Numerical Simulation of Stefan's Problem in a Plane Layer with Selective Optical Properties of a Semitransparent Medium

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ABSTRACT

Numerical investigation of melting of a plane layer with transparent and semitransparent boundaries has been carried out. The mathematical phase change model is a formulation of the One-Phase Stefan problem. The correct statement of radiative-conductive heat transfer (RCHT) problem requires accounting of optical properties as functions of radiation wavelength. To account the selectivity of optical properties the model of rectangular bands was applied. In this model some rectangular bands are taken in the spectrum with constant values of optical coefficients. The algorithm on the basis of modified mean fluxes method has been used for the numerical calculation of the radiation transfer equation. The energy equations are solved by a finite-difference method.

The subject of this paper is to study the effect of the radiation on the temperature distribution and the velocity of the phase change front during melting of semitransparent medium. The first stage of the problem solving is to study RCHT in a solid plane layer by radiation and convection heating. The second stage is to consider Stefan's problem. It is assumed that liquid phase sublimates and it is removed by convection. Numerical results of the temperature distribution, radiation fluxes and the position of the phase change front are presented in this paper. The numerical results are obtained first for the material with selective absorption of radiation with using One-Phase Stefan problem.

INTRODUCTION

Investigations of radiative-conductive heat transfer (RCHT) in a semitransparent medium with phase changes are important in some practical applications. These problems arise in glassmanufacturing, technologies of translucent crystal growth, development of effective methods of heat protection and under the natural conditions, when considering the process of glaciers and ice melting in Arctic. In particular, the presented model of melting the translucent layer with gray coating under the certain boundary conditions simulates the ice melting in the Arctic lake with the snow (gray) coating at solar irradiation.

There are many works simulating the two-phase problems in semitransparent material. The experimental and numerical studies of melting the translucent material [1] as well as pulsed alumina heating and melting by laser radiation [2,3] are the expressive examples of these problems. The numerical solutions of such problems are considered in detail in monographs [4-6]. The strict account for dependence of absorbance of the medium volume on radiation frequency is challenging. To simplify it different models are used. One of the most simple and convenient is model of rectangular bands. In this case, the absorption coefficients and other values that describe the optical properties are assumed constant within a certain frequency band Δv . The required accuracy is achieved by increasing the number of bands and selection of appropriate values of optical coefficients in the spectral range [4]. The singlephase Stefan problem [7-10] as a particular case of the twophase problem has the fundamental differences from the latter and at the same time, it is more complex. This paper reports results of numerical calculation of the single-phase Stefan problem for selectively absorbing medium with transparent and translucent gray boundaries. Consideration of selective conditions of radiation absorption on the right boundary is fundamentally important for the single-phase Stefan problem modeling the processes of melting of translucent crystals. In future it seems possible to simulate the thermal state of the water stratum under the action of solar radiation.

NOMENCLATURE

a	$[m^2/s]$	thermal diffusivity
с	[J/kgK]	heat capacity
h	$[W/(m^2 K)]$	heat-transfer coefficient at sample
Α		absorption factor
D		transmission factor
R		reflection coefficient
п		refraction coefficient
Ε	$[W/m^2]$	hemispherical density of radiation flux
т		coefficient of radiation intensity distribution
l		coefficient of radiation diffusion
L_0	[m]	initial sample thickness
L(i	t) [m]	sample thickness during phase transition
S		dimensionless thickness
Т	[K]	temperature
Т	[s]	time
х	[m]	variable coordinate of sample thickness
Gr	eek symbols	
α	[m ⁻¹]	coefficient of volume absorption
δ	[m]	infinite small distance from coordinate x
3		degree of blackness of sample boundaries
Φ		dimensionless semispherical density of radiation flux
η		dimensionless time
λ	[W/(m K)]	thermal conductivity
γ	[J/kg]	latent heat of phase transition
μ		cosine of radiation propagation angle within solid angle
		$\Omega = \pm 2\pi$
θ		dimensionless temperature
ρ	[kg/m ³]	density of semitransparent sample
σ_0	$[W/(m^2 K^4)]$	Stefan-Boltzmann constant
ξ		dimensionless coordinate
τ		optical thickness
Inc	lexes	
i		left $i=1$, right $i=2$ sides of medium
\pm		intensities forward ($\Omega = 2\pi$) and backwards
		$(\Omega = -2\pi)$
f		phase change
j i		number of rectangular hands
J V		related to frequency
*		the incident radiation flux

PROBLEM STATEMENT

In Figure 1, there is the geometrical scheme of the problem, which is the three-layer system, where semiinfinite layers I and III correspond to the external conditions with air refractive index $n_0=1$ at corresponding air temperatures T_1 and T_2 , and layer II corresponds to the studied solid translucent medium with refractive index n = 1.5.

Heating and following melting of plane layer II of selectively absorbing translucent medium with coefficient of volume absorption of radiation α_{ν} and heat conductivity λ are studied in this work. The boundaries absorb, reflect and transmit radiation so that $A_i + R_i + D_i = 1$, At that, the validity of Kirchhoff law is assumed: $A_i = \varepsilon_i$,

The solution of the problem includes two stages. The first stage is reduced to consideration of non-stationary radiant-convective heat transfer in the process of heating a selective translucent sample with the gray boundaries. At the second step, when the right sample boundary achieves the melting point $T(L(t), t) = T_f$, the Stefan problem is considered. At that, the liquid phase formed at the boundary is carried away by a convective flow.



Figure 1 Geometrical scheme of the problem

Position of interface L(t) is determined from the solution to the boundary problem, reduced to determination of the temperature fields and flow densities in a solid phase layer of a variable (from x = 0 to x = L(t)) thickness (Fig. 1).

The equation of energy conservation takes form:

$$c\rho \frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x} \left(\lambda \frac{\partial T(x,t)}{\partial x} - E_{\nu}(x,t) \right). \tag{1}$$

Here $E_v(x, t)$ is the density of resultant radiation flux in cross-section x at time t.

The boundary conditions of energy equation (1) for arbitrary time $t \ge 0$ are written as:

$$-\lambda \frac{\partial T}{\partial x}\Big|_{x+\delta} + h_1 (T - T_1)\Big|_{x-\delta} + \left|E_{1,\nu}\right| = 0, \ x = 0,$$

$$\lambda \frac{\partial T}{\partial x}\Big|_{x-\delta} + h_2 (T_2 - T)\Big|_{x+\delta} - \left|E_{2,\nu}\right| = \rho \gamma \frac{\partial L}{\partial t}, \ x = L(t),$$
(2)

where $E_{1,\nu} = E_{1,\nu}(0, t)$, $E_{2,\nu} = E_{2,\nu}(L(t), t)$ are the densities of resultant radiation flux at boundary 1 (x = 0) and 2 ($x = L_0, L(t)$) at time $t \ge 0$. $|E_{i,\nu}| = E_{i,\nu}(x-\delta) - E_{i,\nu}(x+\delta)$, i = 1, 2 is the difference of flux densities of resultant radiation. At the layer-medium boundary, $x \pm \delta$ is the coordinate in finitely close to coordinate x; h_i is the coefficient of heat transfer with the ambient medium, T_i is the temperature of the medium, surrounding the flat layer, γ is the latent heat of melting, ρ is the density at the phase change temperature T_f ; indexes i = 1, 2 correspond to the left and right media (layer-sample boundaries). Radiation component $|E_{i,\nu}|$ of boundary conditions (2) takes into account the processes of radiation reflection and transmission by the sample boundaries, and it is written in the form, which considers

$$\begin{split} E_{1,\nu} &= A_1 \Big[E_{\nu}^{-} \left(x + \delta \right) + \sigma_0 T_1^4 \Big] - \varepsilon_1 \left(1 + n^2 \right) \sigma_0 T^4(x,t), \ x = 0, \\ E_{2,\nu} &= A_2 \Big[E_{\nu}^{+} \left(x - \delta \right) + E^* \Big] - \varepsilon_2 \left(1 + n^2 \right) \sigma_0 T^4(x,t), \ x = L(t). \end{split}$$
(3)

only absorption and radiation of boundaries [12]:

It is assumed that the phase transition at boundary 2 does not affect the optic properties, therefore ε_i , A_i , R_i and D_i are considered constant, and in the second equation of system (3) it should be taken into account that $T(x) \equiv T_f$,

x = L(t), t > 0. While considering the first stage of radiantconductive heating of a sample, in the second equation of boundary conditions (2) $T_f \equiv T(x)$, $x = L_0$, . The system of equations (1)–(3) is added by initial condition

$$T(x,0) = f(x), \ L(0) = L_0.$$
(4)

To solve the radiation part of the problem, the modified mean fluxes method for the three-layer system is used. The spectral dependences of absorption coefficient are presented in the Table 1. It takes into account high absorption in the IR region and transparent in the visible region [4].

Table 1

Spectral dependences of absorption coefficient

j	v_j , 10 ¹⁴ ,Hz	$\lambda_j, \mu m$	$\alpha_j, \mathbf{m}^{-1}$
1	0-0.6	∞−5	500
2	0.6-1.2	5-2.5	160
3	1.2-2.3	2.5-1.3	5
4	2.3-3.84	1.3-0.78	0.1
5	3.84-6	0.78-0.5	0.2

The flux densities are set at the external boundaries of the system at n_0 = 1:

$$x = 0 - \infty; \qquad E_{j,1}^{+} = B_{\nu}(T_{1}),$$

$$x = L(t) + \infty; \quad E_{j,III}^{-} = E^{*};$$
(5)

in the intermediate layer at $n > n_0$

$$E_{j,II}^{+} = \left(1 - R_{1}\right) \frac{n_{0}^{2}}{n^{2}} E_{j}^{-} + R_{1}E_{j}^{+}, \ x = 0,$$

$$E_{j,II}^{-} = \left(1 - R_{2}\right) \frac{n_{0}^{2}}{n^{2}} E_{j}^{+} + R_{2}E_{j}^{-}, \ x = L(t),$$
(6)

j is a number of the spectral band Δv , B_v is the Planck function of black body radiation; the Roman figures in the indices indicate the number of layers: I and III are the outer layers, II is the intermediate layer, considered by the current study (further, we will skip index II). Here, we take into account that the reflection coefficient in the intermediate layer is determined by total internal reflection, which is obtained from relationship

$$(1 - R'_i)n^2 = (1 - R_i)n_0^2.$$
⁽⁷⁾

The radiation flux is determined from relationship

$$E_{\nu} = \sum_{j=1}^{3} \left(E_j^+ - E_j^- \right).$$

Transformation of boundary problem (1)–(4) to the dimensionless form is performed with the use of Lagrangian transformations $\xi = x/L(t)$ [7]. This variable allows registration of a coordinate of the phase transition front within $0 \le \xi \le 1$, at that, the front becomes plane-parallel (the method of front straightening). Equation system (1), (2) and (4), with consideration of (3) is transformed to the boundary problem of the following form:

$$\frac{\partial\theta(\xi,\eta)}{\partial\eta} = \xi \frac{\dot{s}}{s} \frac{\partial\theta(\xi,\eta)}{\partial\xi} + \frac{1}{s^2} \frac{\partial^2\theta(\xi,\eta)}{\partial\xi^2} - \frac{1}{sN} \frac{\partial\Phi_{\nu}(\xi,\eta)}{\partial\xi}, \quad 0 \le \xi \le 1,$$
(8)

$$-\frac{\partial\theta(0,\eta)}{\partial\xi} + sBi_1(\theta(0,\eta) - \theta_1) + \frac{s}{N} \left[A_1\left(\Phi_\nu^- + \frac{\theta_1^4}{4}\right) - \varepsilon_1\left(1 + n^2\right) \frac{\theta^4(0,\eta)}{4} \right] = 0, \quad (9)$$

$$\frac{\partial \theta(\mathbf{l},\eta)}{\partial \xi} + s \operatorname{Bi}_{2} \left(\theta_{2} - \theta(\mathbf{l},\eta) \right) - \frac{s}{N} \left[A_{2} \left(\Phi_{\nu}^{+}(\mathbf{l},\eta) + F^{*} \right) - \varepsilon_{2} \left(\mathbf{l} + n^{2} \right) \frac{\theta^{4}(\mathbf{l},\eta)}{4} \right] = \frac{s\dot{s}}{\operatorname{St}},$$
(10)

$$\theta(\xi, 0) = f(\xi), \ s(0) = 1, \ \theta(1, \eta) = 1, \tag{11}$$

here
$$\theta = T/T_f$$
, $\xi = x/L(t)$, $s(\eta) = L(t)/L_0$,
 $\eta = \lambda t / (\rho c_p L_0^2)$ is dimensionless time, $N = \lambda / (4\sigma_0 T_f^3 L_0)$
is radiant-conductive parameter, $\Phi_{\nu}^{\pm}(\xi,\eta) = E_{\nu}^{\pm}(x,t) / (4\sigma_0 T_f^4)$
is dimensionless density of radiation flux, $F^* = E^* / (4\sigma_0 T_f^4)$ is
dimensionless density of radiation flux falling on a plate
from the right, $\operatorname{Bi}_i = h_i L_0 / \lambda$ is the Biot number, $\dot{s} = ds/d\eta$
is the velocity of melting front propagation, $\operatorname{St} = T_f c_p / \gamma$ is

the Stefan number. $\Phi_{\nu} = \sum_{j} \left(\Phi_{j}^{+} - \Phi_{j}^{-} \right)$ in equations

(8)–(10) are determined from the solution of the radiant transfer equation in a plane layer of emitting and absorbing medium with the known temperature distribution over the layer.

A wide field of possibilities in terms of solution simplicity and efficiency of results is offered by the modified method of mean fluxes [4]. In this method, the radiation transfer equation is transformed to the system of two nonlinear differential equations for a plane layer of translucent medium. The differential analogue of transfer equation for hemispherical fluxes Φ_i^{\pm} is written as:

$$\frac{d}{d\tau_{j}} \left(\Phi_{j}^{+}(\tau,\eta) - \Phi_{j}^{-}(\tau,\eta) \right) + \left(m_{j}^{+}(\tau) \Phi_{j}^{+}(\tau,\eta) - m_{j}^{-}(\tau) \Phi_{j}^{-}(\tau,\eta) \right) = n^{2} \Phi_{0},$$

$$\frac{d}{d\tau_{j}} \left(m_{j}^{+}(\tau) l_{j}^{+}(\tau) \Phi_{j}^{+}(\tau,\eta) - m_{j}^{-}(\tau) l_{j}^{-}(\tau) \Phi_{j}^{-}(\tau,\eta) \right) + \left(\Phi_{j}^{+}(\tau,\eta) - \Phi_{j}^{-}(\tau,\eta) \right) = 0.$$
12)

The boundary conditions for equation system (11) in the dimensionless form are obtained from conditions (5) and (6) in the form:

$$\tau_{j,\mathrm{I}} = 0 - \infty : \quad \Phi_{j,\mathrm{I}}^+ = \Phi_0(\theta_1),$$

$$\tau_{j,\mathrm{III}} = L(t) + \infty : \quad \Phi_{j,\mathrm{III}}^- = F^*,$$
 (13)

$$\Phi_{j,\Pi}^{+} = \left(1 - R_{1}\right) \frac{n_{0}^{2}}{n^{2}} \Phi_{j}^{-} + R_{1} \Phi_{j}^{+}, \ \tau = 0,$$

$$\Phi_{j,\Pi}^{-} = \left(1 - R_{2}\right) \frac{n_{0}^{2}}{n^{2}} \Phi_{j}^{+} + R_{2} \Phi_{j}^{-}, \ \tau = L(t).$$
(14)

Here $\Phi_0 = B_v / (4\sigma T_f^4)$, $\tau_j = \alpha_j \cdot x$ is the optic thickness of a layer. In equations (12)-(14), $\Phi_{ji}^{\pm}(\tau_{ji}) = \pm \frac{1}{4\sigma T_f^4} \int_{\Delta V_j} 2\pi \int_{0(-1)}^{1(0)} I_v(\tau_{ji}, \mu) \mu d\mu d\nu$ are the

dimensionless densities of the hemispherical radiation fluxes in the band Δv_j ; The values of coefficients m_j^{\pm} , l_j^{\pm} are determined from the recurrent relationship obtained by means of a formal solution to the equation of radiation transfer [4].

The solution of the problem is to determine of temperature $\theta(\xi, \eta)$ and radiation fluxes $\Phi_v(\xi, \eta)$ in layer II $G = \{0 \le \xi \le 1, 0; 0 \le \eta \le \eta_1\}$. The position of the phase change front $s(\eta)$ changes from 1 to 0. Equations (8)–(11) is solved by the finite-difference method. Implicit finite-difference scheme was developed by integral-interpolation method. The equable mesh was used. The system of finite-difference equations was solved by method of running with method of iteration. When solving the radiation problem, the iterations are used, and at every step of these iterations, the equations (12) – (14) is solved by the method of matrix factorization. Fast convergence of this method allows us to obtain the results with a high degree of accuracy. Numerical algorithm was tested on known analytical results and results by other authors [4].

RESULTS

In this section we present the results of numerical simulation of heating the sample of a translucent material with the following physical parameters: $S_0 = 0,1$ m, $T_1 = 300$ K, $T_2 = 900$ K, $T_f = 1000$ K, $E^* = 200$ kW/m²; the thermal-physical properties of this material are close to the properties of fluorite and they are as follows: $\rho = 2000$ kg/m³, $\lambda = 1$ W/(m·K), $a = 10^{-6}$ m²/s, latent heat of phase transition is $\gamma = 500$ kJ/kg. Absorption coefficients are presented in Table 1.

In the numerical experiment, it was assumed that heat transfer from the layer boundaries corresponds to the conditions of natural convection: $h_{1,2} = 8 \text{ W/(m^2 \cdot K)}$ at $\varepsilon_{1,2} =$ 0 and 0.1, heat transfer on the left boundary at $\varepsilon_{1,2} = 0.2$ was assumed to be $h_1=30 \text{ W/(m}^2 \cdot \text{K})$, at $\varepsilon_{1,2} = 0.3 h_1 =$ $80 \text{ W/(m}^2 \cdot \text{K})$. Heat transfer coefficient on the right boundary h_2 remained unchanged. These values have been chosen considering the fact that at heat transfer $h_1 = 80$ $W/(m^2 \cdot K)$ and high density of radiation flux the temperature of the left boundary undergoes uncharacteristic with increasing its emissivity. The values of emissivity $\varepsilon_{1,2} = 0.3$ were chosen assuming that inner reflection coefficient $R'_{1,2}$, derived from relationship (7), equals 0.6. The inner transmittance according Kirchhoff law takes value $D'_{1,2} = 1 - A'_{1,2} - R'_{1,2} = 0,1$. At $\varepsilon_{1,2} > 0.4$ the boundaries of the considered medium becomes not transmitting, but it reflects and absorbs radiation.

A temperature increase of the left boundary is shown in Figure 2*a*. For $\varepsilon_{1,2} < 0.2$, the growth dynamics can be characterized by three stages: to a certain level a rapid increase in temperature was observed, then there was a slow increase, and then to the end of the process there was a rapid temperature increase to reaching the phase change temperature. The temperature increase of the left boundary at $\varepsilon_{1,2} > 0.2$ is restrained by more intensity heat transfer, and the melting process decelerates, and leads to the fact that the layer is melted incompletely (Figure 2b).





$$\begin{split} I & \longrightarrow \varepsilon_{1,2} = 0, \ h_1 = 8 \ W/(m^2 K), \ 2 & \longrightarrow \varepsilon_{1,2} = 0.1, \ h_1 = 8 \\ W/(m^2 K), \\ 3 & \longrightarrow \varepsilon_{1,2} = 0.2, \ h_1 = 30 \ W/(m^2 K), \ 4 & \longrightarrow \varepsilon_{1,2} = 0.3, \ h_1 = 80 \\ W/(m^2 K). \end{split}$$



Figure 3 Temperature distribution (*a*) and motion of the melting front (*b*) for models of selectively absorbing medium (solid lines) and gray medium (dashed lines). 1- $\theta(1, \eta) = 0.4, 2 - \theta(1, \eta) = 1, 3 - s(\eta) = 0.3, 4 - s(\eta)$ - final.

The model of selectively absorbing medium is compared with the model of gray medium at $\varepsilon_{1,2} = 0.1$ in Figure 3. Absorption coefficient of the gray medium was chosen by means of the numerical experiment and it was assumed $\alpha =$ 40 m^{-1} . The temperature field of the gray medium (Figure 3a) at the stage of heating (dashed lines 1 and 2) differs significantly in the medium volume, and that the boundary temperatures coincide. In the model of gray medium, the temperature increase in the volume is higher than in a layer with selective optical properties, and this is explained by the difference of the optical thicknesses of the medium. At the stage of phase transition (curve 3), the temperature increase for the model with selective radiation is higher than for the model of gray medium, and almost equals it by the end of phase transition. The melting process is two times faster in the gray medium (Figure 3b).

CONCLUSION

The numerical results are obtained first for the material with selective absorption of radiation. To solve the radiant part of the problem, the modified method of mean fluxes for the three-layer system was used. At that, the optic properties were assumed artificially combined: the studied layer of the medium (solid phase) was assumed selective and its boundaries were assumed gray.

Calculation of the temperature on the left boundary of a plane layer showed that the temperature increase of the left boundary at increasing degree of blackness ($\varepsilon_{1,2} > 0.2$) is restrained by more intensity heat transfer, and the melting process decelerates, and leads to the fact that the layer is melted incompletely. This simulation is may be important at flood forecast in the north.

Numerical results of the temperature distribution and motion of the melting front are compared for models of selectively absorbing medium and gray medium. The temperature fields differ significantly in the medium volume, and that the boundary temperatures almost coincide. The melting process is two times faster in the gray medium

Comparison obtained numerical results points at the importance to take into account selective radiation absorption by the medium, when comparing the numerical results with experimental data. On the process of phase transition overheating of the solid layer near the right boundary is observed, which does not exceed 5% of the melting point at front position near $s \approx 0.7$. Overheating of the solid phase is determined by heat exchange at a fixed temperature of phase change, as well as the independence of the determining parameters on the temperature. By the end of the melting process the temperature gradient decreases, the layer becomes almost isothermal. The temperature field around the left boundary depends essentially on heat transfer, which prevents surface overheating.

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