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NUMERICAL SOLUTION OF THE STEFAN PROBLEM WITH A VARIABLE PHASE-TRANSITION TEMPERATURE

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The purpose of this paper is to realize a numerical method for solving two-dimensional Stefan problems in which the free boundary is not a level line. The calculations are based on the method of lines which reduces a multidimensional problem to a sequence of one-dimensional free boundary problems, which are, in turn, reduced to a system of first-order ordinary differential equation by means of a Riccati transform. In this case, the location of the free boundary for each line is found as a root of some scalar equation. The fundamentals of the method are developed in [1, 2].

In this paper, the method is used to solve two-dimensional two-phase free-boundary problems with various boundary conditions at both the lateral boundaries of the rectangular domain considered and the free boundary. Application of this method to the solution of problems with several free boundaries is also described.

1. Formulation of the Problem. We assume that the tree boundary between the solid and liquid phases in domain $D = [0,1] \times [0,1]$ is defined by the equation $y = s(x,t)$, where $s(x,t)$ has the first and second continuous space derivatives and the first continuous time derivative. We seek the functions $u(x,y,t)$, $U(x,y,t)$, and $s(x,t)$ subject to the following conditions:
the heat conduction equations for the liquid and solid phases, respectively,

$$u_t = k_l \Delta u \quad \text{for} \quad 0 < x < 1, \quad 0 < y < s(x,t), \quad t > 0,$$

$$U_t = k_s \Delta U \quad \text{for} \quad 0 < x < 1, \quad s(x,t) < y < 1, \quad t > 0,$$

the condition at the free-boundary

$$u = U = -\sigma/\rho(x,t) - qv \qquad \text{for} \quad y = s(x,t),$$

and the Stefan condition

$$\lambda v = k_l \partial u/\partial \mathbf{n} - k_s \partial U/\partial \mathbf{n} \qquad \text{for} \quad y = s(x,t),$$

where σ, q, λ, k_l, and k_s are fixed positive constants; $\mathbf{n} = (-s_x(x,t), 1)/\sqrt{s_x^2+1}$ is the normal vector to the free boundary; $v = (\partial s/\partial t)/\sqrt{s_x^2+1}$ is the normal velocity of the free boundary; and $\rho(x,t)$ is the curvature radius of the free boundary.

The first term of the condition at the free boundary takes into account the influence of the free boundary curvature on the phase-transition temperature (the Gibbs–Thomson condition). The second term is the so-called kinetic condition, which is used since in the supercooled Stefan problem with a constant melting point an abrupt increase in gradients is possible in a finite time (gradient catastrophe). The free boundary is propagating at an unbounded speed in this case. The kinetic condition takes into account that the phase-transition temperature is proportional to the free-boundary propagation velocity, and this makes it possible to eliminate the effects described above. Many papers have been devoted to problems with such conditions, in particular, [3–5].

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Dirichlet conditions for the functions u and U are specified at the lower ($y = 0$) and upper ($y = 1$) boundaries of the domain considered. At the lateral boundaries, the normal derivatives of the functions u and U are assumed to be equal to zero or Dirichlet conditions are specified. The formulation of the problem is completed by specifying the initial distributions for u and U and the initial location of the free boundary $y = s(x, 0)$.

2. Approximation of the Problem. To reduce our problem to a series of one-dimensional problems with free boundaries for the time level t_n, we approximate the second derivatives of the functions u, U, and s with respect to x by central differences:

$$u_{xx}(x_i, y, t_n) = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}, \quad i\Delta x = i/N_x, \quad i = 1, \ldots, N_x - 1,$$

$$s_{xx}(x_i, t_n) = \frac{s_{i+1} - 2s_i + s_{i-1}}{\Delta x^2}, \quad i\Delta x = i/N_x, \quad i = 1, \ldots, N_x - 1.$$

To approximate the time derivative, we use a "backward" difference approximation:

$$u_t(x_i, y, t_n) = \frac{u_i - u_{i,n-1}}{\Delta t}, \qquad s_t(x_i, t_n) = \frac{s_i - s_{i,n-1}}{\Delta t}.$$

The conditions at the free boundary are approximated by

$$\frac{du}{dx}(x_i, s_i, t_n) = \frac{u_{i+1}(s_{i+1}) - u_{i-1}(s_{i-1})}{2\Delta x}; \tag{2.1}$$

$$\frac{\partial s}{\partial x}(x_i, t_n) = \frac{s_{i+1} - s_{i-1}}{2\Delta x}. \tag{2.2}$$

If the functions u and U are specified at the lateral boundaries, we use one-side difference approximations for the free-boundary conditions:

$$\frac{du}{dx}(x_0, s_0, t_n) = \frac{4u_1(s_1) - u_2(s_2) - 3u_0(s_0)}{2\Delta x},$$

$$\frac{du}{dx}(x_N, s_N, t_n) = \frac{-4u_{N-1}(s_{N-1}) + u_{N-2}(s_{N-2}) + 3u_N(s_N)}{2\Delta x}; \tag{2.1'}$$

$$\frac{\partial s}{\partial x}(x_0, t_n) = \frac{4s_1 - s_2 - 3s_0}{2\Delta x}, \qquad \frac{\partial s}{\partial x}(x_N, t_n) = \frac{-4s_{N-1} + s_{N-2} + 3s_N}{2\Delta x}. \tag{2.2'}$$

Using the identity

$$\frac{d}{dx} u(x, s(x, t)) = u_x + u_y s_x(x, t)$$

to approximate the derivative u_x at the free boundary, we obtain

$$u_x(x_i, y, t_n) = \frac{u_{i+1}(s_{i+1}) - u_{i-1}(s_{i-1})}{2\Delta x} - u_y \frac{s_{i+1} - s_{i-1}}{2\Delta x}.$$

In the case of Dirichlet conditions at the lateral boundaries for $i = 0$ and $i = N$, the corresponding expressions are easily obtained using formulas (2.1′) and (2.2′). The same reasoning can be extended with no changes to the functions U_i.

Thus, we have a system of linear differential equations for the functions $u_i(y)$ and $U_i(y)$

$$L_i(u_i) \equiv u_i'' - \left[\frac{2}{\Delta x^2} + \frac{1}{k_l \Delta t}\right] u_i = F_i(u_{i,n-1}, u_{i-1}, u_{i+1}) \quad \text{on} \quad (0, s_i),$$

$$L_i(U_i) \equiv U_i'' - \left[\frac{2}{\Delta x^2} + \frac{1}{k_s \Delta t}\right] U_i = F_i(U_{i,n-1}, U_{i-1}, U_{i+1}) \quad \text{on} \quad (s_i, 1),$$

where

$$F_i(u_{i,n-1}, u_{i-1}, u_{i+1}) = -\frac{(u_{i+1} + u_{i-1})}{\Delta x^2} - \frac{u_{i,n-1}}{k_l \Delta t};$$

$$F_i(U_{i,n-1}, U_{i-1}, U_{i+1}) = -\frac{(U_{i+1} + U_{i-1})}{\Delta x^2} - \frac{U_{i,n-1}}{k_s \Delta t}$$

with the following conditions at the free boundary $y = s_i$:

$$u = U = -\frac{\sigma(s_{i-1} - 2s_i + s_{i+1})}{\Delta x^2 (1 + s_i'^2)^{3/2}} - q\,\frac{s_i - s_{i,n-1}}{\Delta t (1 + s'^2)^{1/2}},$$

$$\frac{-\lambda(s_i - s_{i,n-1})}{\Delta t} = (k_s - k_l)\,\frac{du}{dx}(x_i, s_i, t_n)\, s_i' - (1 + s_i'^2)(k_l u_i'(s_i) - k_s U_i'(s_i)).$$

Here du/dx and s_i' are given by formulas (2.1) and (2.2). This system of one-dimensional problems with free boundaries will be denoted by A.

3. Algorithm of Numerical Solution. The system of one-dimensional problems with free boundaries for finding the functions $u_i(y)$ and $U_i(y)$ and the constant s_i at the time level $t = t_n$ is solved by a successive over-relaxation method with the iterations

$$L_i(\tilde{u}_i) = F_i(u_{i,n-1}, u_{i-1}^{k+1}, u_{i+1}^{k}), \quad u_i^{k+1} = u_i^k + \omega(\tilde{u}_i - u_i^k) \quad \text{for} \quad y \in (0, s_i^{k+1}); \tag{3.1}$$

$$L_i(\tilde{U}_i) = F_i(U_{i,n-1}, U_{i-1}^{k+1}, U_{i+1}^{k}), \quad U_i^{k+1} = U_i^k + \omega(\tilde{U}_i - U_i^k) \quad \text{for} \quad y \in (s_i^{k+1}, 1), \tag{3.2}$$

where $\omega \in [1,2)$ is an iteration parameter; $i \in [0, N]$ if Neumann conditions are applied at the lateral boundaries of the domain considered, and $i \in [1, N-1]$ for Dirichlet conditions. The location of the free boundary on the ith line s_i^{k+1}, where i varies from zero to N, is found as a root of the scalar equation given below for both Neumann conditions at the lateral boundaries and Dirichlet conditions. This equation is solved by the method of linear interpolation between the grid points y. Thus, the system of problems with free boundaries A for determining the functions $u_i(y)$ and $U_i(y)$ and the numbers s_i at the level $t = t_n$ is reduced to a sequence of problems (3.1) and (3.2); we denote it by $\{A^{k+1}\}$ and solve for a fixed k by moving successively from i to $i+1$.

Each problem A^{k+1} [i.e., (3.1) and (3.2)] will be solved, in accordance with [1], by using a Riccati transform. Let

$$u_i'(y) = v_i(y), \qquad u_i(y) = R_l(y) v_i(y) + w_{l,i}(y),$$

and, similarly,

$$U_i'(y) = V_i(y), \qquad U_i(y) = R_s(y) V_i(y) + w_{s,i}(y).$$

Dropping the subscripts i and k, we write the Cauchy problems for the functions $R_l(y)$ and $w_{l,i}(y)$:

$$R_l' = 1 - R_l^2\left[\frac{2}{\Delta x^2} + \frac{1}{k_l \Delta t}\right], \qquad R(0) = 0; \tag{3.3}$$

$$w_l' = -R_l\left[\frac{2}{\Delta x^2} + \frac{1}{k_l \Delta t}\right] w_l + R_l F, \qquad w_l(0) = u(x_i, 0, t_n). \tag{3.4}$$

The problems for determining $R_s(y)$ and $w_{s,i}(y)$ are written in a similar way.

The first-order explicit Runge–Kutta method for a fixed uniform grid is used for numerical solution of these problems.

The location of the free boundary s_i^{k+1} in the line $x = x_i$ for $i \in [1, N-1]$ can be found as a root of the scalar equation

$$\Phi(y) \equiv \left[\left[\frac{s_{i+1}^k - s_{i-1}^{k+1}}{2\Delta x}\right]^2 + 1\right]\left[k_l\,\frac{I(y) - w_l(y)}{R_l(y)} - k_s\,\frac{I(y) - w_s(y)}{R_s(y)}\right]$$

$$- \left[\frac{s_{i+1}^k - s_{i-1}^{k+1}}{2\Delta x}\right](k_l - k_s)\,\frac{u_{i+1}^k(s_{i+1}^k) - u_{i-1}^{k+1}(s_{i-1}^{k+1})}{2\Delta x} - \lambda\,\frac{y - s_{i,n-1}}{\Delta t} = 0,$$

where $I(y) = u(y) = U(y) = -\sigma(s_{i+1}^k - 2y + s_{i-1}^{k+1})/[\Delta x^2(1 + s'^2)^{3/2}] - q\,(y - s_{i,n-1})/[\Delta t(1 + s'^2)^{1/2}]$ and, in accordance with (2.2), $s' = (s_{i+1}^{k} - s_{i-1}^{k+1})/2\Delta x$. For $i = 0$, this equation has the form

$$\Phi(y) \equiv \left[\left[\frac{4s_1^k - s_2^k - 3y}{2\Delta x}\right]^2 + 1\right]\left[k_l u_y(0,y,t_n) - k_s U_y(0,y,t_n)\right]$$
$$- \left[\frac{4s_1^k - s_2^k - 3y}{2\Delta x}\right](k_l - k_s)\frac{4u_1^k(s_1^k) - u_2^k(s_2^k) - 3u_0^{k+1}(y)}{2\Delta x} - \lambda\frac{y - s_{i,n-1}}{\Delta t} = 0.$$

The equation for $i = N$ will be obtained in a similar way.

In our work, the root of the equation $\Phi(y) = 0$ was found by linear interpolation between two neighboring grid points y, the grid point y nearest to the root being taken as the desired value of s_i^{k+1}. If the equation $\Phi(y) = 0$ had several roots, the root nearest to the location of the free boundary in the previous iteration was chosen as a rule.

Determination of the functions $v(y)$ and $V(y)$ as solutions of the Cauchy problems is the next step:

$$v'(y) = v(y)R_l(y)\left[\frac{2}{\Delta x^2} + \frac{1}{k_l\Delta t}\right] + \frac{w_l(y) - u_{i,n-1}(y)}{\Delta t} - \frac{u_{i+1}(y) - u_{i-1}(y) + 2w_l(y)}{\Delta x^2},$$
$$0 < y < s_i, \quad v(s_i) = \frac{I(s_i) - w_l(s_i)}{R_l(s_i)}; \tag{3.5}$$

$$V'(y) = V(y)R_s(y)\left[\frac{2}{\Delta x^2} + \frac{1}{k_s\Delta t}\right] + \frac{w_s(y) - u_{i,n-1}(y)}{\Delta t} - \frac{u_{i+1}(y) - u_{i-1}(y) + 2w_s(y)}{\Delta x^2},$$
$$s_i < y < 1, \quad V(s_i) = \frac{I(s_i) - w_s(s_i)}{R_s(s_i)}. \tag{3.6}$$

Cauchy problems (3.5) and (3.6) are solved numerically in the same way as problems (3.3) and (3.4), and the value of $u_{i+1}(y)$ is taken from the previous iteration.

The solution of the problem A^{k+1} is completed by reconstructing $u_i^{k+1}(y)$ and $U_i^{k+1}(y)$ using the formulas

$$u_i^{k+1}(y) = R_l(y)v_i(y) + w_{l,i}(y), \qquad U_i^{k+1}(y) = R_s(y)V_i(y) + w_{s,i}(y).$$

4. Analysis of Convergence. The convergence of the iterative process was studied numerically. The root-mean-square norm of the difference between temperature-function values corresponding to two successive iterations was used as a criterion for estimation. In this case, the following results were obtained. Depending on the initial and boundary conditions, the norm was reduced by a factor of 3–10 in one iteration, with the original norm of the order of 10^{-2}. In problem 2 (Section 6), the residual was of the order of 10^{-3}. Variations of Δx, Δy, and Δt within reasonable limits did not have any considerable influence on the convergence, but it should be noted that the best results were obtained for the relation $\Delta y = \Delta x/10$. The parameter ω was chosen in accordance with minimization of the above criterion in each particular problem. A beneficial influence of surface tension ($\sigma > 0$) and kinetic supercooling ($q > 0$) on the stability of the free-boundary form in the supercooled problem (Section 6, problem 5) was noted.

5. Multifront Problems. The method in question can be used for solution of multifront problems. We illustrate this using as an example a problem with two free boundaries.

Let domain $[0,1]^2$ be divided by two free boundaries: $y = s_1(x,t)$ and $y = s_2(x,t)$. We seek to find the functions $u_1(x,y,t)$, $u_2(x,y,t)$, $u_3(x,y,t)$, $s_1(x,t)$, and $s_2(x,t)$ subject to the following conditions:
the heat conduction equations

$$\begin{aligned} (u_1)_t &= k_1\Delta u_1 && \text{in } (0,1)\times(0,s_1),\\ (u_2)_t &= k_2\Delta u_2 && \text{in } (0,1)\times(s_1,s_2),\\ (u_3)_t &= k_3\Delta u_3 && \text{in } (0,1)\times(s_2,1), \end{aligned}$$

the conditions at the free boundaries

$$u_1 = u_2 = -\frac{\sigma_1}{\rho_1(x,t)} - q_1 v_1 \quad \text{on} \quad s_1, \qquad u_2 = u_3 = -\frac{\sigma_2}{\rho_2(x,t)} - q_2 v_2 \quad \text{on} \quad s_2,$$

$$-\lambda_1 v_1 = k_1 \frac{\partial u_1}{\partial n} - k_2 \frac{\partial u_2}{\partial n} \quad \text{on} \quad s_1, \qquad -\lambda_1 v_2 = k_2 \frac{\partial u_2}{\partial n} - k_3 \frac{\partial u_3}{\partial n} \quad \text{on} \quad s_2.$$

Dirichlet and Neumann conditions can be applied at the lateral boundaries, and Dirichlet conditions can be applied at the boundaries $y = 0$ and $y = 1$. The statement is completed by specification of initial conditions.

The calculations will be performed as follows. Let the superscript $k \geqslant 1$ denote the number of iterations made at one time level. We assume that u_1^{k-1}, u_2^{k-1}, u_3^{k-1}, s_1^{k-1}, and s_2^{k-1} are already known. Let us first consider domain $[0,1] \times [0,\, s_2^{k-1}]$ and apply to it the iteration procedure described in Sections 2 and 3 to find a new location of the free boundary and a new temperature distribution. It should be noted that the iterations made within the framework of this procedure are inner and are not related to the iterations denoted by k. The only difference in application of this procedure is that it was previously used in a rectangular domain, and here one boundary of the domain is curvilinear. This, however, does not prevent realization of this algorithm, because it is based on the method of lines. The condition at the curvilinear boundary of the domain remains a Dirichlet condition, because it represents either the temperature-function value in this curve that is taken from the previous iteration if the phase-transition temperature is not constant, or, otherwise, the phase transition temperature.

Thus, a new location of the free boundary s_1 and a new distribution of the temperatures u_1 and u_2 are obtained. Similarly, considering domain $[0,1] \times [s_1^{k-1},\, 1]$, we find s_2, $\tilde{u}_2$, and u_3. Then we assume that

$$\begin{aligned}
u_1^k &= u_1^{k-1} + \omega_1(u_1 - u_1^{k-1}) && \text{on} \quad (0,\, s_2^k), \\
u_2^k &= u_2^{k-1} + \omega_1((u_2 + \tilde{u}_2)/2 - u_2^{k-1}) && \text{on} \quad (s_1^k,\, s_2^k), \\
u_3^k &= u_3^{k-1} + \omega_1(u_3 - u_3^{k-1}) && \text{on} \quad (s_2^k,\, 1),
\end{aligned}$$

where $s_1^k = s_1^{k-1} + \omega_1(s_1 - s_1^{k-1})$ and $s_2^k = s_2^{k-1} + \omega_1(s_2 - s_2^{k-1})$.

The iterative process is continued until a satisfactory result is obtained, and then the next time level is used.

6. Results of Numerical Calculations.

(1) Single-Phase Problem with Surface Tension (Fig. 1):

$$u(x,y,0) = 1 - y/(0.5 - 0.25\cos(\pi x)), \quad U(x,y,0) = 0,$$

$$s(x,0) = 0.5 - 0.25\cos(\pi x), \quad u(x,0,t) = 1, \quad U(x,1,t) = 0.$$

The zero-flux condition is specified at the lateral boundaries $x = 0$ and $x = 1$,

$$Kl = Ks = 1,\ \sigma = 0.001,\ q = 0,\ \lambda = 1,\ \omega = 1.3,\ dx = 0.04,\ dy = 0.004,\ dt = 0.05.$$

Figure 1 shows the front propagation with time.

(2) "Traveling Wave" (Fig. 2):

$$u(x,y,0) = \exp(16(y + x/2 - 0.75)) - 1, \quad U(x,y,0) = 0, \quad s(x,0) = -x/2 + 0.75,$$

$$u(x,0,t) = \exp(16(x/2 - 0.75 + 20t)) - 1, \quad U(x,1,t) = 0,$$

$$u(0,y,t) = \exp(16(y - 0.75 + 20t)) - 1, \quad U(0,y,t) = 0,$$

$$u(1,y,t) = \exp(16(y - 0.25 + 20t)) - 1, \quad U(1,y,t) = 0,$$

$$Kl = 2,\ Ks = 2,\ \sigma = q = 0.001,\ \lambda = 1,\ \omega = 1.5,\ dx = 0.04,\ dy = 0.004,\ dt = 0.018.$$

The front propagation with time is shown in Fig. 2.

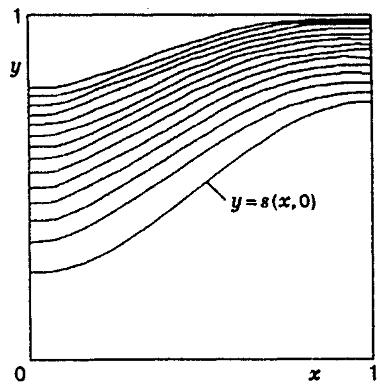

Fig. 1

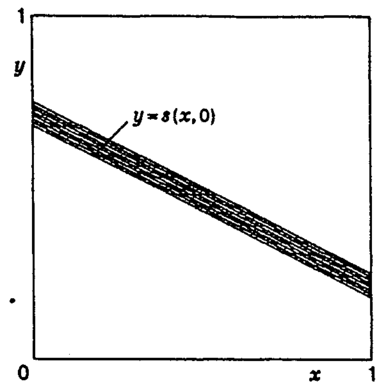

Fig. 2

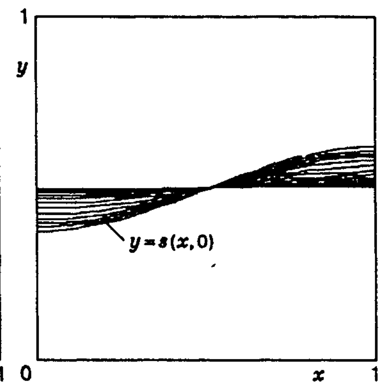

Fig. 3

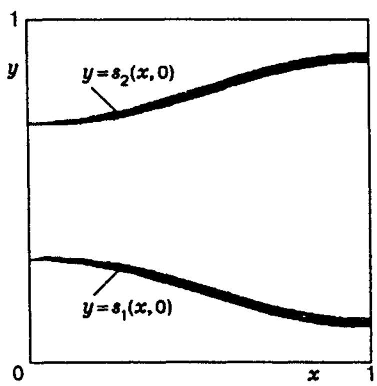

Fig. 4

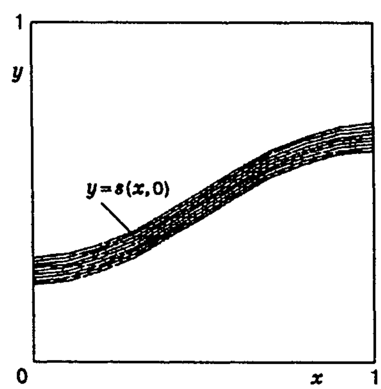

Fig. 5

(3) Two-Phase Problem with Surface Tension and Dynamic Supercooling (Fig. 3):

$$u(x,y,0) = 1 - y/(0.5 - 0.125\cos(\pi x)), \quad s(x,0) = 0.5 - 0.125\cos(\pi x),$$

$$U(x,y,0) = -1 + (y-1)/(-0.5 - 0.125\cos(\pi x)), \quad u(x,0,t) = 1 + 20t, \quad U(x,1,t) = -1 - 20t,$$

zero flux is specified at the lateral boundaries $x = 0$ and $x = 1$,

$$Kl = Ks = 1, \quad \sigma = 0.001, \quad q = 0.0001, \quad \lambda = 1, \quad \omega = 1.5, \quad dx = 0.04, \quad dy = 0.004, \quad dt = 0.018.$$

Figure 3 gives the location of the free boundary at various times.

(4) Two-Phase Problem with Two Fronts (Fig. 4):

$$s_1(x,0) = 0.2 + 0.1\cos(\pi x), \quad s_2(x,0) = 0.8 - 0.1\cos(\pi x),$$

$$u_1(x,y,0) = 1 - y/(0.2 + 0.1\cos(\pi x)), \quad u_2(x,y,0) = 0,$$

$$u_3(x,y,0) = 1 - (y-1)/(-0.2 - 0.1\cos(\pi x)), \quad u_1(x,0,t) = 1, \quad u_3(x,1,t) = 1,$$

zero flux is specified at the lateral boundaries $x = 0$ and $x = 1$,

$$k_1 = 0.1, \quad k_2 = 0.2, \quad k_3 = 0.1, \quad \sigma_1 = q_1 = 0.001, \quad \lambda_1 = 0.8, \quad \sigma_2 = q_2 = 0.001,$$

$$\lambda_2 = 0.8, \quad \omega = 1.3, \quad \omega_1 = 1.3, \quad dx = 0.05, \quad dy = 0.005, \quad dt = 0.005.$$

Figure 4 shows the propagation of the fronts.

(5) Problem with Initial Supercooling (Fig. 5):

$$u(x,y,0) = -1 + y/(0.5 - 0.125\cos(\pi x)), \quad s(x,0) = 0.5 - 0.125\cos(\pi x),$$

$$U(x,y,0) = -1 + (y-1)/(-0.5 - 0.125\cos(\pi x)), \quad u(x,0,t) = -1, \quad U(x,1,t) = -1,$$

zero flux is specified at the lateral boundaries $x = 0$ and $x = 1$,

$$Kl = Ks = 1,\ \sigma = 0.001,\ q = 0.001,\ \lambda = 1,\ \omega = 1.5,\ dx = 0.04,\ dy = 0.004,\ dt = 0.018.$$

Figure 5 gives the location of the free boundary at various times.

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