An effective algorithm of the numerical solution to the Stefan problem

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Abstract. The method of the frontal interval of the numerical solution to Stefan problems is proposed. The method allows the calculation of the position of the phase transition boundary with high accuracy at any time. Using the example of a plane two-phase Stefan problem, which has an exact analytical solution, the advantages of the proposed method in comparison with a variable time stepping method are demonstrated with respect to the calculation of the position of the phase transition boundary. An example of the solution to the one-phase Stefan problem using the frontal interval method is also given.

1. Introduction
Practically, it is important to know the phase transition boundary position with high accuracy in the Stefan problems. It is known numerical methods that explicitly track the motion of the phase transition boundary, for example, a variable time stepping method \cite{1, 2}, a front-fixing method \cite{3}, a phase-field method \cite{4}, a combined finite difference method \cite{5} and numerous other. Reviews of papers utilizing the front-tracking techniques can be found, for example, in \cite{5} and \cite{7}.

In present paper we propose a \textit{frontal interval method} which allows for the calculation of the position of the phase transition boundary with high accuracy at any time. This method relates to the class of front-tracking methods and has similarities with the front-fixing method and the combined finite difference method. However, unlike the variable time stepping method and the front-fixing method, the frontal interval method uses a constant spatial grid and time step. The proposed method, in contrast with the combined finite difference method \cite{5}, is implicit and utilizes different algorithms for the temperature calculation near the phase transition boundary.

2. The frontal interval method
In using this method, assume that there are two stationary phases (for example, the frozen and unfrozen soil) separated by a phase interface (the phase transition boundary). The movement of the phase transition boundary occurs due to changes in the temperature of the primary phase on the outer boundary. For numerical solutions similar Stefan problems a uniform spatial grid is introduced. The \textit{frontal interval} is defined as the only interval between two adjacent grid nodes, that either contains both phases or through one of the nodes of this interval the phase front passes at the considered point in time. The frontal interval method is based on the computation
of both the frontal interval position and the position of the phase interface in it at the every moment of time.

Out of the frontal interval the heat equations in each phase are solved using an implicit difference scheme. At every time step, a starting point of the frontal interval is determined and the movement of the phase interface is computed using difference analog of the Stefan condition, in which the heat fluxes are determined using temperature values of the primary and secondary phases at the previous temporal level. The computational scheme of the front interval method is an implicit non-iterative scheme.

3. Model problem
Let us demonstrate the algorithm of the numerical solution to the Stefan problems using the proposed frontal interval method with the example the well-known 1D two-phase Stefan problem [8] which has an exact analytical solution depending on the values \( x \) and \( t \) through the self-simulated variable \( \xi = x/(a\sqrt{t}) \). We have used the following designations: \( T_\infty \) is the temperature of the secondary phase at infinity (K), \( T_* \) is the phase transition temperature (K), \( T_0 \) is the temperature (K) of the primary phase at \( x = 0 \), \( k = 1, 2 \) is the phase number, \( c_k \) is the coefficient of specific volumetric heat capacity of the \( k \)-th phase (J m\(^{-3}\) K\(^{-1}\)), \( \lambda_k \) is the thermal conductivity coefficient of the \( k \)-th phase (W m\(^{-1}\) K\(^{-1}\)), and \( Q \) is the specific (per unit volume of ice) heat of phase transition (latent heat of melting), (J m\(^{-3}\)).

The statement of this Stefan problem is written as follows:

\[
c_1 \frac{\partial T_1}{\partial t} = \lambda_1 \frac{\partial^2 T_1}{\partial x^2}, \quad t > 0, \quad x \in (0, y(t));
\]

\[
t > 0, \quad x = 0 : \quad T_1 = T_0; \tag{2}
\]

\[
c_2 \frac{\partial T_2}{\partial t} = \lambda_2 \frac{\partial^2 T_2}{\partial x^2}, \quad t > 0, \quad x \in (y(t), \infty); \tag{3}
\]

\[
t = 0, \quad x \in (0, \infty) : \quad T_2(x) = T_\infty; \tag{4}
\]

\[
t > 0, \quad x \to \infty : \quad T_2 = T_\infty; \tag{5}
\]

\[
t > 0, \quad x = y(t) : \quad T_1 = T_2 = T_*; \tag{6}
\]

\[
\left. \lambda_1 \frac{\partial T_1}{\partial x} \right|_{y-0} - \left. \lambda_2 \frac{\partial T_2}{\partial x} \right|_{y+0} = Q \frac{dy}{dt}; \tag{7}
\]

\[
t = 0 : \quad y = 0, \tag{8}
\]

where \( T_k(x, t) \) is the temperature of the \( k \)-th phase \( (k = 1, 2) \) and \( y(t) \) is the coordinate of the phase change boundary.

We assume all thermal and physical characteristics of the phases and the given temperatures are constant. The problem (1)–(8) has a known analytical solution [8]:

\[
T_1(x, t) = A_1 + B_1 \text{erf}(\frac{x}{2a_1\sqrt{t}}), \quad T_2(x, t) = A_2 + B_2 \text{erf}(\frac{x}{2a_2\sqrt{t}}), \quad y(t) = \alpha \sqrt{t}. \tag{9}
\]

The constants \( a_k \) are equal to: \( a_k = (\lambda_k/c_k)^{1/2}, \ k = 1, 2 \); constants \( A_1, A_2, B_1, \) and \( B_2 \) in a known manner [8] are expressed through the parameters of the problem (1)–(8) and the value of \( \alpha \), which is calculated by the transcendental equation given in [16], depends on all parameters of the problem, namely \( T_0, T_*, T_\infty, c_1, c_2, \lambda_1, \lambda_2 \) and \( Q \).
4. Numerical solution to the Stefan problem by the frontal interval method

Let us consider the numerical solution to the Stefan problem (1)–(8) for non-zero initial conditions by the proposed frontal interval method. We assume that the primary phase thickness is $y_0 \neq 0$ in the initial instant of time $t = t_0$. Both, the initial moment $t_0$ and the initial temperatures distributions $T_1^{(0)}(x, t_0)$ and $T_2^{(0)}(x, t_0)$ are calculated using the given $y_0$ from the analytical solution (9). The constant step $h$ was chosen so that $y_0$ was a multiple of $h$. The heat equations in the primary and secondary phases are approximated using an implicit scheme. The difference analogs can be represented as:

$$Ak T_{ki}^{n+1} - Bk T_{ki}^{n+1} + Ck T_{ki}^{n+1} = Dk_i^n,$$

$$Ak = Ck = m_k, \quad Bk = 1 + 2m_k, \quad Dk_i^n = -T_{ki}^n, \quad m_k = \tau a_k^2/h^2, \quad k = 1, 2,$$

$T_{ki}^{n+1}$ is the temperature of the $k$-th phase at the $i$-th nodes on the $(n+1)$-th temporal level. At the $(n)$-th temporal level, the following values are considered to be known: the position of the front interval, which is between the node $s = k^n$ in the primary phase and the node 1 in the secondary phase; temperature arrays $T_{1i}^n, T_{2i}^n$ of the primary and secondary phases; the value $\Delta y^n$ is equal to the sum of all previous displacements inside the frontal interval beginning at the $k$-th node; the position $y^n$ of the phase interface.

5. Transition algorithm from the $n$-th to the $(n+1)$-th temporal level

The displacement $\delta y^{n+1}$ of the phase interface for the time from $t^n$ to $t^{n+1}$ is calculated from the difference analog of the Stefan condition (7), and the heat fluxes using temperature values at the $n$-th temporal level are calculated as:

$$\delta y^{n+1} = \frac{(\tau/h)Q}{a_1(\lambda_1 T_{1s}^n - T_{1s-1}^n) - \lambda_2(T_{22}^n - T_{21}^n)}.$$  \hspace{1cm} (10)

The resulting displacement of the phase interface inside the frontal interval equals

$$\Delta y^{n+1} = \Delta y^n + \delta y^{n+1}.$$  \hspace{1cm} (11)

The relative fraction $\theta^{n+1}$ of the primary phase into the frontal interval is defined from the value $\Delta y^{n+1}$ as

$$\theta^{n+1} = \frac{\Delta y^{n+1}}{h}.$$  \hspace{1cm} (12)

If $\theta^{n+1} < 1$, the position of the frontal interval at the $(n+1)$-th temporal level remains unchanged and the temperatures of the primary and secondary phases on the boundaries of the frontal interval are calculated as follows:

$$T_{1s+1}^{n+1} = T_s - \theta^{n+1}(T_{1s}^n - T_{1s-1}^n), \quad T_{21}^{n+1} = T_s + (1 - \theta^{n+1})(T_{22}^n - T_{21}^n).$$  \hspace{1cm} (13)

If $1 \leq \theta^{n+1} < 2$, the frontal interval at the $(n+1)$-th temporal level moves to the adjacent node and the temperatures of the primary and secondary phases are:

$$T_{1s}^{n+1} = T_{1s}^n, \quad T_{21}^{n+1} = T_s.$$  \hspace{1cm} (14)

The summary displacement $\Delta y^{n+1}$ of the phase change boundary into the new frontal interval is assigned the value

$$\Delta y^{n+1} = \Delta y^n + \delta y^{n+1} - h.$$  \hspace{1cm} (15)

Temperatures in both phases are found from the boundary conditions (2) and (5). The calculation of all other temperature values of the primary and secondary phases at the $(n+1)$-th
temporal level is made by the tridiagonal matrix algorithm. Which scenario of the front interval movement realizes at the \((n+1)\)-th temporal level is defined via the found phases temperatures.

I. If \(T_{2}^{n+1} > T_{*}\), then the frontal interval remains in the same position. In this case, the node number defining the beginning of the frontal interval and position of the change phase boundary are calculated by the following formulas:

\[
k_{n+1} = k_n = s, \tag{16}
\]
\[
y_{n+1} = k_n h + \Delta y_{n+1}, \tag{17}
\]
where \(\Delta y_{n+1}\) is defined by the equality (11).

II. If \(T_{2}^{n+1} \leq T_{*}\) and \(T_{2}^{n+2} > T_{*}\), then the frontal interval moves to the adjacent node and the node number defining a position of the frontal interval is assigned the value

\[
k_{n+1} := k_n + 1 = s, \tag{18}
\]
where the node \((k_n + 1)\) was placed at time instant \(t^n\) in the secondary phase becomes the node belonging to the primary phase at time instant \(t^{n+1}\). The phase boundary position is calculated using the formula (17).

In the frontal interval method it is necessary that for every step in time the boundary of the phase transition either remains in the same spatial interval or passes into the adjacent interval. With this approach it is possible only the considered above scenarios I and II, but fulfillment of this requirement imposes restrictions on the permissible value of step \(\tau\) for specified values of \(h\) and other problem parameters.

6. Basis for the steps selection in the frontal interval method

The formulated requirement for the value of the front displacement during time \(\tau\) is written as follows:

\[
y_{n+1} = y^n + \sigma h, \quad 0 < \sigma < 1. \tag{19}
\]
Condition (19) must be fulfilled for all time moments in the considered problem. If the speed of front moving is a decreasing function of time (as in problem (1)–(8)), then the maximum limit on \(\tau\) occurs when calculating the first step, i.e. at the time instance \(t_0 + \tau\). In this case, an estimation of the admissible value \(\tau\) is easy to calculate from an analytical solution \((y = \alpha \sqrt{t})\).

Indeed, condition (19) implies the equality: \(\alpha \sqrt{t_0^0 + \tau} = \alpha \sqrt{t_0} + \sigma h\), which for \(\tau\) less than \(t_0\) leads to the following estimation:

\[
\tau < \left(2 \frac{s_0 \sigma h}{\alpha}\right). \tag{20}
\]

At the initial instance of time, the primary phase area must contain at least three spatial nodes, since the \(x\)-derivative of the primary phase temperature is used in the calculations for the frontal interval method. Hence the following condition must be satisfied: \(y_0 = s_0 h, s_0 \geq 3\), and the estimation (20) can be written in the form:

\[
\tau < \left(2 s_0 \sigma h^2\right)/\alpha^2, \quad s_0 \geq 3, \quad 0 < \sigma < 1. \tag{21}
\]

7. Comparison of the numerical solution to the Stefan problem by the frontal interval method with the exact analytical solution

For the model problem (1)–(8), the following thermophysical parameters and conditions specific to glaciation problems in saline water were set as:

\[
T_{\infty} = 272.15, \quad T_s = 271.236, \quad T_0 = 265.236, \quad c_1 = 2150500,
\]
\[
c_2 = 3995450, \quad \lambda_1 = 2.0, \quad \lambda_2 = 0.6, \quad Q = 2.805 \cdot 10^8, \tag{22}
\]
where all values in (22) are given in the above units.

At the initial time instance, the thickness of the primary phase is considered equal to \( y_0 = 0.0025 \text{ m} \). The value \( t_0 = 76.27 \text{ sec} \) was found from the analytical solution (9). For the dimensional spatial step \( h = 5 \cdot 10^{-4} \text{ m} \) at the initial time instance, the number of spatial steps in the first phase is \( s_0 = 5 \), and the permissible value of the time step for \( \sigma = 0.5 \) in accordance with (21) should be less than 15 sec. We have set that \( \tau = 15 \text{ sec} \).

The results of the calculations of position \( y^n \) of the phase transition boundary by the proposed method for model problem (1)–(8) under the selected initial conditions and the parameters (22) are shown in Table 1. Table 1 also shows the deviations \( \delta_n \) (\( \delta_n = y^n(t^n) - y^a \)) of the numerically calculated values \( y^n \) from the exact \( y^a(t^n) = \alpha \sqrt{t^n} \) found using the analytical solution (9).

| \((t - t_0)\), days | 1   | 4   | 10  | 16  | 22  | 30  |
|-----------------|-----|-----|-----|-----|-----|-----|
| \(y^n\), cm     | 8.42| 16.83| 26.61| 33.66| 39.46| 46.08|
| \(\delta_n\), cm| \(-6.6 \cdot 10^{-4}\) | \(-8.0 \cdot 10^{-4}\) | \(4.7 \cdot 10^{-4}\) | \(2.7 \cdot 10^{-3}\) | \(4.8 \cdot 10^{-3}\) | \(8.3 \cdot 10^{-3}\) |

The data in the table demonstrates a high computational accuracy of the phase transition boundary position by the frontal interval method. The calculations show that similar accuracy is maintained under other parameters of the problem leading to larger, as well as smaller, Stefan numbers.

Generalizations of the frontal interval method on the multi dimensional Stefan problems and the study of the convergence of this method are beyond the scope of this paper.

Application of the proposed method on the one-dimensional one- and two-phase Stefan problems with other boundary conditions does not pose any difficulties. As an example we presented the solution of the one dimensional one-phase Stefan problem for an infinite cylinder with radius \( R = 0.67 \text{ m} \) under a given constant temperature \( T_1(R, t) = T_0 \) on the lateral surface and with a given heat flux \( q = 30 \text{ (J m}^{-2} \cdot \text{sec}^{-1}) \) into the phase transition boundary from the ambient. The thermophysical parameters of growing ice (the primary phase), the specific heat of phase transition, the values of steps \( h \) and \( \tau \), and the initial conditions are equal to the above. When the condition \( y_0 \ll R \) is met, it is permissible to set the initial temperature distribution \( T_1(r, t_0) \) in an cylindrical layer with the thickness \( y_0 \) in the form of the distribution \( T_1^{(0)}(r, t_0) \) found from the analytical solution to the plane problem (1)–(8).

The calculation results of the ice layer thicknesses \( y^n \) in the time instances \( t^n \) for the one-dimensional problem of the cylinder glaciation by the frontal interval method are presented in Table 2.

| \((t - t_0)\), days | 1  | 3  | 6  | 9  | 14 | 20 | 26 | 30  |
|-----------------|----|----|----|----|----|----|----|-----|
| \(y^n\), cm     | 7.78| 12.58| 16.60| 19.28| 22.35| 24.84| 26.59| 27.50|
8. Comparison of the numerical solution to the Stefan problem by the frontal interval method and the variable time stepping method

In Table 3 we presented the calculation results of the numerical solution to the model problem by the variable time stepping method for the parameters (22), the same step $h$ and under the same initial conditions as in the calculations in Table 1. $y^n_l$ is the position of the phase transition boundary calculated by the variable time stepping method at the time instance $t^n$, the values $\delta l^n = y^n(t^n) - y^n_l$ are the deviations of the numerically calculated values $y^n_l$ from the exact $y^n(t^n) = \alpha \sqrt{t^n}$.

Table 3. The values of the ice layer thicknesses $y^n_l$.

| $(t - t_0)$, days | 0.80 | 4.34 | 8.84 | 12.72 | 28.58 | 35.27 |
|-------------------|------|------|------|-------|-------|-------|
| $y^n_l$, cm       | 7.5  | 17.5 | 25.0 | 30.0  | 45.0  | 50.0  |
| $\delta l^n$, cm  | 0.023| 0.022| 0.016| 0.011 | -0.017| -0.030|

Comparison of Tables 1 and 3 shows that for the considered model problem, the calculation accuracy of the phase transition boundary position by the frontal interval method is two orders of magnitude higher than by the variable time stepping method. This same level of accuracy was similar for long-time processes and other parameters of the problem.

9. Conclusion

In the present study the frontal interval method of the numerical solution to Stefan problems is proposed. This method allows for calculation of the position of the phase transition boundary with a high accuracy at any instance of time. The proposed method is an implicit non-iterative scheme and is distinguished for the algorithmic simplicity. The results of the test calculations of the plane one-dimensional two-phase Stefan problem are presented using the frontal interval method over a long period of time. A comparison with an analytical solution to this problem demonstrates a high accuracy of the phase transition boundary calculation. The comparative results of this problem solution by the frontal interval method and the variable time stepping method are presented. These results indicated the advantage of the proposed method in the accuracy of the phase transition boundary calculation. An example of the one-phase Stefan problem solution for a cylinder using the frontal interval method is given.

10. References

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