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In this paper we propose a model and numerical scheme for quantifying the motion of the phase transition front and the temperature fields in layered materials using boundary conditions of the third kind at the surface.

Keywords: Stefan problem, thermal conductivity, finite-difference scheme.

1. Introduction

Manufacturing of composite materials and their welding occur in a thermal regime that makes phase transitions in materials possible. Mathematical models of heat transfer processes associated with changes in aggregate states are subdivided into models with the formation of fronts (classic frontline Stefan problem) or phase transition zones. Mathematical theory of crystallization and melting of pure substances and classical solutions and applications of various models have been discussed in [1, 2].

In Stefan problem the material in question has a point of phase transition, i.e. it melts or solidifies at a certain temperature. The classical Stefan condition at the phase transition boundary and the generalized Stefan problem describe a physical situation when at the phase transition the energy as function of the temperature changes abruptly by the quantity known as the heat of phase transition. The solution of such problems determines the temperature fields of different phases in the regions with moving boundaries whose position and speed are calculated by considering the balance of energy required for a phase transition. Stefan-type problems are usually solved numerically, for example, by capturing the front at a mesh point and smoothing the coefficients [3] or by local straightening the fronts [4].

The front-capturing method at a mesh point is used only for one-dimensional problems while the front straightening is applied for two-dimensional problems. The main feature of these methods is the explicit tracking of the phase transition front; in this case the position of the free phase boundary is monitored at each time step. This is achieved either through the use of dynamic grids with variable step, or by the introduction of new dynamic independent variables (front straightening methods). The main drawback of these methods is their poor adaptation to the solution in multi-dimensional problems and in problems where there exist several moving fronts some of which can merge or disappear.

The continuous computations scheme and the method of smoothing of coefficients are based on the same idea. In continuous computations scheme the phase transition boundary is not traced explicitly and the discretization is applied uniformly throughout a computational domain. The heat released during a phase transition is introduced as Dirac δ - function representing a localized heat source. The

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resulting discontinuous temperature distribution function is subsequently smoothed and becomes independent of the number of phases and the dimensionality of the problem. The main advantage of such an approach is its relatively low computational cost. Its main disadvantage is the uncertainty in choosing the smoothing method, which depends on a particular grid and is often selected empirically.

In this paper we propose a model and a numerical scheme that enable us to trace the motion of a phase transition front without the use of Stefan condition or a localized heat source. This simplifies the problem while allowing us to consider more complicated geometry and initial conditions and to increase the number of layers in the modeled materials. It becomes possible to track all thermal processes, including melting of individual layers and their subsequent crystallization, within a single model.

2. Mathematical model

Consider a model of melting (crystallization) of the layered material, each layer of which is a pure substance. The basic assumption in modeling of phase transitions in crystalline materials is that the phase transition occurs at a constant temperature T_k^* (each layer has its own melting point); here $\overline{k = 1, K}$ is the layer number in the composite. The transition of crystalline material to a liquid state requires a certain amount of heat Q_k^*, which is called the specific heat of fusion (per unit mass; for many materials it is a known quantity). We introduce the step function $\gamma(t, M)$ into the heat equation that will take into account the continuous accumulation of energy subsequently spent in phase transition. The equation of heat conduction may be written in the form

$$\rho(\mathrm{T})\mathrm{c}(\mathrm{T})(1-\gamma(t,M))\frac{\partial T(t,M)}{\partial t} = div\big(\lambda(T)grad\ T(t,M)\big) - \gamma(t,M)\frac{\partial Q(t,M)}{\partial t}, \tag{1}$$

$$\gamma(M,t) = \begin{cases} 1,\ T = T^* \ \text{ and } -\rho_k^+ Q_k^* < \overline{Q}(M,t) < \rho_k^- Q_k^*,\ M \in \Omega_k, \\ 0,\ T \neq T^* \ \text{ or } \overline{Q} = \rho_k^- Q_k^* \text{ or } \overline{Q} = -\rho_k^+ Q,\ M \in \Omega_k, \end{cases} \tag{2}$$

$$Q(t,M) = \begin{cases} \overline{Q}(t,M), \text{ if } \gamma(t,M) = 1, \\ 0, \qquad \text{if } \gamma(t,M) = 0, \end{cases} \tag{3}$$

$$c(T), \rho(T) = \begin{cases} c_k^+(T), \rho_k^+(T), \text{ if } T < T_{\mathrm{k}}^*,\ M \in \Omega_k, \\ c_k^-(T), \rho_k^-(T), \text{ if } T > T_{\mathrm{k}}^*,\ M \in \Omega_k, \end{cases} \tag{4}$$

$$\lambda(T) = \begin{cases} \lambda_k^+, \text{ if } T \le T_{\mathrm{k}}^* - \delta T_k,\ M \in \Omega_k, \\ \lambda_k^*, \text{ if } T_{\mathrm{k}}^* - \delta T_k < T < T_{\mathrm{k}}^* + \delta T_k,\ M \in \Omega_k,\ \delta T_k \to 0, \\ \lambda_k^-, \text{ if } T \ge T_{\mathrm{k}}^* + \delta T_k,\ M \in \Omega_k, \end{cases} \tag{5}$$

where $\overline{Q}(t, M)$ is a bounded function characterizing heat (per unit volume) generated in the phase transition that is dynamically updated at each time step, $\rho(T)$, $c(T)$ are the density and heat capacity at constant volume of the corresponding layers and phases. The coefficient of thermal conductivity $\lambda(T)$ is continuous and is given by (5) so that conditions $\lambda_k^*(T_{\mathrm{k}}^* + 0) = \lambda_k^+$ and $\lambda_k^*(T_{\mathrm{k}}^* - 0) = \lambda_k^-$ are satisfied. The boundary conditions at the outer boundary and the initial conditions are

$$\left[\lambda\frac{\partial T}{\partial n} - \alpha(T - T_e(t))\right]\Big|_{\partial\Omega} = 0, \qquad \Omega = \bigcup_{k=1}^{K}\Omega_k, \tag{6}$$

$$T\big|_{t=0} = T_k^0, \qquad M \in \Omega_k\ , \tag{7}$$

where $\alpha-$ is the heat transfer coefficient. It depends on the method of heating (or cooling) of the outer surface. It can be constant or function $T_e(t)$ depending on the temperature regime of the technological process.

We assume ideal contact at the boundaries between the layers, i.e. the temperature is continuous and heat fluxes are equal

$$\left[\lambda\frac{\partial T}{\partial n}\right]_{\partial\Omega_k}=0, \qquad M\in\partial\Omega_k. \tag{8}$$

The mathematical model consisting of equation (1) and conditions (2) - (8) has a unique solution. Note that a similar formulation of Stefan problem was proposed in [8], but in our model the term

$\frac{\partial Q(t,M)}{\partial t}=\frac{\partial}{\partial t}\int_{t^*}^{t}\frac{\partial Q(\tau,M)}{\partial\tau}d\tau$ in equation (1) describes the increment of the internal energy of the phase transition over time $t-t^*$.

We show that in a one-dimensional case with $k=1$ the problem described by equation (1) with conditions (2) - (5) where the surface of the solid-liquid interface $x=\xi(t)$ is a plane includes Stefan condition. In this case Stefan problem is

$$\rho(\mathrm{T})\mathrm{c}(\mathrm{T})\frac{\partial T(t,x)}{\partial t}=div\big(\lambda(T)grad\ T(t,x)\big), \quad x\in(0,l), \quad t>0, \tag{9}$$

$$c(T),\rho(T),\lambda(T)=\begin{cases}c^+(T),\rho^+(T),\lambda^+(T), & \text{if} \quad T<T^*,\\ c^-(T),\rho^-(T),\lambda^-(T), & \text{if} \quad T>T^*,\end{cases} \tag{10}$$

$$T(t,\xi)=T^*, \qquad \lambda^+\frac{\partial T}{\partial x}\bigg|_{x=\xi+0}-\lambda^-\frac{\partial T}{\partial x}\bigg|_{x=\xi-0}=\widetilde{Q}\frac{d\xi}{dt}, \qquad t>0, \tag{11}$$

where $\widetilde{Q}$ is the heat of fusion per unit volume, and boundary and initial conditions are given in the form (6) - (7).

If the temperature $T=T^*$, then equation (9) takes the form of

$$\frac{\partial Q(t,x)}{\partial t}=div\big(\lambda(T)grad\ T(t,x)\big). \tag{12}$$

We show that (12) implies (11). Let $T=T^*$ be the melting temperature of a volume element, and let the boundary of phase transition $x=\xi(t)$ move from point x to point $x+\Delta\xi=\xi(t)$ (Figure 1) during the time $\Delta t=t-t^*$. Consider a small cylinder of length $\Delta\xi$ parallel to the x axis with the side surface σ_3 and bases σ_1 and σ_2 perpendicular to the x axis and located at x and $x+\Delta\xi$, respectively. Let $\vec{n}_1$, $\vec{n}_2$ and $\vec{n}_3$ be the unit normal vectors to surfaces σ_1, σ_2 and σ_3. Integrate (12) over the volume of the cylinder (Figure 1) and consider the limit of $\Delta t\to 0$.

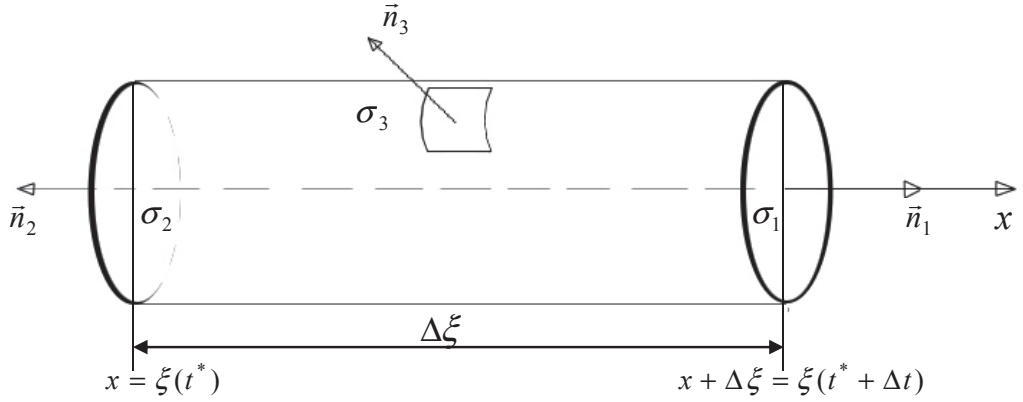

Figure 1: Cylindrical volume element.

Consider the left- and right-hand sides of the obtained result separately

$$\iiint_V div(\lambda(T)grad\,T(t,x))dV = \iint_{\sigma_1} \lambda^+ \frac{\partial T}{\partial \vec{n}_1} d\sigma + \iint_{\sigma_2} \lambda^- \frac{\partial T}{\partial \vec{n}_2} d\sigma + \iint_{\sigma_3} \lambda^* \frac{\partial T}{\partial \vec{n}_3} d\sigma =$$

$$= \iint_{\sigma_1} (\lambda^+ \frac{\partial T}{\partial x} - \lambda^- \frac{\partial T}{\partial x}) d\sigma .$$

Since $\frac{\partial T}{\partial \vec{n}_3} = 0$ and the areas of bases σ_1 and σ_2 are equal and their normals are opposite then

$$\iiint_V \frac{\partial Q(x,t)}{\partial t} dV = \iint_{\sigma_1} \int_x^{x+\Delta\xi} \lim_{\Delta t \to 0} \frac{\Delta Q(x,t)}{\Delta t} dx d\sigma$$

Introducing the limit under the integral we obtain

$$\lim_{\Delta t \to 0} \iint_{\sigma_1} \int_x^{x+\Delta\xi} \frac{\Delta Q(x,t)}{\Delta t} d\xi d\sigma = \lim_{\Delta t \to 0} \widetilde{Q} \iint_{\sigma_1} \frac{1}{\Delta t} \int_x^{x+\Delta\xi} dx d\sigma = \iint_{\sigma_1} \widetilde{Q} \lim_{\Delta t \to 0} \frac{\Delta\xi}{\Delta t} d\sigma = \iint_{\sigma_1} \widetilde{Q} \frac{d\xi}{dt} d\sigma .$$

Since the volume element melts during the time $\Delta t = t - t^*$ then $\Delta Q = \widetilde{Q}$ and thus

$$\iint_{\sigma_1} \widetilde{Q} \frac{d\xi}{dt} d\sigma = \iint_{\sigma_1} (\lambda^+ \frac{\partial T}{\partial x} - \lambda^- \frac{\partial T}{\partial x}) d\sigma .$$

Finally, we obtain

$$\widetilde{Q} \frac{d\xi}{dt} = \lambda^+ \frac{\partial T}{\partial x} - \lambda^- \frac{\partial T}{\partial x} .$$

Thus for temperature $T = T^*$, from equation (12) we obtain the classical Stefan condition (11) at phase boundary.

3. Algorithm of numerical solution for multi-layer one-dimensional problem

The features of the proposed numerical method for solving the problem (1) - (8) are illustrated by solving a one-dimensional multi-layer problem. Consider a layer of finite thickness $0 \le x \le H$ that consists of *K* different layers with thicknesses h_k, where $k = \overline{1,K}$ is the index of the layer and $H = h_1 + h_2 + \ldots + h_K$. We need to find the temperature distribution and track the dynamics of the phase transition in each layer should it take place. The geometry of layers is illustrated in Figure 2, where ξ_1 and ξ_2 denote the boundary of the phase transition in the i-th layer where $\gamma(t, \xi_{1,2}) = 1$.

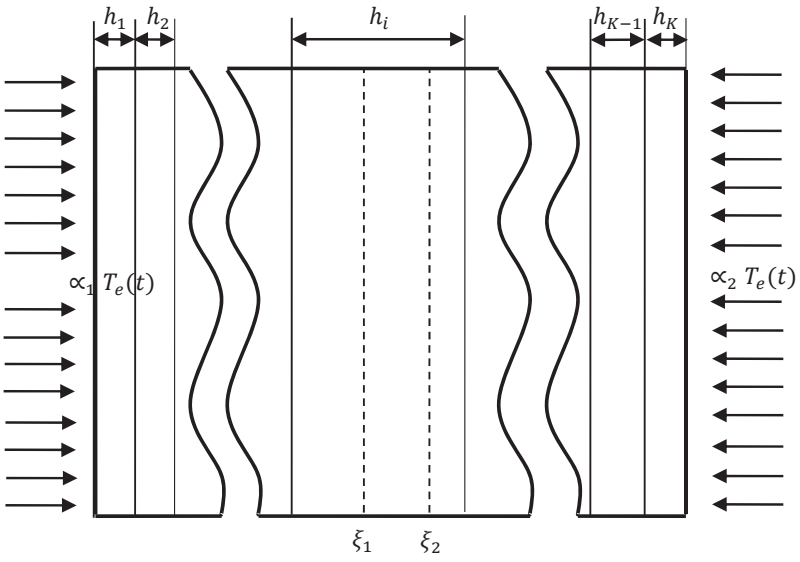

Figure 2: Geometry of a layered material with two fronts in the i-th layer.

We construct a space-time grid $\varpi = \varpi_x \times \varpi_t$, which has piecewise uniform steps in coordinate Δ_k, $\varpi_x = \{x_i = x_{i-1} + \Delta_k, k = 1, i = 0..n_1, k = 2, i = n_1..n_2, .., k = K, i = n_{k-1}..n_K,\}$. The time stepping $\varpi_t = \left\{t_j = t_{j-1} + \Delta_t, j = \overline{1,m}\right\}$ dynamically adapts when melting (crystallization) is detected. We specify the basic time step Δ_t that is associated with a variable step $\Delta_{t,j}$ as follows

$$\Delta_{t,j} = \begin{cases} \Delta_t, \text{ if } -\rho_k^+ Q_k^* - \varepsilon < Q_i^j < \rho_k^- Q_k^* + \varepsilon, \\ \dfrac{\Delta_t}{2^s}, \text{if } -\rho_k^+ Q_k^* + \varepsilon > Q_i^j \text{ or } Q_i^j > \rho_k^- Q_k^* - \varepsilon, \end{cases}$$

where s is the iteration number at the j - th time level. The iterations stop if Q_i^j falls in the interval $(-\rho_k^+ Q_k^* - \varepsilon, -\rho_k^+ Q_k^*]$ or $[\rho_k^- Q_k^*, \rho_k^- Q_k^* + \varepsilon)$.

Since the coefficients c, ρ and λ depend on temperature that changes with time to determine the current values of T_i^j and Q_i^j at the j - th step of their values are taken from the previous time step $(j-1)$.

Upon discretizing (1) using an implicit time integration scheme we obtain the system

$$(1-\gamma_i^j)\rho_i^{j-1} c_i^{j-1} \frac{T_i^j - T_i^{j-1}}{\Delta_t} = \frac{1}{(\Delta_k)^2}(\xi^j_{i+\frac{1}{2}}(T_{i+1}^j - T_i^j) - \xi^j_{i-\frac{1}{2}}(T_i^j - T_{i-1}^j)) - \gamma_i^j \frac{Q_i^j - Q_i^{j-1}}{\Delta_{t,j}},\ j = \overline{1,m} \tag{13}$$

$$\xi^j_{i+\frac{1}{2}} = \frac{1}{2}(\lambda_i^{j-1} + \lambda_{i+1}^{j-1}), \qquad \xi^j_{i-\frac{1}{2}} = \frac{1}{2}(\lambda_i^{j-1} + \lambda_{i-1}^{j-1}).$$

The step function $\gamma(t,x)$ is approximated as

$$\gamma_i^j = \begin{cases} 1, & T_i^j = T_k^* \ \text{и} \ i \in [n_{k-1}+1, n_k - 1],\ k = \overline{1,K} \ \text{и} \ -\rho_k^+ Q_k^* \le Q_i^j \le \rho_k^- Q_k^*, \\ 0, & T_i^j \ne T_k^* \ \text{и} \ i \in [n_{k-1}+1, n_k - 1],\ k = \overline{1,K}. \end{cases} \tag{14}$$

System (13) is supplemented by the approximate initial and boundary conditions

$$T_i^0 = T_k^0, \qquad i = \overline{0, n_K}, \tag{15}$$

$$\lambda^{j-1}_{n_k - 0} \frac{T^j_{n_k} - T^j_{n_k - 1}}{\Delta_k} = \lambda^{j-1}_{n_k + 0} \frac{T^j_{n_k+1} - T^j_{n_k}}{\Delta_{k+1}}, \quad k = 1,.., K-1, \quad j = \overline{1,m}, \tag{16}$$

$$\lambda_0^{j-1} \frac{T_1^j - T_0^j}{\Delta_1} = \alpha_1 (T_0^j - T_e^j), \qquad \lambda^{j-1}_{n_K} \frac{T^j_{n_K} - T^j_{n_K - 1}}{\Delta_K} = \alpha_2 (T^j_{n_K} - T_e^j), \qquad j = \overline{1,m}. \tag{17}$$

It is possible to write the system of equations (13)-(17) for unknown quantities T_i^j, Q_i^j as

$$A_i^j X_{i-1}^j - C_i^j X_i^j + B_i^j X_{i+1}^j = F_i^j, \qquad i \in \overline{1, n_K - 1}, \qquad j = \overline{1,m}, \tag{18}$$

where all coefficients are given by (14) and

$$X_i^j = \begin{cases} T_i^j, & \gamma_i^j = 0, \\ Q_i^j, & \gamma_i^j = 1. \end{cases}$$

System of equations (18) has a tridiagonal matrix and can be solved by the sweep method.

4. Results and discussion

Test computations have been performed for melting a three-layer material (aluminum (1), tin (2), zinc (3)) were performed to test the model and the numerical algorithm in one dimension. Figure 3 shows the results of calculations. The boundary and initial conditions were given by (9) and (10) and the

following parameters were chosen $\dot{O}_1^0 = \dot{O}_2^0 = \dot{O}_3^0 = 20\ ^i\tilde{N}, \dot{O}_e = 2200\ ^i\tilde{N}, \alpha_1 = 500 W/(m^2 \cdot s)$, $\alpha_2 = 500 J/(m^2 \cdot s)$ for layer thicknesses of $h_1 = 0.5\ (m), h_2 = 0.3\ (m)$ and $h_3 = 0.2\ (m)$. The thermophysical properties of materials are given in Table 1.

Table 1. Thermophysical properties of materials.

Material	$T^*, {}^oC$	$c, \frac{J}{kg \cdot m^3}$		$\lambda, \frac{W}{m\,{}^oC}$		$\rho, \frac{kg}{m^3}$		$Q^*, \frac{J}{kg}$
		c^+	c^-	λ^+	λ^-	ρ^+	ρ^-	
Aluminum	660	1131.8	732.8	229	132	2700	2300	398
Tin	232	228	184	86	66.8	7310	7420	59.3
Zink	420	387	357	142	116	7133	7300	111

The graphs in Figure 3 show the phase boundary in the three layers. The material is liquid (liq) above the line, and solid (sol) below it. The vertical lines show the interfaces between layers. The peaks seen the first two layers correspond to the collision of two fronts moving in the opposite directions.

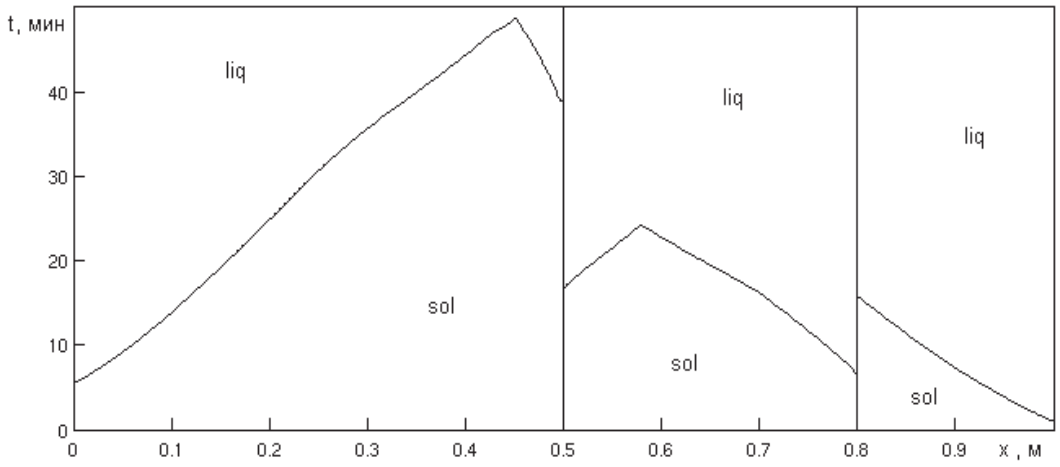

Figure 3: The location of phase transition fronts in a three-layer composite material as functions of time.

For the comparison test, a classical Stefan foundering problem was selected in the interval $0 \le x < \infty,\ t \ge 0$, which has a similar solution. In developing an approximate solution the semi-infinite space was represented by a single layer ($K = 1$) of large thickness $(0 \le x \le H,\ t \ge 0)$, $H = 1\,(м)$. The material selected was aluminum; initial bulk temperature was equal to the melting temperature $T_0 = T^*$ everywhere; the temperature at the boundary $x = 0$ was also constant and equal to $T_e = 670\ ^0C$ and the border $x = H$ was assumed adiabatic (see Figure 4).

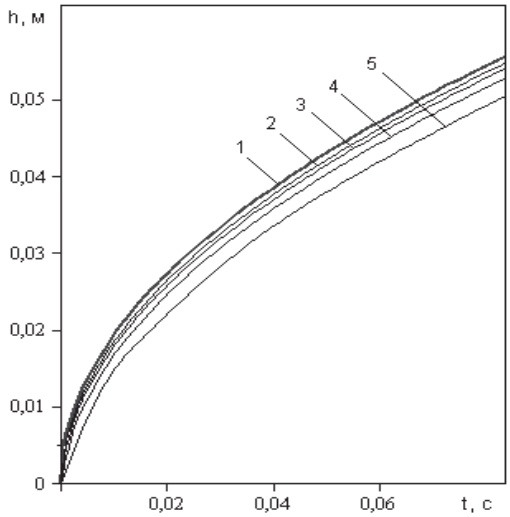

Figure 4: Comparison with Stefan's self-similar solution.

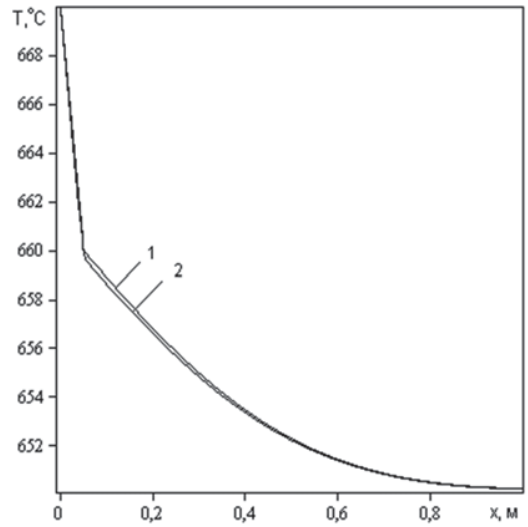

Figure 5: Comparison with the continuous computations scheme.

Graphs of the foundering thickness h are shown in Figure 4: 1 – self-similar Stefan solution, 2, 3, 4, 5 - the current model solutions for different discretizations: $5-\Delta_x = 0{,}01,\ \Delta_t = 0{,}01,$ $4-\Delta_x = 0{,}005,\ \Delta_t = 0{,}005,\ 3-\Delta_x = 0{,}0025,\ \Delta_t = 0{,}0025,\ 2-\Delta_x = 0{,}00125,$ $\Delta_t = 0{,}00125$. Comparing the graphs in Figure 4 we observe the convergence of numerical solutions to the analytical one as both spatial and temporal discretization steps decrease.

The proposed method was also compared with the continuous computations scheme in the example of melting problem in the region $0 \le x \le H$ for $t \ge 0$. The initial temperature and the temperature at the border $x = 0$ were constant and equal to $T_0 = 650\ ^0C$ and $T_e = 670\ ^0C$, respectively, and the border at $x = H$ was assumed to be adiabatic. Thermal characteristics were obtained for aluminum and the results for the temperature distribution over the thickness of the layer 60 seconds after the start of the process are shown in Figure 5. The solutions are obtained using the front-capturing (1) and proposed (2) methods with $\Delta_x = 0{,}05$ and $\Delta_t = 0{,}1$. A very close agreement between the curves

obtained using the two methods with identical discretizations also confirms the accuracy of the proposed method.

5. Conclusions

The process of manufacturing composite materials involving melting and subsequent crystallization of individual layers generally consists of 3 stages: heating, curing and cooling. Baking of layers together usually occurs during the first two stages and sometimes it is followed by the formation of an intermediate phase and the layer interfaces. Tracking the dynamics of the phase transition front enables one to determine thermal and structural stresses and material inhomogeneities in layered materials and especially at the contact surfaces between different materials and phases.

In the present work a fictitious heat source given by function (3) is used to determine the shape and location of the boundary between various phases. The introduction of such function simplifies the problem on one hand but enables one to consider more complicated geometry, boundary and initial conditions and materials with the arbitrary number of layers on the other. The proposed method also allows modeling situations when several merging phase transition boundaries are present in a layer. The obtained computational results agree well with a self-similar solution of Stefan problem and the numerical solution obtained using the continuous computations scheme.

The proposed method can be successfully used not only for modeling the fabrication of layered composite materials but also for developing he quality control procedures of welding and other technological processes that can lead to melting of one of the layers. The total welding time is one of the control parameters that have a strong influence on the quality of the manufactured material. It must include the time required for three stages: establishing the contact between materials that are being welded, formation of the reaction activation, and development of a diffusion process. The method suggested here enables one to monitor efficiently the processes taking place in the welded materials and in particular, to optimize the total welding time.

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