Approximate Solutions of Mathematical Models of Supercooling Solidification

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By

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Abstract

In [1], [2], some one-dimensional mathematical models of supercooling solidification have been established, and some existence theorems have been proven by a difference method. In this paper, the models and the method are shown again in §§ 1, 2 and another analytic method of approximate solution is proposed in § 3. It is based on the assumption that a profile of temperature distribution at any time may be considered linear in every inner region. By some numerical examples, solutions by the approximate method are compared with some solutions given by the difference method. It is then realized that the approximate solutions come sufficiently close to the difference solutions.

§ 1 Mathematical models

It is assumed that some supercooling matter of a liquid phase is first contained quietly in a tube, starts to be solidified by some shock at one end of the tube, and then the solidification proceeds to the other end of the tube. Here, it is considered that a front surface of solidification is always perpendicular to the axis of the tube, that is, the process is substantially one-dimensional.

We consider two problems, a one-phase problem and a two-phase problem. In the former, it is assumed that only the temperature of a solid phase may change, but that of liquid phase is constant during the process. Heat balance is, as well known, formulated like that in the inner region of a solid phase:

$$(1) \qquad \rho c \frac{\partial u}{\partial t} = k \frac{\partial^2 u}{\partial x^2} \, (0<t<T, \ 0<x<y(t))$$

and at the front surface of solidification:

$$(2) \qquad \rho \{b - cu(y(t), \ t)\} \, \dot{y} = k \frac{\partial u}{\partial x} \quad (0<t<T),$$

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where $u=u(x, t)$ is the normalized temperature, $y(t)$ is the distance of the front surface from the starting end, ρ is the density of the solid, c is the specific heat, k is the heat conductivity and b is the latent heat. In the last equation, the term $cu(y(t), t)$ signifies the heat quantity used when the temperature of the quiet liquid $(u=0)$ rises suddenly to $u(y(t), t)$ at the front surface. Furthermore, a boundary and an initial condition must be imposed. They are here taken, for example, as

$$u(0, t)=0 \qquad (0<t<T) \tag{3}$$

and

$$y(0)=0. \tag{4}$$

One more condition is essential for the present problem. It is given by the formula:

$$\dot{y}(t)=\alpha\{u_E-u(y(t), t)\} \quad (0<t<T) \tag{5}$$

which means that the solidification speed is proportional to the degree of supercooling, where u_E is the melting point and α is a proportional constant.

In the other problem, the two-phase problem, it is assumed that the temperature may change in both regions of a solid and liquid phase. In this case, heat balance is formulated by the following set of equations:

$$\rho c_1\frac{\partial u}{\partial t}=k_1\frac{\partial^2 u}{\partial x^2} \qquad (0<x<y(t),\ 0<t<T), \tag{6}$$

$$\rho c_2\frac{\partial u}{\partial t}=k_2\frac{\partial^2 u}{\partial x^2} \qquad (y(t)<x<l,\ 0<t<T), \tag{7}$$

$$\rho b\dot{y}(t)=k_1\frac{\partial u}{\partial x}(y(t)-0, t)-k_2\frac{\partial u}{\partial x}(y(t)+0, t) \quad (0<t<T), \tag{8}$$

where c_1 and c_2 are the specific heat of the solid and liquid phase respectively, k_1 and k_2 are the heat conductivity of the solid and liquid phases respectively. The density ρ is, however, assumed to be common for both the solid and liquid phases. Other conditions are like those in the one-phase problem as follows:

$$u(0, t)=u(l, t)=0 \qquad (0<t<T), \tag{9}$$

$$y(0)=0, \quad u(x, 0)=0 \qquad (0<x<l), \tag{10}$$

$$\dot{y}(t)=\alpha\{u_E-u(y(t), t)\} \qquad (0<t<T). \tag{11}$$

In the following, we want to construct approximate solutions of both problems. In §2, the difference method in [1] and [2] is reproduced for giving numerical solutions in §4, as the objects of comparison with the approximate solutions given by the analytic method, which itself is proposed in §3.

§ 2 Difference method

As in [1] and [2], we introduce a net of rectangular meshes with a uniform space width h and variable time steps $\{\tau_n\}$ $(n=1, 2, 3, \ldots)$. The time steps $\{\tau_n\}$ are assumed to be unknown a priori and to be determined in the process of computation by the rule that h/τ_n might give the gradient of a front surface at each time $t=t_n$, so that the front boundary might cross each line of ordinate $x=x_j$ just at each corresponding mesh point. (See Fig. 1). Here, the discrete coordinates are given by:

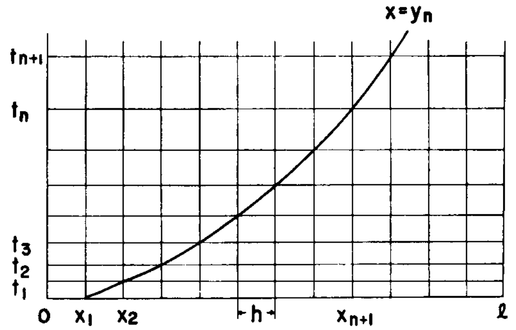

Fig. 1. The net of meshes of the difference scheme.

$$x_j=jh \qquad (j=0, 1, 2, \ldots, L;\ Lh=l),$$
$$t_n=\sum_{p=1}^{n}\tau_n \qquad (n=1, 2, 3, \ldots).$$

Unknown functions are denoted by y_n and u_j^n which correspond to $y(t_n)$ and $u(x_j, t_n)$ respectively. By the rule mentioned above we can put

$$y_n=J_nh \qquad (J_n\text{: integer, } n=0, 1, \ldots, J_{n+1}=J_n+1).$$

It must be noted that the real unknown variables are $\{\tau_n\}$ and $\{u_j^n\}$ in the difference net established above.

In the case of the one-phase problem, the equations (1)–(5) are replaced by the following difference equations. For $n=0, 1, 2, \ldots,$

$$(12) \qquad \rho c\frac{u_j^{n+1}-u_j^n}{\tau_{n+1}}=k\frac{u_{j+1}^{n+1}-2u_j^{n+1}+u_{j-1}^{n+1}}{h^2} \quad (j=1, 2, \ldots, J_{n+1}-1),$$

$$(13) \qquad \rho(b-cu_{J_{n+1}}^{n+1})\frac{h}{\tau_{n+1}}=k\frac{u_{J_{n+1}}^{n+1}-u_{J_{n+1}-1}^{n+1}}{h},$$

$$(14) \qquad u_0^{n+1}=0,$$

$$(15) \qquad J_0=1, \qquad u_1^0=0,$$

$$(16) \qquad \frac{h}{\tau_{n+1}}=\alpha(u_E-u_{J_n}).$$

In the case of the two-phase problem, the equations (6) – (11) are replaced by the following difference equations. For $n=0, 1, 2, \ldots$,

(17) $$\rho c_1 \frac{u_j^{n+1}-u_j^n}{\tau_{n+1}} = k_1 \frac{u_{j+1}^{n+1}-2u_j^{n+1}+u_{j-1}^{n+1}}{h^2} \quad (j=1, 2, \ldots, J_{n+1}-1),$$

(18) $$\rho c_2 \frac{u_j^{n+1}-u_j^n}{\tau_{n+1}} = k_2 \frac{u_{j+1}^{n+1}-2u_j^{n+1}+u_{j-1}^{n+1}}{h^2} \quad (j=J_{n+1}+1, \ldots, L-1),$$

(19) $$\rho \frac{bh}{\tau_{n+1}} = k_1 \frac{u_{J_{n+1}}^{n+1}-u_{J_{n+1}-1}^{n+1}}{h} - k_2 \frac{u_{J_{n+1}+1}^{n+1}-u_{J_{n+1}}^{n+1}}{h},$$

(20) $$u_0^{n+1}=u_L^{n+1}=0,$$

(21) $$J_0=1, \quad u_j^0=0 \quad (j=1, 2, \ldots, L-1),$$

(22) $$\frac{h}{\tau_{n+1}} = \alpha(u_E - u_{J_n}^n).$$

In both systems, that is, (12) – (16) and (17) – (22), τ_{n+1} is first determined from the last equation, (16) or (22). Then, $\{u_j^{n+1}\}$ is found by solving equations (12) – (14) or (17) – (20).

§ 3 Approximate solution

i) The one-phase problem

We regard a profile of temperature distribution at any time as a straight line and put

(23) $$u(x, t) = \frac{v}{y(t)}x, \quad v=v(t)=u(y(t), t).$$

Then condition (2) becomes

(24) $$\rho(b-cv)\dot{y}(t) = k\frac{v}{y}$$

and (5) is written as

(25) $$\dot{y}(t) = \alpha(u_E - v)$$

Elimination of v from (24) and (25) gives a quadratic equation with respect to $\dot{y}$:

(26) $$\rho c \dot{y} y^2 + (\rho\alpha b y - \rho\alpha c u_E y + k)\dot{y} - \alpha k u_E = 0.$$

From this, we have

(27) $$\dot{y} = \frac{1}{2\rho c y}\{-(\rho\alpha b y - \rho\alpha c u_E y + k) + \sqrt{(\rho\alpha b y - \rho\alpha c u_E y + k)^2 + 4\rho\alpha c k u_E y}\}$$

or

(28) $$dt=\frac{-2\rho c y\, dy}{\rho\alpha(b-cu_E)y+k-\sqrt{\rho^2\alpha^2(b-cu_E)^2y^2+2\rho\alpha k(b+cu_E)y+k^2}}\,.$$

If we put

(29) $$\mathrm{A}=\rho\alpha(b-cu_E)\quad\text{and}\quad \mathrm{B}=2\rho\alpha k(b+cu_E),$$

the last equation becomes

(30) $$dt=\frac{-2\rho c y\, dy}{Ay+k-\sqrt{A^2y^2+By+k^2}}\,.$$

In order to solve this ordinary differential equation, we put

$$z=Ay+\sqrt{A^2y^2+By+k^2}\,.$$

Then it is easy to see that

$$y=\frac{z^2-k^2}{2Az+B}$$

and

$$dy=\frac{2(Az^2+Bz+Ak^2)}{(2Az+B)^2}dz.$$

From this and (30), we get

$$\frac{dz}{dt}=\frac{(B-2Ak)(2Az+B)^2}{4\rho c(z+k)(Az^2+Bz+Ak^2)}$$

$$=\frac{\alpha k u_E(2Az+B)^2}{(z+k)(Az^2+Bz+Ak^2)}\,.$$

Since $dy/dt=dy/dz\cdot dz/dt$,

$$\frac{dy}{dt}=\frac{2\alpha k u_E}{z+k}\,.$$

Hence,

$$t=\frac{1}{2\alpha k u_E}\int(z+k)\,dy$$

$$=\frac{1}{2\alpha k u_E}\int(Ay+\sqrt{Ay^2+By+k^2}+k)\,dy$$

$$=\frac{1}{2\alpha k u_E}\left\{\frac{A}{2}y^2+ky+\frac{\sqrt{B^2-4A^2k^2}}{2A}\int\sqrt{\frac{(2A^2y+B)^2}{B^2-4A^2k^2}-1}\,dy\right\}.$$

For the computation of the last integration, we put

$$\xi=\frac{2A^2y+B}{\sqrt{B^2-4A^2k^2}}\,.$$

Then,

$$t=\frac{1}{2\alpha k u_E}\Big[\frac{A}{2}y^2+ky+\frac{B^2-4A^2k^2}{4A^3}\int\sqrt{\xi^2-1}\,d\xi\Big]$$

$$=\frac{1}{2\alpha k u_E}\Big[\frac{A}{2}y^2+ky+\frac{B^2-4A^2k^2}{8A^3}\{\xi\sqrt{\xi^2-1}-\log(\xi+\sqrt{\xi^2-1})\}+C\Big]$$

(C : a constant)

$$=\frac{1}{2\alpha k u_E}\Big[\frac{A}{2}y^2+ky+\frac{2A^2y+B}{4A^2}\sqrt{A^2y^2+By+k^2}-$$
$$-\frac{B^2-4A^2k^2}{8A^3}\log\Big(\frac{2A^2y+B+2A\sqrt{A^2y^2+By+k^2}}{\sqrt{B^2-4A^2k^2}}\Big)+C\Big]$$

Considering condition (4), we have

$$C=-\frac{Bk}{4A^2}+\frac{B^2-4A^2k^2}{8A^3}\log\frac{B+2Ak}{\sqrt{B^2-4A^2k^2}}\ .$$

Thus, we finally obtain

$$t=\frac{A}{4\alpha k u_E}y^2+\frac{1}{2\alpha u_E}y+\frac{1}{8\alpha k u_E A^2}\{(2A^2y+B)\sqrt{A^2y^2+By+k^2}-Bk\}-$$
$$-\frac{B^2-4A^2k^2}{16\alpha k u_E A^3}\log\frac{2A^2y+B+2A\sqrt{A^2y^2+By+k^2}}{B+2Ak} \tag{31}$$

which determines the function $x=y(t)$ implicitly.

It is also found from (25) and (30) that

$$v=u(y(t),\ t)=u_E+\frac{Ay+k-\sqrt{A^2y^2+By+k^2}}{2\rho\alpha c y}\ . \tag{32}$$

ii) The two-phase problem

We again regard a profile of temperature distribution at any time as a sectionally straight line and put

$$u(x,\ t)=\begin{cases}\dfrac{v}{y}x & 0\leqq x\leqq y,\\[2mm] \dfrac{v}{(l-y)}(l-x) & y\leqq x\leqq l.\end{cases} \tag{33}$$

Then, condition (8) becomes

$$b\dot{y}(t)=k_1\frac{v}{y}+k_2\frac{v}{l-y} \tag{34}$$

Elimination of v from the last equation and (11), $\dot{y}(t)=\alpha(u_E-v)$, produces the equation

$$dt=\frac{\rho\alpha b y^2-(l\rho\alpha b-k_1+k_2)y-lk_1}{\alpha u_E\{(k_1-k_2)y-lk_1\}}dy.$$

By integration, we have

$$t=\frac{1}{\alpha u_E(k_1-k_2)}\int\frac{\rho\alpha b y^2-(l\rho\alpha b-k_1+k_2)y-lk_1}{y-\frac{lk_1}{k_1-k_2}}dy$$

$$=\frac{1}{\alpha u_E(k_1-k_2)}\left[\frac{1}{2}\rho\alpha b y^2+\frac{l\rho\alpha bk_2+(k_1-k_2)^2}{k_1-k_2}y+\right.$$

$$\left.+\frac{l^2\rho\alpha bk_1k_2}{(k_1-k_2)^2}\log\left(y-\frac{lk_1}{k_1-k_2}\right)+C\right]$$

The integration constant C is determined by the initial condition (10) as

$$C=-\frac{l^2\rho\alpha bk_1k_2}{(k_1-k_2)^2}\log\left(-\frac{lk_1}{k_1-k_2}\right).$$

Thus, we obtain

(36) $$t=\frac{\rho b}{2u_E(k_1-k_2)}y^2+\frac{l\rho\alpha bk_2+(k_1-k_2)^2}{\alpha u_E(k_1-k_2)^2}y+$$

$$+\frac{l^2\rho bk_1k_2}{u_E(k_1-k_2)^3}\log\left(1-\frac{k_1-k_2}{lk_1}y\right).$$

It is also found from (11) and (35) that

(37) $$v=\frac{\rho\alpha bu_E y(y-l)}{\rho\alpha by^2-(l\rho\alpha b-k_1+k_2)y-lk_1}.$$

The formulas (36), (37) and (33) give an approximate solution of the two phase problem.

§4 Numerical examples

For the exhibition of numerical examples, we consider the cases of solidification of supercooling water. Constant data are as follows;

$\rho=0.917$ (gram/cm^3),

$c=c_1=0.487$ (cal/deg · gram),

$c_2=1.0$ (cal/deg · gram),

$k=k_1=0.00526$ (cal/cm · sec · deg),

$k_2=0.00123$ (cal/cm · sec · deg),

$b=79.8$ (cal/gram),

$u_E=10.0$ (deg),

$l=0.1$ (cm)

$\alpha=0.01.$

All computations by difference schemes are done with the mesh size $h=0.0001$.

Fig. 2 shows the profiles of temperature in the solid phase computed for the one-phase problem by the forementioned difference scheme. Fig. 3 shows the profiles for the two-phase problem. Figs. 4–7 are given in order to compare the two kinds of solutions by the difference method (real lines) and the analytic method (broken lines). Figs. 4 and 5 show the changes of temperature on the front surface of solidification for the one- and two-phase problem respectively. It is seen in Fig. 4 that the difference solution shows an unnatural change near the equilibrium temperature. (Here, it

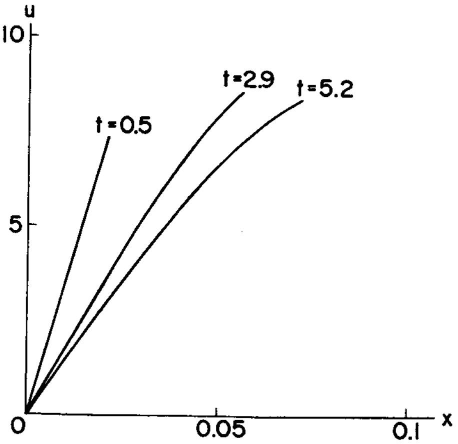

Fig. 2. The profile of temperature distribution at the assigned times in the case of the one-phase problem.

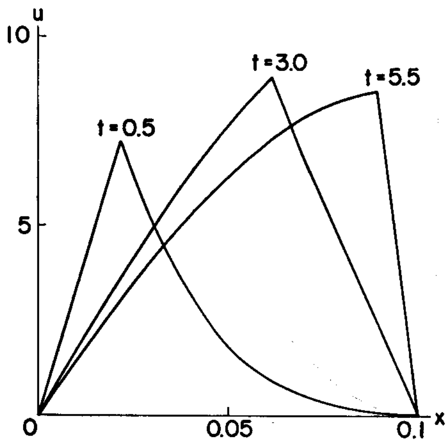

Fig. 3. The profile of temperature distribution at the assigned times in the case of the two-phase problem.

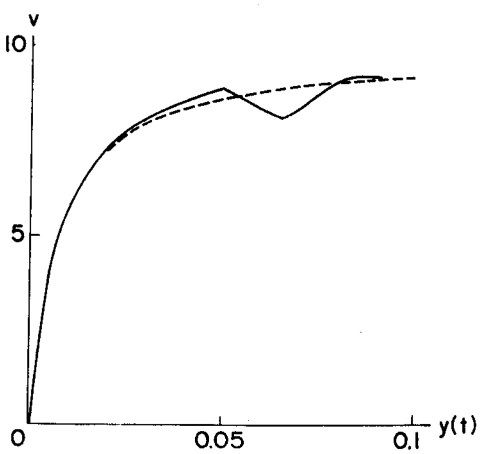

Fig. 4. The change of temperature on the front surface of solidification in the case of the one-phase problem. (The real line : the soution by the difference method ; the broken line : the solution by the proposed method.)

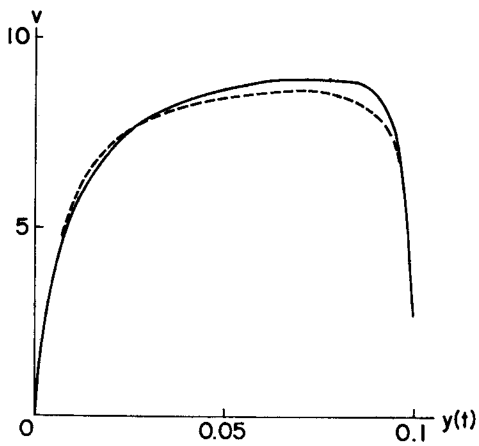

Fig. 5. The change of temperature on the front surface of solidification in the case of the two-phase problem. (The real line : the solution by the difference method; the broken line : the solution by the proposed method.)

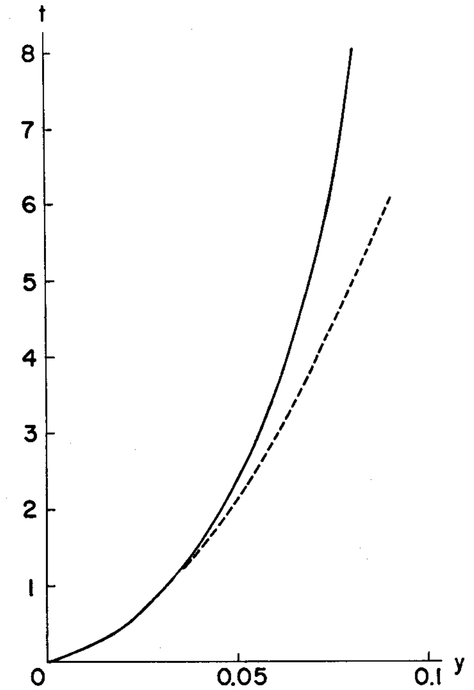

Fig. 6. The change of position of the front surface in the case of the one-phase problem. (The real line : the solution by the difference method; the broken line: the solution by the proposed method.)

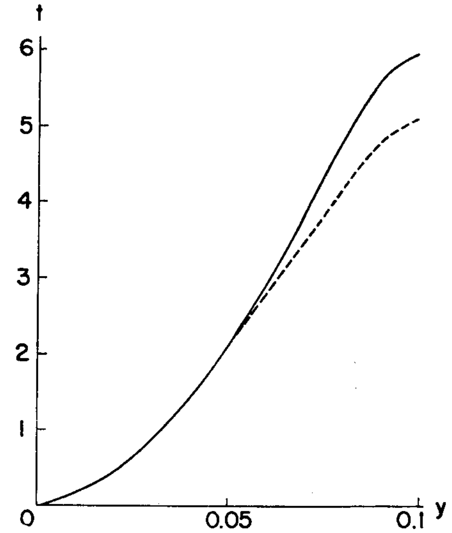

Fig. 7. The change of position of the front surface in the case of the two-phase broblem. (The real line : the solution by the difference method; the broken line: the solution by the proposed method.)

is equal to 10). It depends only on the difference scheme itself, and may be diminished by tending the mesh width h to zero. Except for this, comparatively good coincidences are found. Figs. 6 and 7 show the changes of position of the front surface for the one and two-phase problem respectively. It is found in those figures that the analytic approximate solution has a higher speed of the front surface than that of the difference solution. The difference increases as the solidification temperature comes near the equilibrium temperature. In conclusion, the two solutions coincide well for a small time interval from the start. However they have their differences later. Thus, it has been found that the approximate method proposed here is useful for a restricted time interval.

References

1) T. Nogi, A Mathematical One-Dimensional Model of Supercooling Solidification, (a private communication).
2) R. Kobayashi, A Mathematical One-Dimensional One-Phase Model of Supercooling Solidification (a private communication).