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DYNAMIC ADAPTATION METHOD FOR MODELLING OF MELTING AND EVAPORATION PROCESSES WITH CONVECTION

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Abstract. The application of the dynamic adaptation method for the explicit tracking of interfaces in two-dimensional phase change problems with convection is presented. The results of computational experiments in modelling the action of high energy fluxes on metal target are given.

Key words: Stefan problem, natural convection, melting, evaporation, adaptive method, curvilinear coordinate systems, difference scheme

1. Introduction

Concentrated energy fluxes are wide-spread tools for the treatment of different materials. Laser and electron-beam techniques are used in many technological operations, such as drilling, cutting, welding and so on. Most of the applications for laser irradiation are connected with the phase transformations of metals, dielectrics and semiconductors (melting-crystallization and evaporation processes). The main feature of such processes is the presence of moving interfaces where phase changes occur. Due to the complexity of the problem the numerical methods are used for its study [5].

Two alternative approaches are widely used for numerical solution of phase transition (or Stefan-like) problems: explicit tracking of moving interfaces [1]

and the use of smoothing procedures [6]. In the first method the governing equations are solved on a moving body-fitted grid. In the second method the heat and mass transfer conditions on interfaces are incorporated into the governing equations which are solved on a fixed grid.

A numerical algorithm for the explicit tracking of interfaces in melting-solidification and evaporation is presented. An unsteady natural convection in a liquid phase is also taken into account. Difference schemes for the solution of such problem in an arbitrary region on non-staggered grids are developed. The method is based on the idea of a transition to a non-stationary curvilinear coordinate system.

2. Mathematical Model

The mathematical formulation of the two-dimensional Stefan problem describing melting and crystallization processes with convection in an arbitrary physical region $\Omega(t)$ contains heat and mass transfer equations in the Boussinesq approximation

$$\left[c_p\rho\left(\frac{\partial T}{\partial t}+C(\mathbf{v})T\right)=\lambda\Delta T\right]_m, \quad x\in\Omega^m(t), \quad m=s,l, \tag{2.1}$$

$$\frac{\partial \mathbf{v}}{\partial t}+C(\mathbf{v})\mathbf{v}-\nu\Delta\mathbf{v}=-\frac{1}{\rho}\mathrm{grad}p+\mathbf{g}\beta_T T, \quad \mathrm{div}\mathbf{v}=0, \quad x\in\Omega^l(t), \tag{2.2}$$

$$\mathbf{v}\equiv 0, \quad x\in\Omega^s(t), \quad 0<t\leqslant t_0. \tag{2.3}$$

An a priori unknown interface $\Gamma_{sl}(t)$ separates the solid $\Omega^s(t)$ and liquid $\Omega^l(t)$ phases:

$$\Omega(t)=\Omega^s(t)\cup\Omega^l(t).$$

On $\Gamma_{sl}(t)$ the differential Stefan condition and the temperature continuity equation are fulfilled

$$\lambda_l\frac{\partial T_l}{\partial \mathbf{n}}-\lambda_s\frac{\partial T_s}{\partial \mathbf{n}}=L_m\rho v_{sl}^n, \tag{2.4}$$
$$T_s=T_l=T_m,$$

where T_m is the temperature of melting. The boundary conditions for the temperature on $\partial\Omega(t)$ are presented in the form

$$\left.\frac{\partial T}{\partial \mathbf{n}}\right|_{\partial\Omega}=f, \tag{2.5}$$

where $\mathbf{n}$ is the external normal to $\partial\Omega(t)$, f is the function defined on $\partial\Omega(t)$.

Accounting of the evaporation leads to the appearance of the second movable interface $\Gamma_{lv}(t)$ on the boundary $\partial\Omega(t)$. The process of the advanced surface evaporation on this boundary is described by the mass, momentum and energy conservation laws

$$\begin{cases} \rho_l v_{lv}^n = \rho_v (u - v_{lv}^n), \\ P_l + \rho_l (v_{lv}^n)^2 = P_v + \rho_v (u - v_{lv}^n)^2, \\ -\lambda \dfrac{\partial T}{\partial n} = G^n - L_v \rho_l v_{lv}^n \end{cases} \tag{2.6}$$

and two additional relations of the kinetics of phase transformations

$$T_v = T_v(T_l, \mathrm{M}), \quad \rho_v = \rho_v(\rho_H, \mathrm{M}),$$

that are determined from the Knudsen layer approximation [4]. Here $G = (G^n, G^\tau)$ is the energy source intensity, u is the gas-dynamic velocity, v_{lv}^n is the velocity of evaporation front, L_v is the heat of vaporization, M is the Mach number, and ρ_H is the saturated vapor density.

The conditions of no-slip and no-penetration give the uniform boundary conditions of the first kind for the velocity

$$\mathbf{v}(x,t) = 0, \quad x \in \partial\Omega^l(t) \backslash \Gamma_{lv}(t), \quad 0 < t \leqslant t_0. \tag{2.7}$$

The initial conditions can be written in the form

$$T(x,0) = T_l(x) < T_m, \quad \mathbf{v}(x,0) = 0, \quad x \in \Omega. \tag{2.8}$$

3. Transition to a Nonstationary Curvilinear Coordinate System

We assume that there is a nonsingular one-to-one transformation $\xi = \xi(x,y,t)$, $\eta = \eta(x,y,t)$, converting a physical region Ω of an arbitrary shape into the square region $\Omega_{\xi\eta} = \left\{(\xi,\eta)\,,\, 0 \leqslant \xi \leqslant 1, 0 \leqslant \eta \leqslant 1\right\}$ in the space of curvilinear coordinates. The boundary $\partial\Omega_{\xi\eta}$ and the interfaces Γ_{sl}, Γ_{lv} in $\Omega_{\xi\eta}$ coincide with the corresponding coordinate lines and are constant in time.

Equations (2.1) and (2.2) in the new variables (ξ,η) are presented as follows:

$$\left[c_p \rho \left(\frac{\partial (JT)}{\partial t} + JC_{\xi\eta}(\mathbf{v})T + M_{\xi\eta}T \right) = \lambda J \Delta_{\xi\eta} T \right]_m, \ \theta \in \Omega_{\xi\eta}^m, \ m = s, l, \tag{3.1}$$

$$\frac{\partial (J\mathbf{v})}{\partial t} + JC_{\xi\eta}(\mathbf{v})\mathbf{v} + M_{\xi\eta}\mathbf{v} - \nu J \Delta_{\xi\eta}\mathbf{v} = -\frac{J}{\rho}\mathrm{grad}_{\xi\eta} p + J\mathbf{g}\beta_T T, \tag{3.2}$$

$$\mathrm{div}_{\xi\eta}\mathbf{v} = 0, \quad \theta \in \Omega_{\xi\eta}^l, \quad 0 < t \leqslant t_0, \tag{3.3}$$

where

$$\mathrm{div}_{\xi\eta}\mathbf{v} = \frac{1}{J}\left[\frac{\partial}{\partial\xi}\left(\frac{\partial y}{\partial\eta}u\right) - \frac{\partial}{\partial\eta}\left(\frac{\partial y}{\partial\xi}u\right) - \frac{\partial}{\partial\xi}\left(\frac{\partial x}{\partial\eta}v\right) + \frac{\partial}{\partial\eta}\left(\frac{\partial x}{\partial\xi}v\right)\right],$$

$$\mathrm{grad}_{\xi\eta} p = \frac{1}{J}\left(\frac{\partial y}{\partial\eta}\frac{\partial p}{\partial\xi} - \frac{\partial y}{\partial\xi}\frac{\partial p}{\partial\eta}, -\frac{\partial x}{\partial\eta}\frac{\partial p}{\partial\xi} + \frac{\partial x}{\partial\xi}\frac{\partial p}{\partial\eta}\right),$$

$$C_{\xi\eta}(\mathbf{v})\mathbf{v} = \frac{1}{2}\left(\left(\mathbf{v}\cdot\mathrm{grad}_{\xi\eta}\right)\mathbf{v} + \mathrm{div}_{\xi\eta}(\mathbf{vv})\right),$$

$$\Delta_{\xi\eta}u = \frac{1}{J}\left[\frac{\partial}{\partial\xi}\left(B_{11}\frac{\partial u}{\partial\xi} + B_{12}\frac{\partial u}{\partial\eta}\right) + \frac{\partial}{\partial\eta}\left(B_{12}\frac{\partial u}{\partial\xi} + B_{22}\frac{\partial u}{\partial\eta}\right)\right],$$

$$B_{11} = \frac{g_{22}}{J}, \quad B_{12} = -\frac{g_{12}}{J}, \quad B_{22} = \frac{g_{11}}{J},$$

$$g_{11} = \left(\frac{\partial x}{\partial\xi}\right)^2 + \left(\frac{\partial y}{\partial\xi}\right)^2, \quad g_{22} = \left(\frac{\partial x}{\partial\eta}\right)^2 + \left(\frac{\partial y}{\partial\eta}\right)^2,$$

$$g_{12} = \frac{\partial x}{\partial\xi}\frac{\partial x}{\partial\eta} + \frac{\partial y}{\partial\xi}\frac{\partial y}{\partial\eta}, \quad J = \frac{\partial x}{\partial\xi}\frac{\partial y}{\partial\eta} - \frac{\partial y}{\partial\xi}\frac{\partial x}{\partial\eta},$$

$$M_{\xi\eta}u = \frac{\partial}{\partial\xi}\left(A_1 u\right) + \frac{\partial}{\partial\eta}\left(A_2 u\right),$$

$$A_1 = \frac{\partial x}{\partial t}\frac{\partial y}{\partial\eta} - \frac{\partial y}{\partial t}\frac{\partial x}{\partial\eta}, \quad A_2 = \frac{\partial y}{\partial t}\frac{\partial x}{\partial\xi} - \frac{\partial x}{\partial t}\frac{\partial y}{\partial\xi}.$$

Here g_{11}, g_{12}, g_{22} are the metric coefficients, J is the Jacobian of the inverse transformation $x = x(\xi,\eta,t)$, $y = y(\xi,\eta,t)$.

Normal derivatives are transformed to the following form:

$$\left.\frac{\partial T}{\partial\mathbf{n}}\right|_{\xi=const} = \frac{1}{g_{22}^{1/2}}\left[B_{11}\frac{\partial T}{\partial\xi} + B_{12}\frac{\partial T}{\partial\eta}\right], \tag{3.4}$$

$$\left.\frac{\partial T}{\partial\mathbf{n}}\right|_{\eta=const} = \frac{1}{g_{11}^{1/2}}\left[B_{12}\frac{\partial T}{\partial\xi} + B_{22}\frac{\partial T}{\partial\eta}\right]. \tag{3.5}$$

The velocities of the moving coordinate system are determined from the system of differential equations

$$\left[\frac{\partial x}{\partial t} = -\frac{Q_x}{\rho}\right]_m, \quad \left[\frac{\partial y}{\partial t} = -\frac{Q_y}{\rho}\right]_m, \quad m = s, l, \tag{3.6}$$

where $\mathbf{Q} = (Q_x, Q_y)$ is the mass flow through the coordinate lines.

We rewrite problem (2.1)-(2.7) according to (3.1)-(3.5) and additional system of equations (3.6) and solve it numerically in the rectangular region $\Omega_{\xi\eta}$.

4. Computational Algorithm

The computational algorithm is based on the application of the dynamic adaptation method to the solution of multi-interface Stefan problems with a convection process in a liquid phase. The problem in the new independent variables (ξ,η) is solved in the computational space on a rectangular uniform difference grid making it possible to use classical finite–difference schemes.

The algorithm is divided into two enclosed iteration cycles at each time level.

1. In the first cycle, the velocities of the grid nodes and their positions are determined by the values of the temperatures from the previous iteration [3].
2. In the second cycle the temperature distribution in the domains $\Omega^s(t)$, $\Omega^l(t)$ and flow parameters in $\Omega^l(t)$ are calculated.

For determination of velocities and pressure in a liquid phase the method of incompressible fluid flow computation in an arbitrary region on nonstaggered grids is applied [2]. The second order approximations in the grid nodes and the Douglas-Rachford splitting method are used in the algorithm implementation. The convective difference operator is skew-symmetric and the diffusion difference operator is self-adjoint and positive definite. To eliminate the oscillations of the discrete solution arising on nonstaggered grids the regularization term is added to the incompressibility condition.

5. Numerical Experiment

The proposed algorithm has been applied to simulate the action of high energy fluxes on the square aluminium target 2×1 cm. The source intensivity $G = 10^5$ W/cm^2 has been considered. The first stage of heating occurs without phase transformation $\Omega(t) = \Omega^s(t)$. A liquid phase is introduced when the melting temperature on the irradiated surface is reached. The second stage of computations includes heating with solid-liquid and liquid-vapour transitions. A moving grid is used from this moment (see Fig. 1). The isotherms and stream lines in a liquid phase are given in Fig. 2.

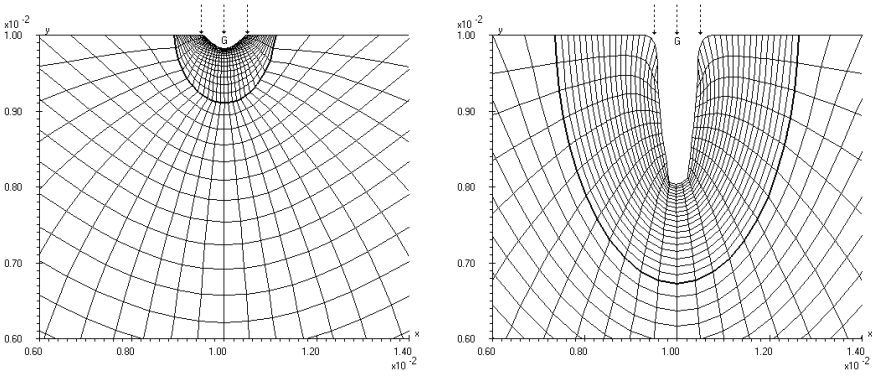
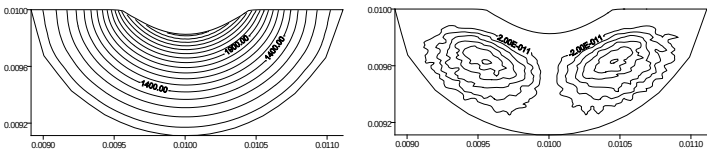
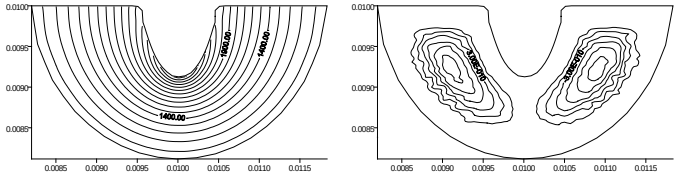


Figure 1. Fragments of moving grid in the physical space.

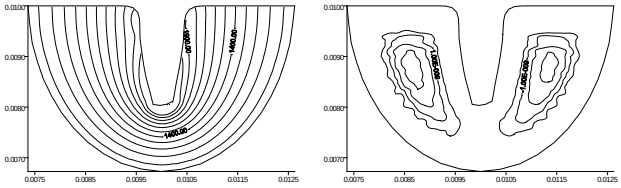
The results of modelling under such conditions show, that the natural convection does not have a significant influence on the shape of interfaces. It might be due to a small volume of a liquid phase together with high velocities of moving interfaces and the absence of thermocapillary effects in the problem formulation.



(a)



(b)



(c)

Figure 2. Isotherms and stream lines in a liquid phase; (a) t=0.0075; (b) t=0.030; (c) t=0.080.

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