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# APPLICATION OF THE HEAT-BALANCE INTEGRAL METHOD TO THE FREEZING OF A CUBOID

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## NOMENCLATURE

- $a$, semi-length of cuboid;
- $c_p$, specific heat at constant pressure;
- $L$, latent heat of fusion;
- $\kappa$, thermal diffusivity;
- $T_0$, ambient temperature;
- $T_F$, fusion temperature;
- $\beta$, $L/c_p(T_F - T_0)$;
- $\theta$, temperature, non-dimensionalised and normalised by subtracting $T_0$ and dividing by $T_F - T_0$;
- $\tau$, time, non-dimensionalised with respect to $\kappa/a^2$;
- $V_s$, volume of solidified phase, non-dimensionalised with respect to $a^3$;
- $X, Y, Z$, coordinates, non-dimensionalised with respect to $a$;
- $K, E$, complete elliptic integrals of the first and second kinds, respectively;
- $g, \varepsilon$, free-parameters in temperature profile;
- $\mathbf{R}$, $(X, Y, Z)$;
- $S_0$, $S_0(\mathbf{R}) = 0$ denotes the surface of the cuboid;
- $S_i$, $S_i(\mathbf{R}, \tau) = 0$ denotes the inter-phase surface;
- $d\mathbf{S}$, directed element of area, non-dimensionalised with respect to $a^2$.

## 1. INTRODUCTION

THERE is considerable interest in the group of problems collectively known as the Stefan problem, as is shown in the Proceedings of the Conference on Moving Boundary Problems in Heat Flow and Diffusion [1]. However, there is comparatively little information of an analytical or approximate nature available and so the development of numerical methods to deal with Stefan problems is inhibited.

In this paper the heat balance integral method is applied to the three-dimensional problem of the freezing of a cuboid, which has previously been examined numerically by Lazaridis [4], using an explicit finite difference scheme. There are in practice two approaches to the method: there is the one adopted in this paper due to Poots [2, 3], which leads to the need to solve coupled differential equations, and there is also Goodman's approach [5], which minimises the number of differential equations to be solved by using conditions leading to algebraic equations for the coefficients. Whilst the latter approach is certainly more appealing, it is also much more difficult to implement when multi-dimensional problems are considered (Goodman's method apparently breaks down even for the freezing cylinder and sphere problems, which are both one-dimensional problems [2]).

Finally, the question of accuracy of this method is still unresolved; an attempt to establish some criteria was made by Langford [6], who applied the method to the semi-infinite region.

## 2. ANALYSIS

In what follows, we shall assume that: (i) all thermal properties are constant; (ii) the temperature of the molten phase is constant, and equal to that of fusion; and (iii) the material has a definite fusion temperature (which implies a sharp inter-phase boundary). The heat balance method can cope with some relaxation of these conditions, for example the thermal conductivity may be taken to be temperature dependent. However just how general a problem the method can deal with is a matter for further investigation.

For convenience we shall work in terms of dimensionless quantities (see nomenclature for details). We consider a cuboid consisting of molten material at the fusion temperature 1, bounded by the surface

$$S_0(\mathbf{R}) = (1 - X^2)(1 - Y^2)(1 - Z^2) = 0.$$

At time $\tau = 0$ a uniform temperature 0 is imposed and maintained at the outer boundary; the body subsequently solidifies inwards. The problem is to determine the temperature distribution in the solidified phase and the location of the solidification front.

Following Poots we form two heat-balance integrals by integrating the heat conduction equation and its first moment over the solidified phase (cf. Poots [3], equations (3.3) and (3.4)), viz.:

$$\beta \frac{dV_s}{d\tau} + \iint_{S_0=0} \nabla\theta \cdot d\mathbf{S} = \iiint_{V_s} \frac{\partial\theta}{\partial\tau}\, dV \tag{1}$$

and

$$\beta \frac{dV_s}{d\tau} = \iiint_{V_s} \left\{ \nabla\theta \cdot \nabla\theta - \theta \frac{\partial\theta}{\partial\tau} \right\} dV. \tag{2}$$

In order to apply the heat-balance integral method we need to guess the shape of the solidification front this we do guided by Poots' arguments for the two-dimensional prism. We assume that for small time the inter-phase surface will be a cube with rounded corners (cf. Lazaridis' results: Figs. 15–18), and that eventually it becomes spherical. Hence it seems reasonable to assume that the phase interface is given by

$$S_i(\mathbf{R}, \tau) = (1 - X^2)(1 - Y^2)(1 - Z^2) - \varepsilon(\tau) = 0 \tag{3}$$

where $\varepsilon(0) = 0$ and at the instant of solidification $\varepsilon = 1$.

### (a) *One-parameter method*

We assume the one-parameter temperature distribution

$$\theta = \frac{(1 - X^2)(1 - Y^2)(1 - Z^2)}{\varepsilon}. \tag{4}$$

which automatically satisfies the isothermal boundary conditions:

$$\left.\begin{aligned} \theta &= 0 \quad \text{on} \quad S_0 = 0 \\ \theta &= 1 \quad \text{on} \quad S_i = 0 \end{aligned}\right\}. \tag{5}$$

On substituting (4) into the heat-balance integral (1) there results a first order differential equation for $\varepsilon(\tau)$, the solution of which is given by

$$\tau = \beta I_0(\varepsilon) + I_1(\varepsilon) \tag{6}$$

where

$$I_0(\varepsilon) = \tfrac{3}{16} \int_0^{\varepsilon} \int_0^{\sqrt{(1-\varepsilon)}} (1 - \sigma) K \, dZ \, d\varepsilon,$$

$$I_1(\varepsilon) = \int_0^{\varepsilon} \left\{ \frac{1}{9\varepsilon} + \tfrac{1}{24} \int_0^{\sqrt{(1-\varepsilon)}} (5 - 3\sigma) K - \left( \frac{5 - \sigma}{1 - \sigma} \right) E \, dZ \right\} d\varepsilon,$$

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Table 1. The universal functions $I_0(\varepsilon)$, $I_1(\varepsilon)$ for the solution to the cube by the one-parameter method

| $\varepsilon$ | $I_0$ | $I_1$ |
|---|---|---|
| 0.00 | 0.0000 | 0.0000 |
| 0.04 | 0.0010 | 0.0006 |
| 0.08 | 0.0031 | 0.0019 |
| 0.12 | 0.0061 | 0.0037 |
| 0.16 | 0.0097 | 0.0059 |
| 0.20 | 0.0138 | 0.0085 |
| 0.24 | 0.0184 | 0.0114 |
| 0.28 | 0.0232 | 0.0146 |
| 0.32 | 0.0284 | 0.0181 |
| 0.36 | 0.0337 | 0.0217 |
| 0.40 | 0.0393 | 0.0255 |
| 0.44 | 0.0449 | 0.0296 |
| 0.48 | 0.0507 | 0.0337 |
| 0.52 | 0.0565 | 0.0380 |
| 0.56 | 0.0623 | 0.0424 |
| 0.60 | 0.0680 | 0.0469 |
| 0.64 | 0.0737 | 0.0515 |
| 0.68 | 0.0793 | 0.0561 |
| 0.72 | 0.0846 | 0.0608 |
| 0.76 | 0.0898 | 0.0655 |
| 0.80 | 0.0947 | 0.0702 |
| 0.84 | 0.0992 | 0.0750 |
| 0.88 | 0.1033 | 0.0797 |
| 0.92 | 0.1068 | 0.0843 |
| 0.96 | 0.1096 | 0.0889 |
| 1.00 | 0.1111 | 0.0935 |

$\sigma = 1-[\lambda(1-Z^2)]$, and the complete elliptic integrals $K$ and $E$ have modulus $\sqrt{\sigma}$ (see Dwight [7]). In the integral for $I_1(\varepsilon)$, the $K$ term in the integrand has a weak logarithmic singularity [likewise in $I_0(\varepsilon)$], whilst the pole at $\lambda = 0$ in the term $1/9\lambda$ cancels out with the pole obtained by subtracting out the singularity in the $E$ term. Gaussian quadrature, which avoids evaluations of the integrand at the limits of the integral, was used to evaluate the resulting integrals.

Information on the complete or partial solidification of a cube may be obtained for any specified substance by simply substituting the relevant value of $\beta$ in (6) and using Table 1. However to try to improve the accuracy of the results, which are suspect for large times, we now apply the two-parameter method.

(b) *Two-parameter method*

We assume the two-parameter temperature distribution:

$$\theta = \frac{(1-g)(1-X^2)(1-Y^2)(1-Z^2)}{\varepsilon} + g\left\{\frac{(1-X^2)(1-Y^2)(1-Z^2)}{\varepsilon}\right\}^2 \quad (7)$$

which satisfies the isothermal boundary conditions (5). $g(\tau)$ and $\varepsilon(\tau)$ are unknown parameters determined by the heat balance integrals (1) and (2). Substituting (7) into these two equations yields the following two coupled differential equations

$$\left(a_0 + a_1 g + a_2 \frac{dg}{d\varepsilon}\right)\frac{d\varepsilon}{d\tau} + a_3(g-1) = 0, \quad (8)$$

$$\left(b_0 + b_1 g + b_2 g^2 + (b_3 + b_4 g)\frac{dg}{d\varepsilon}\right)\frac{d\varepsilon}{d\tau} + b_5 + b_6 g + b_7 g^2 = 0, \quad (9)$$

where the coefficients $a_i$, $b_j[i = 0(1)3;\ j = 0(1)7]$ involve elliptic integrals and polynomials in $1/\varepsilon$*. By eliminating $d\varepsilon/d\tau$ from (8) and (9), a first order differential equation governing $g(\varepsilon)$ is obtained; the solution to this is substituted back into (8) and the solution for $\varepsilon(\tau)$ found. Unfortunately $dg/d\varepsilon$ turns out to be singular as $\varepsilon \to 0$, and so the differential equation cannot be integrated numerically outwards from the origin. The usual expedient to circumvent this difficulty is to find a series representation valid for $\varepsilon \sim 0$, and then to use this series to start the numerical solution away from the singularity (see Poots [3]). In this case, however, the algebra was too prohibitive and another approach had to be used.

The first point to note is that by finding the asymptotic form of the differential equation for $g$, it is possible to show that the value of $g$ at $\varepsilon = 0$, $g_0$ say, must satisfy the cubic equation:

$$7g_0^3 + (60\beta + 48)g_0^2 + (180\beta + 75)g_0 + 30 = 0. \quad (10)$$

This is, in fact, exactly the same cubic as that found by Poots in the two-dimensional analogue, i.e. the uniform prism of square cross-section. By invoking a minimum energy principle, we took the smallest root of this cubic to be the initial value. Given this value (for a particular $\beta$), solutions were first computed for $g(\varepsilon)$ by applying the initial condition at a point away from the origin. A second approach was used whereby the equation was again solved starting at some given $\varepsilon$, away from the origin, but this time using the value of $g$ at this $\varepsilon$ obtained by Poots for the prism. Essentially, this latter procedure makes use of the fact that away from the vertices of the cube, the solidification process for the cube must resemble that for the uniform prism, i.e. that away from the vertices, three-dimensional edge effects are unimportant for small times.

Having obtained $g(\varepsilon)$, (8) was easily integrated to obtain $\tau(\varepsilon)$. The integration was initiated at the same value of $\varepsilon$ as that used in solving for $g(\varepsilon)$; the starting value being $\tau$ as given by the one-parameter method at this $\varepsilon$. Here it has been assumed that, for small time, the one- and two-parameter solutions agree (this result being indicated by the work of Poots [2, 3]).

All integrations were carried out using a fourth-order Runge–Kutta procedure.

Finally, these results may be extended to a cuboid of sides 2a, 2b, 2c by replacing $\tau$ by $\tau^*$ given by

$$\tau^* = \tfrac{1}{3}\tau(1+\gamma^2+\chi^2) \quad (11)$$

where

$$\gamma = a/b \quad \text{and} \quad \chi = a/c.$$

### 3. RESULTS AND DISCUSSION

Figure 1 shows graphically the results of solving the first order differential equation for $g(\varepsilon)$ using the initialising procedures suggested in the previous section. It is at once apparent that $g$ quickly settles down and that, for moderate freezing times (we have only investigated the case when $\beta \sim 1$ in this paper), it is immaterial which starting procedure is used. However it should be emphasized that it is far easier to use Poots' solution for the prism, rather than perform the rather lengthy algebra necessary to obtain equation (10).

Four quadratures were performed to obtain $\tau(\varepsilon)$ using the four solutions $g(\varepsilon)$ obtained previously. The results indicated that the actual starting point and values had negligible effect on $\tau(\varepsilon)$ [and $g(\varepsilon)$] for $\varepsilon \geqslant 0.28$. It is suggested therefore that for practical purposes a combination of the two methods should be used the one-parameter method being used for small time up to $\varepsilon \sim 0.3$, say, and thereafter the two-parameter method with the one-parameter method results being used to start off the two-parameter solution. However, if results are required only for small depths of solidification, then the one-parameter method should be sufficient. Figure 2 shows the results of the suggested procedure for $\beta = 1.5613$ and $\beta = 5$, which are typical values of $\beta$ for substances such as aluminium, copper, iron, zinc, etc. when the temperature difference $T_F - T_0$ is of the order of 200°C.

*Details may be obtained from the authors.

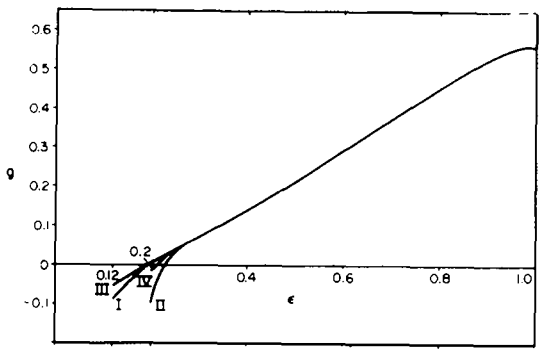


FIG. 1. $g$ vs $\varepsilon$. I—solution using $g_0$ [from equation (10)] when $\beta = 1.5613$] applied at $\varepsilon = 0.12$; II -as I but with $g_0$ applied at $\varepsilon = 0.20$; III- solution using Poots' value of $g$ (for prism) evaluated at $\varepsilon = 0.12$; IV as III but with $g$ evaluated at $\varepsilon = 0.20$.

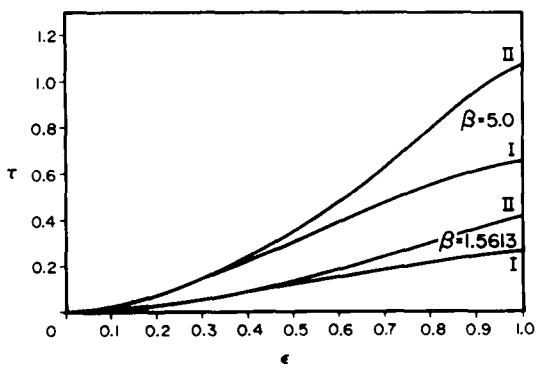


FIG. 2. Location history of the freezing isotherm in the cube when $\beta = 1.5613$ and $\beta = 5.0$. I - one-parameter method; II - two-parameter method.

Figure 3 shows the solid fraction along one of the main diagonals and along one of the axes of the cube, for $\beta = 1.5613$ and 5.

The above results should provide a basis for comparison with purely numerical methods, and as remarked earlier, they also allow numerical solutions to be started away from the singularity at $t = 0$. We do not give a comparison with Lazaridis' results since he has presented them only for times $\tau \leqslant 0.047$ ($\beta = 1.5613$).

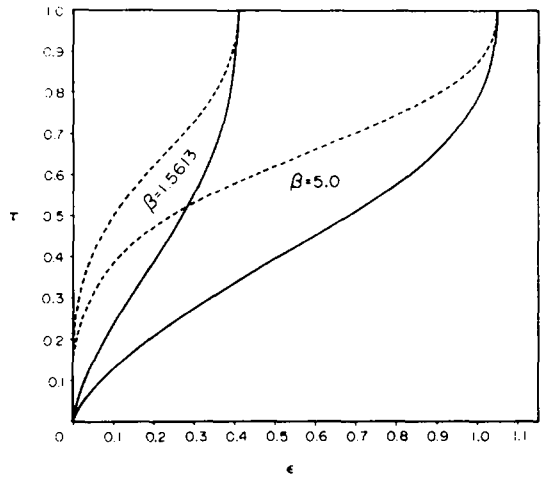


FIG. 3. Solid fraction along the diagonals of a cuboid as a function of time. -- Main diagonal ($X = Y = Z$); — Sub-diagonal ($Y = Z = 0$).

Unfortunately the overall accuracy of the present results cannot be assessed and at present there is no obvious criterion to optimise the choice of profile to be used in the heat balance method.

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