Spherical solidification by the enthalpy method and heat balance integral method

J. Caldwell & Y.Y. Kwan

Department of Mathematics,
City University of Hong Kong, Hong Kong.

Abstract

The heat balance integral method (HBIM), a front tracking method, has been previously applied successfully to problems involving plane and cylindrical geometries. In this paper the method is applied to spherical solidification. For validation purposes a numerical scheme based on the enthalpy method is also used. This method provides a means of tracking the position of the phase front with very little additional effort. The results show that the two methods compare well over a wide range of Stefan number.

1 Introduction

Phase change problems occur naturally in physical and industrial processes. Examples include freezing and thawing of food, production of ice-cream, ice cap formation, solidification of alloys and chemical reactions. These problems possess a moving boundary for which a flux condition expressing the conservation of heat and release of latent heat is satisfied. Very few analytic solutions to this type of Stefan problem are known.

In view of the difficulty in obtaining analytic solutions, numerical solutions are far more common. There are two main approaches to the solution of the Stefan problem. One is the front tracking method, which explicitly tracks the position of the phase front and the condition on the moving boundary is enforced. The heat balance integral method (HBIM) presented here is one such example.

Another approach is to use a fixed domain formulation. In this approach the computational domain is fixed via an application of change of variables. A common method here is the enthalpy method, which introduces
an enthalpy function. The flux condition is automatically satisfied across the phase front, which is realized as a jump discontinuity of the enthalpy.

There are different ways of tracking the boundary using the enthalpy method. Some researchers have used continuous tracking methods, which may only be applicable to plane geometry or which may not take the geometry into consideration. Other methods presented are rather complicated and may not provide a continuous track of the phase front. In past work Caldwell and Chiu \[1\] have used the HBIM to solve one-dimensional solidification problems. Also Caldwell and Chan \[2\] have applied an enthalpy formulation to Stefan problems with cylindrical geometry and have obtained results showing good agreement with those obtained from the HBIM. Date \[3\] has developed an enthalpy method which tracks the phase front easily. He has applied this method to one and two dimensional problems in plane geometry and has obtained good agreement with existing solutions. In this paper, this method is generalized to a spherical geometry and the numerical results obtained are compared to those from the HBIM. This comparison shows that the two methods agree well over a wide range of Stefan number.

\section{Problem formulation}

Consider the idealized problem of solidification of a liquid, initially at its freezing temperature \(T_f\), in contact with the surface of a sphere maintained at a constant, lower temperature \(T_s\) (see Figure 1). The liquid solidifies on the surface and the process may be described by

\[
\frac{\partial T}{\partial t} = \frac{\kappa}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial T}{\partial r} \right], \quad a < r < R(t), \quad t > 0,
\]

(1)

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{spherical_solidification}
\caption{Spherical solidification.}
\end{figure}
where \( T(r,t) \) is temperature and \( R(t) \) is the position of the solid-liquid interface. It is assumed that the physical properties of the material remain constant throughout the process and there is no change of volume on solidification. Suitable initial and boundary conditions for this problem are

\[
T = T_f, \quad r \geq R(t), \quad t > 0, \quad (2)
\]

\[
T = T_s, \quad r = a, \quad t \geq 0, \quad (3)
\]

and for the solid-liquid interface

\[
ck\left( \frac{\partial T}{\partial r} \right)_{R(t)} = L \frac{dE(t)}{dt}. \quad (4)
\]

The constants \( \kappa, c \) and \( L \) are thermal diffusivity, specific heat and latent heat of freezing, respectively.

It is further assumed that the material is initially cooled sufficiently rapidly that a discontinuous change in the temperature takes place at \( r = a \) when \( t = 0 \). This provides the initial condition for the solid-liquid interface, that is \( R(0) = a \).

To change into non-dimensional form, we simplify the above equations by introducing the variables

\[
z = \frac{r}{a}, \quad \tau = \frac{\kappa t}{a^2},
\]

\[
U = \frac{T - T_s}{(T_f - T_s)}, \quad Z = \frac{R}{a},
\]

\[
\alpha = \frac{L}{c(T_f - T_s)}. \quad (5)
\]

The set of equations then becomes

\[
\frac{\partial U}{\partial \tau} = \frac{1}{z^2} \frac{\partial}{\partial z} \left[ z^2 \frac{\partial U}{\partial z} \right], \quad 1 < z < Z(\tau), \quad \tau > 0,
\]

\[
U = 1, \quad z \geq Z(\tau), \quad \tau > 0,
\]

\[
U = 0, \quad z = 1, \quad \tau \geq 0, \quad (6)
\]

and for the solid-liquid interface, we have

\[
\left( \frac{\partial U}{\partial z} \right)_{Z(\tau)} = \alpha \frac{dZ(\tau)}{d\tau}, \quad Z(0) = 1, \quad (7)
\]

where \( \alpha \) is a dimensionless latent heat parameter, and is sometimes called the Stefan number.

### 3 Heat balance integral method

The heat balance integral method (HBIM) was first propounded by Goodman [4, 5]. Goodman's idea is to assume a particular temperature profile, and then integrate the heat equation over an appropriate interval to obtain
a set of heat-balance integral equations, the equations are then solved to obtain the motion of the phase boundary. Later Bell [6] proposed a systematic method to improve the accuracy of HBIM, which we will present below. The main idea is to subdivide the dependent variable $U$, and assume a linear profile within each subdivision. Accuracy can be improved by increasing the number of subdivisions.

Here is the method. First we divide the range $[0, 1]$ into $n$ parts, that is

$$U_i = \frac{i}{n}, \quad i = 0, 1, 2, \ldots, n$$

and denote the corresponding position of the isotherm by $Z_i$. Assuming a linear profile within each subdivision $[Z_i, Z_i+1]$, we have

$$U(z) = \frac{i}{n} + \frac{z - Z_i}{n(Z_{i+1} - Z_i)} \quad \text{for } Z_i \leq z \leq Z_{i+1}.$$ 

Multiplying eqn (6) by $z^2$ and integrating over $[Z_i, Z_{i+1}]$ gives

$$\int_{Z_i}^{Z_{i+1}} z^2 \frac{\partial U}{\partial \tau} \, dz = \int_{Z_i}^{Z_{i+1}} \frac{\partial}{\partial z} \left( z^2 \frac{\partial U}{\partial z} \right) \, dz.$$ 

Taking the derivative outside the integral sign, we obtain

$$\frac{d}{d\tau} \left( \int_{Z_i}^{Z_{i+1}} z^2 U \, dz - \frac{Z_{i+1}^3 U_{i+1}}{3} + \frac{Z_i^3 U_i}{3} \right) = \left( z^2 \frac{\partial U}{\partial z} \right)_{Z_{i+1}} - \left( z^2 \frac{\partial U}{\partial z} \right)_{Z_i}.$$ 

Replacing $U$ by the linear profile and ensuring that the expression representing change in flux is approximated by the discontinuous change in adjacent profile gradients, we obtain a system of ordinary differential equations for the penetration depth $Z_i$, namely,

$$\begin{align*}
(3Z_i^2 + 2Z_i + 1)\dot{Z}_i &= \frac{12}{Z_i - 1} - \frac{12Z_i^2}{Z_i - Z_{i+1}}, \\
(3Z_{i+1}^2 + 2Z_{i+1}Z_i + Z_i^2)\dot{Z}_{i+1} &= \frac{12Z_{i+1}^2}{Z_{i+1} - Z_i} - \frac{12Z_i^2}{Z_i - Z_{i+1}}, \quad i = 1, 2, \ldots, n - 2, \\
[3(1 + 4an)Z_n^2 + 2Z_nZ_{n-1} + Z_{n-1}^2]\dot{Z}_n &= \frac{12Z_{n-1}^2}{Z_n - Z_{n-1}}. 
\end{align*}$$

It is easily seen that the above system is singular when $\tau = 0$, since the positions of the isotherms are all the same. This is unavoidable, since at $\tau = 0$ the phase front will move out with infinite velocity. The velocity becomes finite only for $\tau > 0$. Hence a small time starting solution is
The initial motion of each isotherm \( Z_i \) is assumed to have the form

\[
Z_i(\tau) = 1 + \mu_{i,0} \tau^{1/2} + \mu_{i,1} \tau + \mu_{i,2} \tau^{3/2} + \cdots \tag{11}
\]

The coefficients \( \mu_{i,j} \) can be found by substituting eqn (11) into eqns (8–10) and hence obtaining a system of non-linear equations, which can be effectively solved by Newton's method. The method is effective since the Jacobian is tri-diagonal and each iteration can be computed efficiently. In this paper we retain terms up to \( \tau^{3/2} \), and use \( \tau = 0.01 \) to obtain the initial positions of the isotherms.

It can be seen that the system of eqns (8–10) is stiff, at least for \( \tau \) small where the distances between adjacent isotherms are small. For this reason standard ODE solvers, for example the 4th order Runge-Kutta method with adaptive step size control, will require an extremely small time step for a given accuracy. For this reason we have used a semi-implicit version of the Bulirsch-Stoer method to solve the system. Readers may refer to [8] for details of the method.

### 4 Enthalpy method

The enthalpy formulation is one of the most popular fixed-domain methods for solving the Stefan problem. The major advantage is that the method does not require explicit treatment of the moving boundary. To introduce the formulation, we define an enthalpy function \( h \) as a function of temperature \( T \)

\[
h = \int_{T_s}^{T} \rho c \, dT + \rho L f_1(T),
\]

where \( \rho \) is density and \( f_1 \) is the local liquid fraction given by

\[
f_1 = \begin{cases} 
1 & \text{if } T \geq T_f, \\
0 & \text{if } T < T_f.
\end{cases}
\]

Writing in non-dimensional form (letting \( H = h/(\rho c(T_f - T_s)) \)) gives

\[
H = U + \alpha f_1(U) \tag{12}
\]

Hence \( H \) is identical to the temperature except when phase change occurs, in which case \( H \) has a jump of \( \alpha \). Thus a change of phase is realized as a jump discontinuity in \( H \). Substituting \( H \) into the heat equation, we obtain

\[
\frac{\partial H}{\partial \tau} = \frac{1}{z^2} \frac{\partial}{\partial z} \left( z^2 \frac{\partial U}{\partial z} \right). \tag{13}
\]

Discretization of eqn (13) will result in a set of non-linear equations. Date [3] introduces a simple method which at the same time provides an
effective means of tracking the phase boundary. From eqn (12) we can write

\[ U = H + H' \]

where \( H' = -\alpha f_1(U) \). However, we can express \( H' \) in terms of \( H \) as

\[
H' = \begin{cases} 
-\alpha & \text{if } H \geq \alpha + 1, \\
1 - H & \text{if } 1 < H < \alpha + 1, \\
0 & \text{if } H \leq 1.
\end{cases}
\] (14)

Also, we note that \(-H'/\alpha\) is the local liquid fraction while \(1 + H'/\alpha\) is the local solid fraction. This provides a means of determining the phase boundary, as we shall see later.

To solve the phase-change problem, we first construct uniform grids placed between \( z = 1 \) and \( z = 2 \), as shown in Figure 2.

\[
\begin{array}{c|cccc}
\text{z} & 1 & 2 & \ldots & \text{N} \\
\hline
\text{i} & 1 & 2 & \ldots & N
\end{array}
\]

Figure 2: Arrangement of uniform grids between \( z = 1 \) and \( z = 2 \).

To obtain unconditional stability, we use an implicit discretization of eqn (13). Also, to advance from time level \( j \) to \( j + 1 \), we have

\[
\frac{H_{i,j+1} - H_{i,j}}{\Delta \tau} = \frac{1}{\Delta z^2} \left[ \left(1 + \frac{\Delta z}{z_i}\right)U_{i+1,j+1} - 2U_{i,j+1} + \left(1 - \frac{\Delta z}{z_i}\right)U_{i-1,j+1} \right],
\] (15)

where \( \Delta z \) and \( \Delta \tau \) are the space and time steps, respectively, and \( z_i \) denotes the position of the \( i \)th grid, which is given by \( z_i = 1 + i\Delta z \). Note that \( U_0 = 1 \). For simplicity we use \( U_N = 1 \) as the other boundary condition, which is valid as long as the phase front is not close to \( z = 2 \). Now using the relation \( U_{i,j} = H_{i,j} + H'_{i,j} \) with \( H'_{i,j} \) obtained from eqn (14), we have

\[
-\left(1 - \frac{\Delta z}{z_i}\right)\gamma H_{i-1,j+1} + \left(1 + 2\gamma\right)H_{i,j+1} - \left(1 + \frac{\Delta z}{z_i}\right)\gamma H_{i+1,j+1} = H_{i,j} + \gamma \left[\left(1 - \frac{\Delta z}{z_i}\right)H'_{i-1,j+1} - 2H'_{i,j+1} + \left(1 + \frac{\Delta z}{z_i}\right)H'_{i+1,j+1}\right],
\] (16)

where \( \gamma = \Delta \tau / \Delta z^2 \). This results in a set of nonlinear equations. To solve this system we employ an iterative scheme, where terms involving \( H' \) are set to lag behind terms involving \( H \) for one iteration. Using the result of \( H \) from the previous time step as the initial guess, the values of \( H' \) are
calculated from eqn (14). The new value of $H$ is then obtained from eqn (16). This process is continued until the maximum fractional change in $H$ between successive iterations is less than $10^{-5}$. Then we can continue to the next time step. Note that each iteration involves solving a tridiagonal system, and can be done effectively by the Thomas algorithm.

Recalling that $1 + H_i'/\alpha$ is the solid fraction in the $i$th control volume, there is a simple way to calculate the position of the phase front. Consider the integral $I$, which represents the volume of solid in the range $1 \leq z \leq Z(\tau)$:

$$I = \int_1^{Z(\tau)} z dz \approx \Delta z \sum_{i=1}^{N} z_i \left(1 + \frac{H_i'}{\alpha}\right) + \frac{\Delta z}{2}.$$

The last term is due to the fact that the temperature in the first cell is always zero. Here, the summation can be done over all the cells since the cells behind the phase-front give zeros to $1 + H_i'/\alpha$. Hence we have

$$Z(\tau) = \sqrt{2I + 1}.$$

### 5 Numerical results

In this section we present the computational results obtained by using the two methods outlined in the previous sections. Note that we use $n = 32$ in the HBIM and $\Delta z = 0.01$ in the enthalpy method throughout the paper. In Figure 3 the position of the phase front is plotted against non-dimensional time $\tau/\alpha$ for $\alpha = 1$. It can be seen that the agreement of the two methods is very good. The cases for $\alpha = 5$ and $\alpha = 0.2$ are shown in Figure 4 and Figure 5, respectively. Again the two methods compare well.

![Figure 3: Position of phase front versus non-dimensional time $\tau/\alpha$ for $\alpha = 1$.](image-url)
Figure 4: Position of phase front versus non-dimensional time $\tau/\alpha$ for $\alpha = 5$.

Figure 5: Position of phase front versus non-dimensional time $\tau/\alpha$ for $\alpha = 0.2$. 
Table 1: Position of the phase-front versus dimensional time for $\alpha = 1$. 

| Time $\tau$ | HBIM $Z_H$ | Enthalpy $Z_E$ | $\frac{|Z_H - Z_E|}{Z_H} \times 100\%$ |
|------------|-----------|------------|----------------------------------|
| $0.05$     | 1.258676  | 1.260232   | 0.1236%                          |
| $0.10$     | 1.357523  | 1.359662   | 0.1576%                          |
| $0.15$     | 1.430808  | 1.433675   | 0.2004%                          |
| $0.20$     | 1.490971  | 1.494397   | 0.2298%                          |
| $0.25$     | 1.542886  | 1.546565   | 0.2384%                          |

Table 1 shows the numerical values of the position of the phase-front obtained from the HBIM and enthalpy method at various non-dimensional time, for $\alpha = 1$. From the table, we see that the percentage differences between the results obtained by HBIM and enthalpy method are very small. The percentage differences for the cases $\alpha = 5$ and $\alpha = 0.2$ are shown in Table 2 and Table 3, respectively. Again the percentage differences are small. Clearly the agreement improves with increasing values of Stefan number, $\alpha$.

Table 2: Position of the phase-front versus dimensional time for $\alpha = 5$. 

| Time $\tau$ | HBIM $Z_H$ | Enthalpy $Z_E$ | $\frac{|Z_H - Z_E|}{Z_H} \times 100\%$ |
|------------|-----------|------------|----------------------------------|
| $0.05$     | 1.286181  | 1.282527   | 0.2841%                          |
| $0.10$     | 1.390242  | 1.388581   | 0.1195%                          |
| $0.15$     | 1.467231  | 1.466822   | 0.0278%                          |
| $0.20$     | 1.530413  | 1.530868   | 0.0298%                          |
| $0.25$     | 1.584831  | 1.586001   | 0.0738%                          |

Table 3: Position of the phase-front versus dimensional time for $\alpha = 0.2$. 

| Time $\tau$ | HBIM $Z_H$ | Enthalpy $Z_E$ | $\frac{|Z_H - Z_E|}{Z_H} \times 100\%$ |
|------------|-----------|------------|----------------------------------|
| $0.05$     | 1.201104  | 1.205508   | 0.3666%                          |
| $0.10$     | 1.280582  | 1.285713   | 0.4007%                          |
| $0.15$     | 1.340071  | 1.346091   | 0.4492%                          |
| $0.20$     | 1.389534  | 1.396271   | 0.4849%                          |
| $0.25$     | 1.432756  | 1.439915   | 0.4997%                          |
6 Conclusions

We have presented the heat balance integral method (HBIM) and the enthalpy method for solving the solidification problem in spherical geometry. It is found that the two methods agree well for a wide range of Stefan number.

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References


