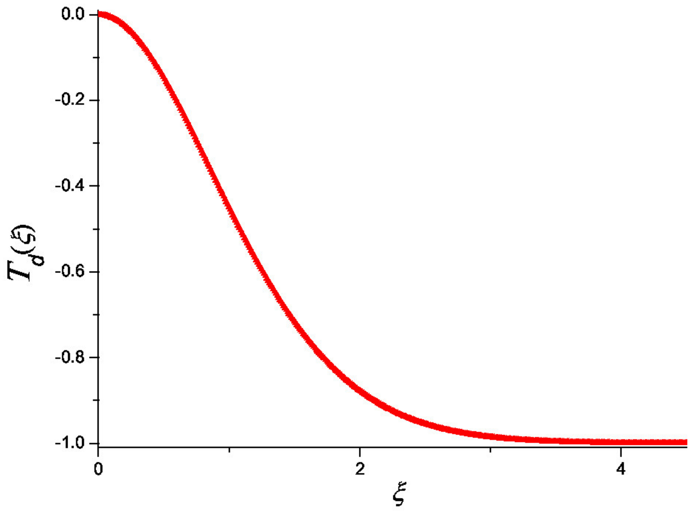

Figure 2. The temperature as a function of parabolic variable ξ at the fixed values of $b = 0.009$, $\eta = 1$ and $\varphi = \pi$.

and

$$p(x, y, z) = -\left(\frac{4}{3}z + b^2 + x^2 + y^2\right). \tag{23}$$

The parabolic coordinates are often used to describe the dendritic growth. The relations between the parabolic coordinates (ξ, η, φ) and the Cartesian coordinates (x, y, z) are

$$x = \xi\eta\cos\varphi, \quad y = \xi\eta\sin\varphi, \quad z = \frac{1}{2}(\xi^2 - \eta^2). \tag{24}$$

For a steady-state isothermal dendrite growing in the z-direction, the dendrite surface has the form $\xi = f(\eta, \varphi)$. The elliptical paraboloid in the parabolic coordinate system is given by

$$\xi^2\eta^2\left[\frac{\cos^2\varphi}{\omega - b} + \frac{\sin^2\varphi}{\omega + b}\right] = \omega - \xi^2 + \eta^2. \tag{25}$$

This relation defines ω as a function of the parabolic coordinates

$$\omega(\xi, \eta, \varphi) = \frac{\xi^2 - \eta^2}{3} + \sqrt[3]{\frac{-q_1 + \sqrt{q_1^2 + \frac{4p_1^3}{27}}}{2}} + \sqrt[3]{\frac{-q_1 - \sqrt{q_1^2 + \frac{4p_1^3}{27}}}{2}}, \tag{26}$$

where

$$q_1(\xi, \eta, \varphi) = \frac{2(\eta^2 - \xi^2)^3}{27} + \frac{(\eta^2 - \xi^2)(b^2 + \xi^2\eta^2)}{3} + b^2(\xi^2 - \eta^2) - \xi^2\eta^2 b(\cos^2\varphi - \sin^2\varphi), \tag{27}$$

and

$$p_1(x, y, z) = -\left(\xi^2\eta^2 + b^2 + \frac{(\eta^2 - \xi^2)^2}{3}\right). \tag{28}$$

3. Conclusions

Figures 1 and 2 demonstrate the solution given by Eq. (20) for the ice-water system ($T_M = 0^\mathrm{o}$C, $T_\infty = -1^\mathrm{o}$C, $P_T = 0.01$).

Let emphasize in conclusion the main output of our study. By leaning upon the previously developed theory of the thermo-solutal boundary-integral method [33], we have sewed together the Horvay and Cahn analytical solutions derived for the elliptical paraboloid [42] and the boundary integrals given by expressions Eq. (3) and Eq. (4) [33]. The temperature distribution in the liquid phase for the elliptical paraboloid is analyzed and illustrated as well.

4. References

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