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Numerical solution of Stefan problems in annuli

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Abstract

A novel enthalpy formulation is applied to Stefan problems in annuli and is compared with the heat balance integral method (HBIM). Both methods are applied to inward and outward solidification in cylindrical geometry, and the results are combined to give numerical solutions in annuli. It is found that the enthalpy method gives comparable accuracy with the HBIM except for small Stefan number, and is more efficient and flexible.

1 Introduction

Change of phase occurs naturally in many physical and industrial processes. The classical phase change problem is that of melting or solidification via the conduction of heat, which is referred to in the literature as the Stefan problem. The main difficulty in solving this problem is the presence of a moving phase boundary. Hill [1] gives an account of analytical solutions to the Stefan problem. Due to difficulties in obtaining such analytical solutions, numerical techniques are more widely used. A useful account of these is given by Crank [2].

Of the two main approaches in the solution of Stefan problems, one is the front-tracking method. Here the position of the phase boundary is continuously tracked. An example is the heat balance integral method (HBIM) which explicitly tracks the motion of isotherms (the phase boundary being one of them). One can also employ finite difference schemes and let the grids deform as the phase boundary moves. These provide a means for tracking the phase front explicitly. In past work Caldwell and Chiu [3,4] have used the HBIM to solve one-dimensional solidification problems.

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A second approach is the fixed-domain formulation, where the computational domain is fixed via a change of variable. An example is the enthalpy formulation, which uses an enthalpy function together with the temperature as dependent variables. In this formulation the flux condition on the phase boundary is automatically satisfied and the phase boundary appears as a jump discontinuity of the enthalpy. One disadvantage of the enthalpy method is that the phase front cannot be determined accurately.

Date [5] introduces a new enthalpy formulation which provides a simple and efficient means of tracking the phase boundary. In this paper, the method is generalized to cylindrical geometry, in particular to annuli, and is compared to the HBIM. Using various numerical experiments, it is found that the new method gives comparable accuracy to the HBIM while being more efficient and flexible.

2 Problem formulation

Consider a freezing vessel in the shape of an annulus, which contains liquid initially at its freezing temperature T_f. The configuration is shown in Figure 1. The two surfaces of the annulus are maintained at a temperature T_s, which is lower than the freezing temperature for $t>0$. If the density change from liquid to solid is neglected, the system is governed by the equations

$$\frac{\partial T_1}{\partial t} = \frac{k}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T_1}{\partial r}\right), \qquad r_1 < r < R_1(t),$$
$$\frac{\partial T_2}{\partial t} = \frac{k}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T_2}{\partial r}\right), \qquad R_2(t) < r < r_2, \tag{1}$$

where k is the thermal diffusivity, $R_1(t)$ and $R_2(t)$ are positions of phase boundaries, where $R_i(0)=r_i$. The initial and boundary conditions are

$$T = T_f, \qquad r_1 \le r \le r_2, \qquad t = 0$$
$$T_i(r_i, t) = T_s, \qquad t > 0, \qquad i = 1,2$$

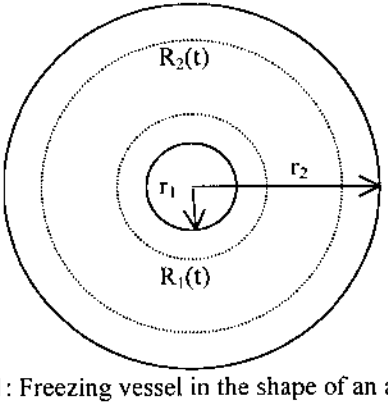

Figure 1: Freezing vessel in the shape of an annulus.

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and at the solid-liquid interface

$$K\left(\frac{\partial T}{\partial r}\right)_{R_i(t)} = L\rho\frac{dR_i(t)}{dt}, \qquad i = 1,2 \tag{2}$$

where we have assumed that the physical properties of the material remain constant throughout the process. The constants K, ρ and L represent thermal conductivity, density and latent heat of freezing, respectively.

To simplify the formulation we introduce non-dimensional variables

$$z = \frac{r}{r_1}, \tau = \frac{kt}{r_1^2}, U_i = \frac{T_i - T_s}{T_f - T_s},$$

$$r^* = \frac{r_2}{r_1}, \alpha = \frac{L}{c(T_f - T_s)}.$$

Then the equations in (1) become

$$\begin{aligned} \frac{\partial U_1}{\partial \tau} &= \frac{1}{z}\frac{\partial}{\partial z}\left(z\frac{\partial U_1}{\partial z}\right), & 1 < z < Z_1(\tau), \\ \frac{\partial U_2}{\partial \tau} &= \frac{1}{z}\frac{\partial}{\partial z}\left(z\frac{\partial U_2}{\partial z}\right), & Z_2(\tau) < z < r^*, \end{aligned} \tag{3}$$

and for the initial and boundary conditions, we have

$$U_i = 1, \qquad \tau = 0$$

$$U_1(1,\tau) = U_2(r^*,\tau) = 0, \qquad \tau > 0.$$

Finally the flux condition (2) becomes

$$\left(\frac{\partial U_i}{\partial z}\right)_{Z_i(\tau)} = \alpha\frac{\partial Z(\tau)}{\partial \tau}, \tag{4}$$

where α is the Stefan number which is a dimensionless latent heat parameter.

3 Heat balance integral method (HBIM)

For problems in cylindrical geometry, there are no exact solutions when the temperature on the boundary is a prescribed constant value. The HBIM, originally proposed by Goodman [6] and later modified by Belt [7], explicitly tracks the motion of isotherms (the phase boundary being one of them).

Consider the non-dimensional equations in (3), For simplicity we consider the outward solidification first, since the problem can be separated into two independent parts, namely, inward solidification and outward solidification. First, we divide the range [0,1] into n equal parts, that is

$$U_{1,i} = \frac{i}{n}, \qquad i = 0,1,2,\ldots,n$$

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and denote the corresponding position of the isotherm by Z_i, Assuming a linear profile within each subdivision $[Z_i, Z_{i+1}]$, then

$$U_1 = \frac{i}{n} + \frac{z - Z_i}{n(Z_{i+1} - Z_i)} \quad \text{for } Z_i \le z \le Z_{i+1}.$$

Multiplying the heat equation (1) by z and integrating over $[Z_i,Z_{i+1}]$ gives

$$z\frac{\partial U_1}{\partial \tau} = \frac{\partial}{\partial z}\left(z\frac{\partial U_1}{\partial z}\right)$$

$$\int_{Z_i}^{Z_{i+1}} z\frac{\partial U_1}{\partial \tau}\,dz = \int_{Z_i}^{Z_{i+1}} \frac{\partial}{\partial z}\left(z\frac{\partial U_1}{\partial z}\right)dz$$

and taking the derivative outside the integral gives

$$\frac{d}{d\tau}\left(\int_{Z_i}^{Z_{i+1}} zU_1\,dz - \frac{Z_{i+1}^2 U_{1,i+1}}{2} + \frac{Z_i^2 U_{1,i}}{2}\right) = \left(z\frac{\partial U_1}{\partial z}\right)_{Z_{i+1}} - \left(z\frac{\partial U_1}{\partial z}\right)_{Z_i}.$$

Replacing U_1 by the linear profile and ensuring that expressions representing change in flux are approximated by the discontinuous change in adjacent profile gradients, we obtain a system of ODE's for the penetration depth Z_i, namely,

$$\begin{aligned}
&(2Z_1 + 1)\dot{Z}_1 = \frac{6}{Z_1 - Z_0} - \frac{6Z_1}{Z_2 - Z_1},\\
&(2Z_{i+1} + Z_i)\dot{Z}_{i+1} + (Z_{i+1} + 2Z_i)\dot{Z}_i\\
&= \frac{6Z_i}{Z_{i+1} - Z_i} - \frac{6Z_{i+1}}{Z_{i+2} - Z_{i+1}}, i = 1,2,3,\ldots,n-2,\\
&[2(1 + 3\alpha n)Z_n + Z_{n-1}]\dot{Z}_n + (Z_n + 2Z_{n-1})\dot{Z}_{n-1} = \frac{6Z_{n-1}}{Z_n - Z_{n-1}},
\end{aligned} \tag{5}$$

where Z_0=1 for outward solidification. The above system can be solved by standard ODE solvers. In this paper, a fourth order Runge-Kutta method with adaptive step size control is used.

It is easily seen that the system of equations (5) is singular when τ=0, since the positions of isotherms coincide. This is unavoidable, since at τ=0 the phase front will move out with infinite velocity. The velocity becomes finite only for τ>0. Hence a small time starting solution is needed. The appropriate starting solution is given by Poots [8] and the initial motion of each isotherm Z_i is given by a power series in $\tau^{1/2}$, namely,

$$Z_i(\tau) = 1 + \mu_{i,0}\tau^{1/2} + \mu_{i,1}\tau + \mu_{i,2}\tau^{3/2} + \ldots \tag{6}$$

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The coefficients $\mu_{i,j}$ can be found by substituting (6) into the heat balance integral equations (5) to obtain a system of non-linear algebraic equations, which can be effectively solved by Broyden's method. In this paper we retain terms up to $\tau^{3/2}$, and use τ=0.01 to obtain the initial positions of the isotherms.

It can be seen that the problem of inward solidification is completely analogous to that of outward solidification. The only change in the heat balance equations (5) is that now $Z_0=\tau^*$, and that an appropriate starting solution is

$$Z_i(\tau) = r^* - \eta_{i,0}\tau^{1/2} - \eta_{i,1}\tau - \eta_{i,2}\tau^{3/2} - \ldots \tag{7}$$

Throughout this work we use the HBIM with 8 subdivisions. On checking we find that doubling the number of subdivisions does not significantly improve the results.

4 Enthalpy formulation

The enthalpy formulation is one of the most popular fixed-domain methods for solving Stefan problems. 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:

$$h = \int_{T_s}^{T} \rho\, c\, dT + \rho\, L\, f_l(T),$$

where f_l is the local liquid fraction given by

$$f_l = \begin{cases} 1 & if \quad T \geq T_f \\ 0 & if \quad T < T_f. \end{cases}$$

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

$$H = U + \alpha\, f_l(U). \tag{8}$$

Hence H is identical to the temperature except when phase change occurs, when H has a jump of α. Thus a change of phase is realized as a jump discontinuity in H. Substituting H into the heat equation gives

$$\frac{\partial H}{\partial \tau} = \frac{1}{z}\frac{\partial}{\partial z}\left(z\frac{\partial U}{\partial z}\right). \tag{9}$$

It can be proved that a weak solution of equation (9) is a solution of the Stefan problem. Discretization of equation (9) will result in a set of nonlinear equations. There are a number of ways of implementing the numerical scheme and some of them are summarized by Voller [9]. One approach is to use a source based method which isolates the nonlinear part as a source term (see Voller and Swaminathan [10]).

Date [5] introduces a simple method which at the same time provides an effective means of tracking the phase boundary. From equation (8) we can write $U=H+H'$ where $H'=-\alpha f_l(U)$. However, we can express H' in terms of H as follows:

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$$H' = \begin{cases} -\alpha & if \quad H \geq \alpha \\ -H & if \quad 0 < H < \alpha. \\ 0 & if \quad H \leq 0 \end{cases} \tag{10}$$

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 in annuli with constant temperature at the boundary, we first construct uniform grids placed between z=1 and $z=r^*$ as shown in Figure 2. To obtain unconditional stability, we use an implicit discretization of (9). To advance from time level j to j+1, we have

$$\frac{H_{i,j+1} - H_{i,j}}{k} = \frac{1}{h^2}\left[\left(1+\frac{1}{2z_i}\right)U_{i+1,j} - 2U_{i,j} + \left(1-\frac{1}{2z_i}\right)U_{i-1,j}\right], \tag{11}$$

for i=1,2,3,...,N, where h and k are the space and time steps respectively, and z_i denotes the position of the i-th grid, which is given by $z_i=1+ih$. Note that $U_0=U_{N+1}=0$. Now, using the relation $U=H+ H'$ with H' defined by (10), we have

$$\begin{aligned} &-\left(1-\frac{1}{2z_i}\right)\gamma\, H_{i-1,j+1} + (1+2\gamma)H_{i,j+1} - \left(1+\frac{1}{2z_i}\right)\gamma\, H_{i+1,j+1} \\ &= H_{i,j} + \gamma\left[\left(1-\frac{1}{2z_i}\right)H'_{i-1,j+1} - 2H'_{i,j+1} + \left(1+\frac{1}{2z_i}\right)H'_{i+1,j+1}\right], \end{aligned} \tag{12}$$

where $\gamma=k/h^2$. 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 1 iteration. Using the value of H from the previous time step as initial guess, the values of H' are calculated from (10). The new values of H are then obtained from the system (12). This process is continued until the maximum fractional change in H between successive iterations is less than 10^{-5}. Then we proceed to the next time step. Note that each iteration involves solving a tri-diagonal system and can be done effectively by the Thomas algorithm.

Since $H'=-\alpha f_l$, the solid fraction f_s in the i-th control volume is given by $1+ H_i'/\alpha$. This provides a simple way to calculate the position of the phase front. For instance, suppose we want to find R_1. Consider the integral I which represents the volume of solid in the range $1\leq z \leq R_1$,

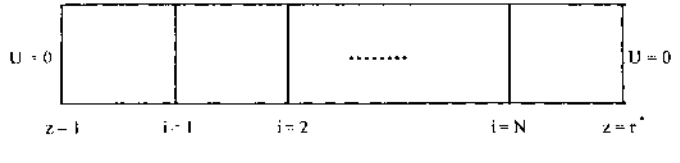

Figure 2: Arrangement of uniform grids between z=1 and $z=r^*$

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$$I = \int_{1}^{R_1} z\,dz \approx h\sum_{i=1}^{m_1-1} z_i\left(1+\frac{H_i'}{\alpha}\right)+\frac{h}{2},$$

where m_1 is the first integer such that $1+H'/\alpha$ is zero, and the last term is due to the fact that the temperature at the boundary is zero. Hence we have $R_1 = \sqrt{\frac{1}{2}+I}$. The value of R_2 can be found similarly. This method assumes there is a node m for which the whole control volume is in the liquid state. Such a node might exist when the phase fronts come close together, and from then on tracking of individual phase fronts is impossible. One remedy is to decrease h so that we can track the front longer. However, if we are interested in the complete solidification time only, as is often the case, there is a simple way to do it. Consider the integral J which represents the total volume of solid in the annulus. Then we have

$$J = \int_{1}^{R_1} z\,dz + \int_{R_2}^{r^*} z\,dz = \frac{1}{2}\left(R_1^2 - R_2^2 + r^{*2} - 1\right)$$

Hence $R_2^2 - R_1^2 = r^{*2} - 1 - 2J$.

On the other hand J can be approximated by

$$J \approx h\sum_{i=1}^{N} z_i\left(1+\frac{H_i'}{\alpha}\right)+\frac{h}{2}\left(1+r^*\right)$$

Therefore the difference of positions of the phase fronts can be calculated easily. The instance at which $R_2^2 - R_1^2 = 0$ gives the complete solidification time. For the cases of inward and outward solidification of a cylinder, the phase front can be tracked similarly.

5 Numerical results

5.1 Inward and outward solidification

As mentioned before, one-phase solidification in a cylinder can be split up into two independent problems of inward and outward solidification. Therefore we present results for inward and outward solidification here, and combine them to give results for an annulus in the next subsection.

In Figure 3 the position of the phase front is plotted versus non-dimensional time τ/α for $\alpha=1$. Computational results using the HBIM and the enthalpy method are compared. Also plotted are the results from Voller and Cross [11], who also use an enthalpy formulation. They used a "latent heat at node" approach to determine the time for the phase front to pass through a grid point. Clearly the present results agree with those of Voller and Cross for h=0.025. The advantage of the present method is that it provides a continuous tracking of the phase front. For h=0.1 the motion of the phase front shows a

non-physical oscillation, which is a common weakness of the enthalpy method. This can be reduced by decreasing h.

A comparison with the HBIM shows that the results agree closely except at the centre. Near the centre the HBIM predicts a much faster motion of the phase front and thus a shorter solidification time. This effect is more prominent when the Stefan number α is large. It is well known that for very small α (e.g. α=0.1) the enthalpy method is unable to give the correct solution (see, for example, Shamsundar and Rooz [12]). This is verified by the results in Figure 4. The enthalpy method predicts a much earlier solidification time.

Numerical results for the motion of the phase front for outward solidification for the cases α=0.1, 1 and 10 show that the situation is similar. Again the enthalpy method and the HBIM agree closely except for α=0.1.

5.2 Solidification in annulus

The results are similar to those mentioned above, namely, that the enthalpy method is good except when α is very small. Since, in the case of annulus solidification, the phase front will not hit the centre, the problem associated with the HBIM near the centre will disappear.

We take r^*=2 in all cases. The main focus is on the positions of phase fronts and prediction of complete solidification time. Figure 5 shows the position of the phase front for α=1. It is clear that the enthalpy method and the HBIM agree closely. The waviness of the motion of the phase front for the case h=0.1 persists. For the enthalpy method we cannot track the position of the phase front down to the moment of complete solidification. In Figure 6 R_2^2- R_1^2 is plotted versus non-dimensional time. The solidification time is the point where R_2^2- R_1^2=0. Again results from the enthalpy method and the HBIM agree closely. Further results show that for large α (e.g. α=10) there is excellent agreement in the position of the phase front. However, for small α (e.g. α=0.1) the enthalpy method fails.

6 Conclusions

In this paper we have extended the enthalpy method proposed by Date [5] to cylindrical geometry. It is shown that the enthalpy method gives comparable accuracy to the HBIM, except for very small Stefan number α.

One of the advantages of the enthalpy method over the HBIM is that it is more flexible. Although it is possible to solve 2-phase problems (i.e. the liquid is not at its freezing temperature initially), the formulation becomes more complicated. However, the enthalpy method needs no modification. Also the enthalpy method can be easily adapted to other geometries, whereas applying the HBIM to more complicated domains will result in extremely tedious algebraic work.

The weakness of the enthalpy method is that it does not give satisfactory results for small Stefan number. Also the waviness in the position of the phase front is non-physical. Date [5] proposed a method which successfully

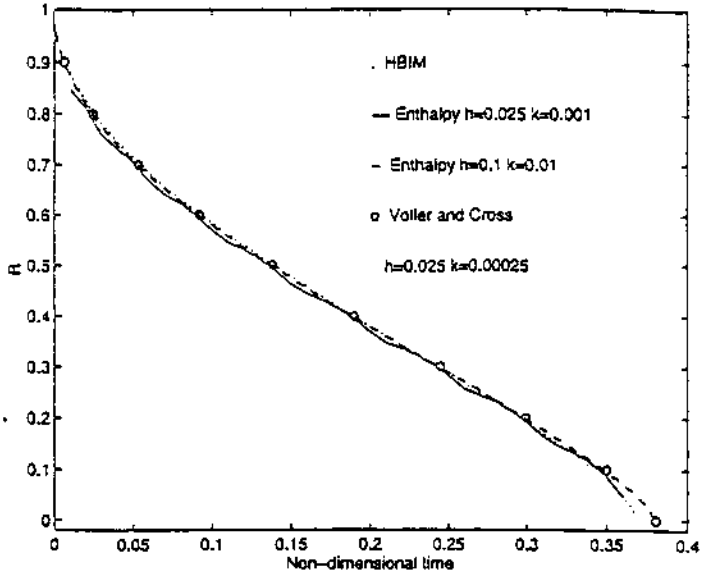

Figure 3: Position of phase front versus non-dimensional time τ/α for α=1, inward solidification.

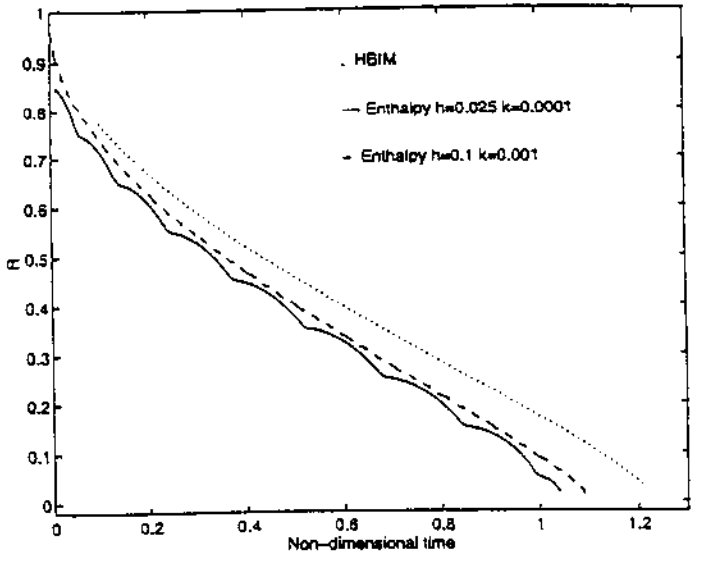

Figure 4: Position of phase front versus non-dimensional time τ/α for α=0.1, inward solidification.

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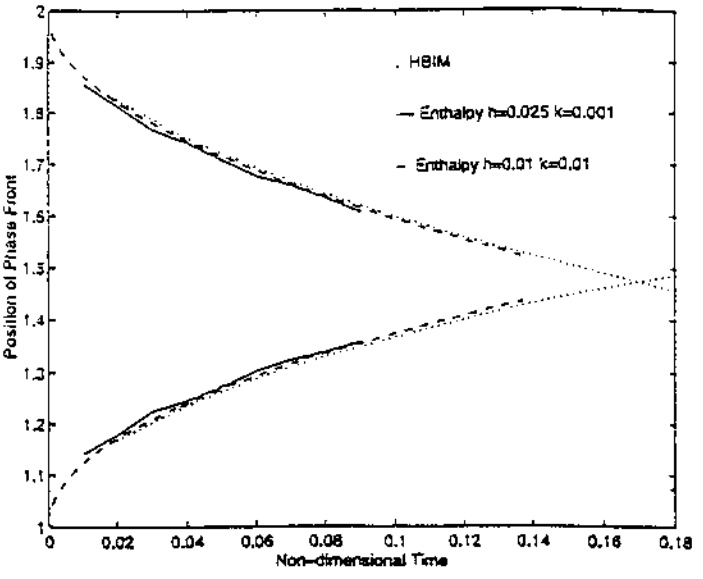

Figure 5: Position of phase front versus non-dimensional time τ/α for α=1, solidification in annulus.

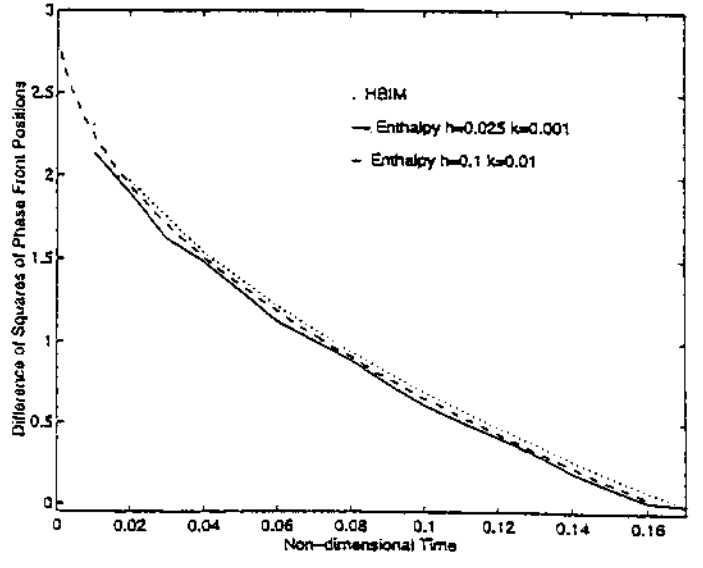

Figure 6: $R_2^2 - R_1^2$ versus non-dimensional time τ/α for α=1.

eliminates the waviness, and at the same time obtained good results for small Stefan number. Date's method is applied to plane geometry, and the possibilities of extension to other geometries are worth investigation.

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