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AN ALGORITHM FOR THE NUMERICAL SOLUTION OF THE PROBLEM OF THE SURFACE VAPORIZATION OF A SUBSTANCE BY LASER RADIATION*

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An algorithm is proposed for the numerical solution of the problem of surface vaporization in the case when the Mach number on the boundary of separation is a variable quantity.

1. Introduction

In general, an analysis of the laser vaporization of a substance requires a treatment of the processes in the condensed medium and the kinetics of phase transfer together with the gas-dynamic processes in the flux of the vaporized substance. The crux of the problem lies in the correct formulation of the boundary conditions on the boundary of separation between the phases which also, strictly, model the surface vaporization process. The boundary conditions with a description of the phase transfer kinetics may be correctly formulated, for example, within the framework of surface vaporization with a Knudsen layer /1/, /2/.

There is also another simplified approach to the analysis of vaporization processes. This is the so-called model of vaporization with an isothermal discontinuity /3/, /4/ in which the phase transition is not taken into account explicitly.

It has been proved in /5/, /6/ that the only fundamental difference in the solutions obtained using these models lies in the description of the structure of the vaporization wave but no detailed comparison of the results was carried out. Without such an analysis, it is, for example, difficult to answer the question concerning the applicability of the isothermal discontinuity model in describing vaporization under the conditions which arise close to the surface of a laser plasma. Although it is likely that the approach in /2/, /3/ and its different modifications /7/-/9/ have a definite region of applicability, questions concerning the boundaries of this region for a number of important practical problems remains open.

It is obvious that the numerical solution of the problem is carried out differently depending on the mathematical model which is assumed. The choice of the mathematical model in multidimensional vaporization problems is particularly important.

The principal aim of this paper was to develop a numerical algorithm for solving the surface vaporization problem under conditions where the rate of vaporization may not only be subsonic but may also take negative values. The process involved in the laser vaporization of aluminium under conditions where a plasma is created in the vapours was investigated using the proposed algorithm.

2. Formulation and analysis of the problem.

A mathematical model of surface vaporization, disregarding hydrodynamic processes in the condensed medium, is described by a system of equations consisting of a non-linear heat transfer equation for the condensed medium and the radiation gas-dynamic equations for the vaporized substance. In a Eulerian system of coordinates connected to the motion of the breakdown front, this system of equations has the form

$$\rho_i(T)c_p(T)\left[\frac{\partial T}{\partial t}-v\frac{\partial T}{\partial z}\right]=\frac{\partial}{\partial z}\left[\lambda(T)\frac{\partial T}{\partial z}\right], \tag{1a}$$

$$-h<z<0, \qquad \lambda\frac{\partial T}{\partial z}\Big|_{z=-h}=0,$$

$$\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial z}(\rho u)=0, \qquad \frac{\partial}{\partial t}(u-v_*)+u\frac{\partial u}{\partial z}=-\frac{1}{\rho}\frac{\partial p}{\partial z} \tag{1b}$$

$$\frac{\partial}{\partial t}\left[\varepsilon+\frac{(u-v_*)^2}{2}\right]+u\frac{\partial}{\partial z}\left(\varepsilon+\frac{u^2}{2}\right)= \tag{1c}$$

$$-\frac{1}{\rho}\left[\frac{\partial}{\partial z}(pu)+\frac{\partial W}{\partial z}+\frac{\partial G_\varepsilon}{\partial z}\right],$$

$$\mu\frac{dI_\nu}{dz}+\varkappa_\nu I_\nu=\varkappa_\nu I_{\nu f}, \qquad W=\int_0^\infty d\nu\int_{-1}^{1}\mu I_\nu\,d\mu, \tag{1d}$$

$$\frac{dG^-}{dz}+\varkappa_\nu G^-=0, \qquad \frac{dG^+}{dz}-\varkappa_\nu G^+=0, \tag{1e}$$

$$\varkappa_\nu=\varkappa_\nu(\nu,\rho,T), \qquad p=p(\rho,T), \qquad \varepsilon=\varepsilon(\rho,T),$$

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$$G^-(z_0)=[1+R(T_s)]G\exp\left(-\int_L^0 \varkappa_\nu dz\right), \quad G^+(z_L)=G,$$
$$0<z<L, \quad G_\Sigma=G^++G^-.$$

The notation employed here is as follows: s and 0 denote that a quantity refers to the condensed medium or the gaseous medium respectively; the quantities with the indices SAT and B refer to saturation and boiling regimes; t and z are time and spatial coordinates; v and ρ_l are the velocity and density of the condensed medium; $c_p(T)$ and $\lambda(T)$ are the heat capacity and thermal conductivity; T is the temperature; p, ε, u, and ρ are the pressure, energy, velocity, and density in the gaseous medium; I_ν and W are the spectral intensity and the flux of the characteristic radiation; G is the intensity of the laser radiation; $R(T_s)$ is the reflection coefficient of the laser radiation; L_v is the specific heat of vaporization; $\gamma=5/3$ is the ratio of the specific heat capacities; $M=u_0/u_c$ is the Mach number, and u_c is the velocity of sound.

Boundary conditions. The reverse side of the irradiated plate $z=-h$ was assumed to be thermally isolated: $\lambda\partial T/\partial z=0$. The conditions $p=0, G_\Sigma=G, I_\nu=0$ were specified in the case of the gas dynamic equations and the equation for the transport of radiation from the vacuum side $z=L$.

At the present time two approaches are made use of in specifying the conditions on the boundary of separation between the condensed medium and the gaseous phase. The first approach utilizes the concept of a non-equilibrium Knudsen layer while the second approach makes use of the isothermal discontinuity hypothesis.

The existence of a sharp boundary of separation, which corresponds to a region of strong gas dynamic discontinuity on the surface of which the boundary conditions are written out, surmises that there is widespread surface vaporization of the condensed medium. In this sense, both mathematical models, i.e. the Knudsen layer and the isothermal discontinuity models, are surface vaporization models. In both models, a number of the boundary conditions for the gas dynamic equations and the heat transfer equation on the surface of discontinuity $z=0$ are written out in the form of the laws for the conservation of mass, momentum, and energy:

$$\rho_s v_s=\rho_0 u_0, \qquad P_s+\rho_s v_s^2=p_0+\rho_0 u_0^2, \qquad -\lambda\frac{\partial T}{\partial z}=G_s+W_s-L_v\rho_s v_s. \tag{2}$$

In the model with a Knudsen layer two additional relationships are formulated on this discontinuity. These characterize the kinetics of the phase transition and are simultaneously boundary conditions for the gas-dynamic equations /2/:

$$T_0=T_s\left\{\left[1+f^2\left(\frac{\gamma-1}{\gamma+1}\right)^2 M^2\right]^{1/2}-f\left(\frac{\gamma-1}{\gamma+1}\right)M\right\}^2, \quad f=\left(\frac{\pi\gamma}{8}\right)^{1/2}. \tag{3a}$$

$$\rho_0=\frac{1}{2}\rho_{SAT}\left\{\left(\frac{T_s}{T}\right)^{1/2}\left[(\gamma M^2+1)\exp(b^2M^2)\operatorname{erfc}(bM)-\frac{4f}{\pi}M\right]+\right. \tag{3b}$$
$$\left.\frac{T_s}{T}[1-2fM\exp(b^2M^2)\operatorname{erfc}(bM)]\right\}, \quad b=\left(\frac{\gamma}{2}\right)^{1/2},$$
$$\rho_{SAT}=\frac{p_{SAT}}{RT_s}, \qquad p_0=\rho_0 RT_0, \qquad p_{SAT}=p_s\exp\left[\frac{L_v}{RT_s}\left(1-\frac{T_s}{T_s}\right)\right].$$

In a rigorous treatment it is necessary to solve the kinetic equation in order to obtain these expressions. However, their explicit form is usually obtained subject to certain assumptions concerning the form of the non-equilibrium distribution function in the region of the discontinuity /2/, /2/, /10/, /11/. In the general case the Mach number M in these relationships is an unknown parameter.

In the isothermal discontinuity model /3/, /4/ which was apparently intended for carrying out exploratory calculations under conditions close to equilibrium conditions, the equalities

$$T_s=T_0, \qquad P_s=p_{SAT}(T_s), \qquad u_0\approx u_c, \text{ i.e. } M\approx 1 \tag{4}$$

are written instead of (3).

Let us now briefly analyse the physical meaning of expressions (3) and (4). The existence of a non-equilibrium Knudsen layer is brought about by a reverse flux of particles which return to the surface from the gas phase. The magnitude of this reverse flux is determined by the conditions of gas-dynamic dispersion beyond the limits of the Knudsen layer which can be characterized by one of the gas dynamic parameters such as the number M, for example. On account of this, the parameter M plays a special role in the problem. Its magnitude determines the effect of the gas dynamic factor on the extent by which the vaporization process deviates from equilibrium and, in the final analysis, it determines the magnitude of the two parameters which are the most important in practical applications. These are the amount of vaporized mass m and the back pressure P_s. It is usually assumed that the value of M has an upper limit of $M=1$. A maximum in the non-equilibrium nature of the phase transition, for which a maximum flux of the substance $\rho_0 u_0$ through the boundary of separation and a minimum value of the back pressure $P_s\approx(1+\gamma M^2)p_0$, which constitutes approximately half of the saturated vapour pressure $P_s\approx 0.55p_{SAT}$. are characteristic, corresponds to this value of M. In a state of phase

equilibrium, i.e. when there is no vaporization, $M=0$, $\rho_0 u_0=0$, $T_*=T_0$ and the value of P_* is identical to p_{SAT} and p_0: $P_*=p_{SAT}=p_0$. A very low pressure of the surrounding gas in comparison with p_{SAT} such as, for example, during vaporization into a vacuum is a necessary condition for the realization of a regime with $M=1$. In the case when a laser plasma is created in the vapour, the pressure in the gaseous medium may significantly exceed the pressure p_{SAT}. When this occurs, the value of M falls into the region of values less than 1 and its actual value is unknown.

From a mathematical point of view the value of the parameter M determines the degree of complexity of the description and subsequent solution of the problem. In the extreme case when $M=1$ the description of the vaporization process is substantially simplified since the behaviour of the condensed medium may be treated independently of the dynamics of the vapour. When $M<1$, this separation is not possible and it becomes necessary to solve the problems of the condensed medium and the gas dynamics simultaneously. When this is done, a difficult question arises concerning the method of determining the actual value of M in the boundary conditions.

Strictly speaking, the additional conditions (4), which are used in the isothermal model, only model the case when $M=0$, i.e. a situation when there is no vaporization. One's attention is drawn to the lack of consistency between the first two equalities and the last equality in which it is assumed that $M=1$. The inconsistent nature of expressions (4) manifests itself when there is any deviation in the value of M and 0 and is maximal when $M=1$.

Two models have been employed for the numerical modelling of the surface vaporization of a substance by laser radiation. In /12/-/17/, the vaporization, warming up, and the two-dimensional dispersion of vapour into air at atmospheric pressure were studied numerically. A representation involving a Knudsen layer was used in modelling the vaporization process /1/. At the same time, it was indicated in /13/ and /14/ that the parameters on the boundary of separation should be calculated taking into account the fact that $0\leqslant u_0\leqslant u_*$ if the pressure of the surrounding medium (i.e. air) is comparable with the pressure of the saturated vapour. However, neither of these papers makes any mention of how u_0 is determined in the case when $u_0<u_*$. Moreover, no data are given on how the parameter M behaves in actual calculations.

A representation of vaporization with an isothermal discontinuity on the boundary of separation was employed for the calculations in /5/-/9/ and /18/-/20/. In /5/, /6/, /18/, and /19/, the value of M in the boundary conditions was either assumed to be 1 or the behaviour of M was not discussed at all. A numerical algorithm for solving a non-stationary, spatially two-dimensional vaporization problem is presented in /7/, /8/. This algorithm is based on the breakdown of the discontinuity and enables one to determine the value of M on a boundary with $M\leqslant 1$. This method of determining the boundary conditions has been used in the calculations in /9/ and /20/. There is, however, no information in any of these papers concerning the behaviour of the parameter M. In all of the papers, no qualitative changes were noted on the formation of a plasma apart from the effect of the screening of the laser radiation.

Hence, the behaviour of M on the boundary of separation between the phases in problems where a plasma arises in the vapour has hardly been investigated in practive. At the same time, the importance of taking account of the effect of a plasma on the kinetics of vaporization was noted on a qualitative level in /11/ and /21/. The development of a numerical algorithm which enables one to solve the problem with a previously unknown value of M in the boundary conditions is a problem of top priority in the investigation of vaporization processes with $M<1$.

We will now consider one possible method of constructing such an algorithm.

3. Approximation of the equations.

A finite difference approach, according to which the differential problem is approximated by a difference problem /22/, was used to solve problem (1)-(3). Consideration of the phase transition in the heat transfer problem (1a) leads to the need to solve the Stefan problem which was approximated by a difference scheme of direct calculation without explicitly separating out the phase transition front /23/:

$$\rho_{i,i+1/2}\tilde{c}(T_{i+1/2})\left(\frac{T^{j+1}_{i+1/2}-T^{j}_{i+1/2}}{\tau}-v_*^{j}\frac{T^{j+1}_{i-1/2}-T^{j}_{i+1/2}}{h_i}\right)= \tag{5}$$

$$\frac{1}{h_i}\left(A_iT^{j+1}_{i-1/2}-C_iT^{j+1}_{i+1/2}+B_iT^{j+1}_{i+1/2}\right),$$

$$T_i=\frac{T_{i-1/2}h_i+T_{i+1/2}h_{i-1}}{h_i+h_{i-1}},\qquad C_i=A_i+B_i,$$

$$A_i=\frac{\tilde{\lambda}(T_i)}{h_i},\qquad B_i=\frac{\tilde{\lambda}(T_{i+1})}{h_{i+1}},$$

$$h_i=0.5(h_i+h_{i-1}),\quad h_i=z_{i+1}-z_i,\quad h_1=h_N=0,\quad i=1,\ 2,\ldots,N-1,$$

$$T^{j+1}_{1/2}=T^{j+1}_0,\qquad -\lambda(T_N)\frac{T_{N+1/2}-T_{N-1/2}}{h_N}=G_N+W_N-L_*\rho_{N+1/2}v_{N+1/2};$$

$\tilde{c}(T)$ and $\tilde{\lambda}(T)$ are the smoothed heat capacity and thermal conductivity. The values of A_i, B_i, C_i, $\tilde{c}$, $\tilde{\lambda}$, and G were recalculated at each iteration. The gas dynamic equations were solved using the FLIC finite difference method (see /24/, /25/) which is carried out in two stages.

Stage 1:

$$\tilde{u}_{i+1/2}=u^j_{i+1/2}-\frac{\tau^j}{\rho^j_{i+1/2}}\frac{p^j_{i+1/2}-p^j_{i-1/2}}{2}+\omega^j_{i+1}-\omega_i{}^j, \qquad i=0,1,\ldots,L-1,$$

$$\tilde{u}_{-1/2}=\tilde{u}_0=u_0, \qquad \tilde{u}_{L+1/2}=\tilde{u}_L=0,$$

$$\tilde{\varepsilon}_{i+1/2}=\varepsilon^j_{i+1/2}-\frac{\tau^j}{2\rho^j_{i+1/2}h_i}\left[p^j_{i+1/2}(\tilde{u}_{i+1/2}-\tilde{u}_{i-1/2})+\omega_{i+1}(\tilde{u}_{i+1/2}-\tilde{u}_{i+1/2})+\right.$$

$$\left.\omega_i(\tilde{u}_{i+1/2}+\tilde{u}_{i-1/2})\right], \qquad \bar{u}_{i+1/2}=(u^j_{i+1/2}+\tilde{u}_{i+1/2})/2,$$

$$\omega_i=\begin{cases} Bu_c\dfrac{\rho^j_{i+1/2}+\rho^j_{i-1/2}}{2}\delta u, & \text{if } \dfrac{K}{4}(\delta u)^2<u_c^2 \text{ and } \delta u>0,\\ 0 & \text{otherwise}\end{cases}$$

$$i=0,1,\ldots,L, \qquad B=0.5, \qquad K=0.8, \qquad \delta u=u^j_{i-1/2}-u^j_{i+1/2},$$

$$u_c=\left\{\frac{1}{2}\left[\left(\frac{\partial p}{\partial\rho}\right)_{i-1/2}+\left(\frac{\partial p}{\partial\rho}\right)_{i+1/2}\right]\right\}^{1/2},$$

$$\tilde{E}_{i+1/2}=\tilde{\varepsilon}_{i+1/2}+\tilde{u}^2_{i+1/2}/2, \qquad i=0,1,\ldots,L-1,$$

$$\tilde{E}_{-1/2}=E_0=\varepsilon_0{}^j+\tilde{u}_0{}^2/2, \qquad \tilde{E}_{L+1/2}=E_L=\varepsilon_L{}^j+\tilde{u}_L{}^2/2,$$

E is the total energy and ω is the artificial viscosity.

Stage 2:

$$\Delta M_i=\tau^j\frac{\tilde{u}_{i-1/2}+\tilde{u}_{i+1/2}}{2}\begin{cases}\rho^j_{i-1/2}, & \tilde{u}_{i-1/2}+\tilde{u}_{i+1/2}>0,\\ \rho^j_{i+1/2}, & \tilde{u}_{i-1/2}+\tilde{u}_{i+1/2}\leq 0,\end{cases} \tag{6a}$$

$$\Delta U_i=\tau^j\frac{\tilde{u}_{i-1/2}+\tilde{u}_{i+1/2}}{2}\begin{cases}\rho^j_{i-1/2}\tilde{u}_{i-1/2}, & \tilde{u}_{i-1/2}+\tilde{u}_{i+1/2}>0,\\ \rho^j_{i+1/2}\tilde{u}_{i+1/2}, & \tilde{u}_{i-1/2}+\tilde{u}_{i+1/2}\leq 0,\end{cases} \tag{6b}$$

$$\Delta E_i=\tau^j\frac{\tilde{u}_{i-1/2}+\tilde{u}_{i+1/2}}{2}\begin{cases}\rho^j_{i-1/2}\tilde{E}_{i-1/2}, & \tilde{u}_{i-1/2}+\tilde{u}_{i+1/2}>0,\\ \rho^j_{i+1/2}\tilde{E}_{i+1/2}, & \tilde{u}_{i-1/2}+\tilde{u}_{i+1/2}\leq 0,\end{cases} \tag{6c}$$

$$i=0,1,\ldots,L,$$

$$\rho^{j+1}_{i+1/2}=\rho^j_{i+1/2}-\frac{1}{h_i}(\Delta M_{i+1}-\Delta M_i), \tag{6d}$$

$$u^{j+1}_{i+1/2}=\frac{1}{\rho^{j+1}_{i+1/2}}\left[\rho^j_{i+1/2}\tilde{u}_{i+1/2}-\frac{1}{h_i}(\Delta U_{i+1}-\Delta U_i)\right], \tag{6e}$$

$$E^{j+1}_{i+1/2}=\frac{1}{\rho^{j+1}_{i+1/2}}\left[\rho^j_{i+1/2}\tilde{E}_{i+1/2}-\frac{1}{h_i}(\Delta E_{i+1}-\Delta E_i)\right], \quad i=0,1,\ldots,L-1, \tag{6f}$$

$$\rho^{j+1}_{-1/2}=\rho_0{}^{j+1}=\rho_0{}^j, \qquad \rho^{j+1}_{L+1/2}=\rho_L{}^{j+1}=\rho_L{}^j, \tag{6g}$$

$$u^{j+1}_{-1/2}=u_0{}^{j+1}=u_0{}^j=u_0, \qquad u^{j+1}_{L+1/2}=u_L{}^{j+1}=u_L{}^j=0. \tag{6h}$$

The work due to compressive forces is

$$\left(\frac{dB}{dt}\right)_{i+1/2}=E^{j+1}_{i+1/2}-\frac{1}{2}(u^{j+1}_{i+1/2})^2-\varepsilon^j_{i+1/2}, \qquad i=0,1,\ldots,L-1.$$

In determining the characteristic radiation flux W, use was made of the multigroup quasidiffusion approximation /26/ with difference averaging with respect to frequency /27/:

$$\frac{d}{dz}\varkappa_k\frac{d\Phi_k}{dz}+\frac{\varkappa_k}{D_k}\Phi_k=4\varkappa_k\sigma_kT^4, \tag{7a}$$

$$-l_k\frac{d\Phi_k}{dz}\Big|_{z=0}=\frac{C_{k0}}{D_k}\Phi_k, \qquad -l_k\frac{d\Phi_k}{dz}\Big|_{z=L}=\frac{C_{kL}}{D_k}\Phi_k, \tag{7b}$$

$$\Phi_k=D_kU_k, \qquad l_k=1/\varkappa_k,$$

where k is the number of groups, $\varkappa_k$ is the Planck-averaged group absorption coefficient, C_{k0}, C_{kL}, and D_k are quasidiffusion coefficients which are determined from the relationships

$$C_{k0}=\left[\int_{-1}^{1}I_k(z_0,\mu)\,d\mu\right]^{-1}\int_{-1}^{1}\mu I_k(z_0,\mu)\,d\mu,$$

$$C_{kL}=\left[\int_{-1}^{1}I_k(z_L,\mu)\,d\mu\right]^{-1}\int_{-1}^{1}\mu I_k(z_L,\mu)\,d\mu,$$

$$D_k = \left(\int_{-1}^{1} I_k d\mu\right)^{-1} \int_{-1}^{1} \mu^2 I_k d\mu;$$

and I_k was determined from the solution of the multigroup transport equation

$$\mu \frac{dI_k}{dz} + \varkappa_k I_k = 2\varkappa_k \sigma_k T^4 \tag{8}$$

with the boundary conditions

$$I_k(z_0, \mu) = 0, \quad \mu \geqslant 0, \qquad I_k(z_L, \mu) = 0, \quad \mu < 0.$$

The difference scheme from /28/:

$$I_{ip} = I_{i-1,p} \exp\left(-\varkappa_{i-1/2} \frac{z_i - z_{i-1}}{\mu_p}\right) + \tag{9a}$$
$$\left[1 - \exp\left(-\varkappa_{i-1/2} \frac{z_i - z_{i-1}}{\mu_p}\right)\right] 2\sigma T^4_{i-1/2}, \quad i = 1, 2, \ldots, L, \quad \mu_p \geqslant 0, \quad I_{0p} = 0,$$

$$I_{ip} = I_{i+1,p} \exp\left(-\varkappa_{i+1/2} \frac{z_i - z_{i+1}}{\mu_p}\right) + \tag{9b}$$
$$\left[1 - \exp\left(-\varkappa_{i+1/2} \frac{z_i - z_{i+1}}{\mu_p}\right)\right] 2\sigma T^4_{i+1/2}, \quad i = L-1, \ldots, 1, 0, \quad \mu_p < 0, \quad I_{Lp} = 0,$$

where p is an angular index and the index k is omitted, was used to approximate the multigroup transport Eq. (8).

The system of quasidiffusion equations was approximated by the difference scheme

$$A_i^k \Phi^k_{i-1/2} - C_i^k \Phi^k_{i+1/2} + B_i^k \Phi^k_{i+1/2} - K_i^k \Phi^k_{i+1/2} + F_i^k = 0, \tag{10a}$$

$$\Phi^k_{-1/2} = \Phi_0^k = \alpha^k \Phi^k_{1/2}, \qquad \Phi^k_{L+1/2} = \Phi_L^k = \gamma^k \Phi^k_{L-1/2}, \qquad i = 0, 1, \ldots, L-1, \tag{10b}$$

where

$$A_i^k = 2\frac{h_{i-1} l^k_{i+1/2} + h_i l^k_{i-1/2}}{(h_{i-1} + h_i)^2}, \qquad B_i^k = 2\frac{h_i l^k_{i+1/2} + h_{i+1} l^k_{i+1/2}}{(h_i + h_{i+1})^2}$$

$$C_i^k = A_i^k + B_i^k, \qquad K_i^k = \frac{h_i}{l^k_{i+1/2} D^k_{i+1/2}}, \qquad F_i^k = 4\varkappa^k_{i+1/2} \sigma^k_{i+1/2} T^4_{i+1/2} h_i,$$

$$\alpha^k = \left(\frac{1 - 0.5\varkappa^k_{1/2} h_1 C_0^k}{D^k_{1/2}}\right)^{-1}, \qquad \gamma^k = \left(\frac{1 + 0.5\varkappa^k_{L-1/2} h_{L-1} C_L^k}{D^k_{L-1/2}}\right)^{-1}.$$

In the problem being considered the temperature is determined from the combined solution of the energy equation and the quasidiffusion equations. An implicit difference scheme /29/ was used to approximate these equations which, taking into account the linearization of ε^{j+1} and F^{j+1} was reduced to the form

$$T^{s+1}_{i+1/2} = T^s_{i+1/2} + \frac{1}{\rho^{j+1}_{i+1/2} h_i (\partial\varepsilon/\partial T)^s_{i+1/2}} \left[\rho^{j+1}_{i+1/2} h_i \left(\frac{dB}{dt}\right)^{j+1}_{i+1/2} + \tau^j (G_{g,i+1} - G_{gi}) + \right. \tag{11a}$$
$$\left. \tau^j (A_i \Phi^{s+1}_{i-1/2} - C_i \Phi^{s+1}_{i+1/2} + B_i \Phi^{s+1}_{i+1/2}) - \rho^{j+1}_{i+1/2} h_i (\varepsilon^s_{i+1/2} - \varepsilon^j_{i+1/2}) \right],$$

$$(1 + g_{i+1/2})(A_i \Phi^{s+1}_{i-1/2} - C_i \Phi^{s+1}_{i+1/2} + B_i \Phi^{s+1}_{i+1/2}) - K_i \Phi^{s+1}_{i+1/2} + F_i^s + \tag{11b}$$
$$\left(\frac{\partial F}{\partial T}\right)^s_i \left[\left(\frac{dB}{dt}\right)^{j+1}_{i+1/2} + \varepsilon^j - \varepsilon^s\right] \left[\left(\frac{d\varepsilon}{dT}\right)^s_{i+1/2}\right]^{-1} +$$
$$g_{i+1/2}(G_{g,i+1} - G_{gi}) = 0,$$

$$\Phi_0^{s+1} = \alpha \Phi^{s+1}_{1/2}, \qquad \Phi_L^{s+1} = \gamma \Phi^{s+1}_{L-1/2}. \tag{11c}$$

where

$$A_i = \left(\sum_k \Phi^k_{i-1/2}\right)^{-1} \sum_k A_i^k \Phi^k_{i-1/2}, \ldots, \Phi_{i+1/2} = \sum_k \Phi^k_{i+1/2}, \quad F_i = \sum_k F_i^k,$$

$$\alpha = (\Phi_{1/2})^{-1} \sum_k \alpha^k \Phi^k_{1/2}, \qquad \gamma = (\Phi_{L-1/2})^{-1} \sum_k \gamma^k \Phi^k_{L-1/2}.$$

4. Thermophysical characteristics.

The thermophysical characteristics of aluminium in the solid and liquid state which were used in the calculations are shown in Fig. 1. The solid lines are based on reference data while the broken lines are the result of interpolation between the last known value and the value of the property at the critical temperature $T_{cr} = 8000$ K (see /30/).

The dependences $c_p(T)$, $\lambda(T)$, and $\rho_t(T)$ for aluminium were taken from /31/, /32/. The data from /15/:

$$R(T_s)=\begin{cases}0.769, & T_s<T \text{ melting point},\\ 1-0.64T_s^{0.4}, & T_s\geqslant T \text{ melting point},\end{cases}$$

were used as the reflection coefficient of the laser radiation.

Tabulated data from /32/ were used in the calculations in order to determine the pressure of the saturated vapour $p_{SAT}(T_s)$. The equations of state $p=p(\rho,T)$ and $\varepsilon=\varepsilon(\rho,T)$ were calculated using the technique in /33/. The technique from /34/ was employed in calculating the absorption coefficients $\varkappa_\nu=\varkappa_\nu(\nu,\rho,T)$. The calculations were carried out over a spectral range $h\nu=10^{-2}-80$ eV. The whole range was divided into 9 intervals in each of which Planck-averaging of the coefficient $\varkappa_\nu$ with respect to frequency was carried out.

5. An algorithm for solving the problem.

When relationships (2) and (4), which are characteristic of an isothermal discontinuity, are used as the boundary conditions on the boundary of separation of the phases $z=0$, no difficulties arise. The problems for the condensed medium and the gaseous medium are separated and solved independently. The heat transfer problem (1a), (2) is initially solved on each step in time, the boundary conditions (4) for the gas dynamic equations are then determined and the radiation-gas dynamic problem (1b-e) is solved.

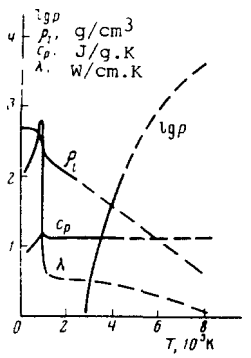

Fig. 1

The algorithm for the solution also cannot be reorganized in the case when the relationships from the Knudsen layer vaporization model (2), (3) are employed as the boundary conditions on $z=0$ if the parameter M in these relationships has a fixed value such as 1 or 0, for example. In this case the heat transfer and radiation-gas dynamic problems are not formally interdependent.

The situation changes radically in the case when the value of M is not fixed, $M<1$ for example. The heat transfer and radiation-gas dynamic problems now turn out to be interdependent and the value of the parameter M in the boundary conditions (3) is unknown and must be determined from the solution of the gas dynamic equations. When this is done, the change in u_0 has an effect on the thermal regime of the surface of the condensed medium, since the efflux velocity of the vapours u_* occurs in the boundary condition for the heat transfer equation via the law of conservation of mass flow $\rho_* v_* = \rho_0 u_0$. The algorithm for the solution which has been described above cannot be used due to the instability of the calculation. A special algorithm, consisting of several embedded iterative loops and organized in a similar manner to that described in /35/, was developed for the numerical solution of vaporization problems in regimes with $M<1$, i.e. $u_0<u_*$. According to this algorithm, the computational process on passing from t^j to t^{j+1} is divided up into several stages.

Algorithm.

Step 1. An inner loop, consisting of relationships (3) and (4) and the gas dynamic Eqs. (1b) is executed. The quantities ρ_0^l, T_0^l, and u_0^l and thereby M^l, where l is the number of iterations, are determined from (4) and (6) by a simple iterative method using the known values of T_* and ρ_{SAT}.

Step 2. An outer iterative loop, where the Stefan problem (5) is jointly solved with relationships (2) is executed. In this loop the quantities T_*^k, v_*^k, ρ_*^k, where k is the number of iterations, are determined using the known value of u_0. On each k-th iteration it is necessary to carry out l iterations of the inner loop. The heat transfer difference Eq. (5) is solved on k iterations by pivotal condensation with iterations /22/.

Step 3. The magnitude of the averaged flux W is determined. In order to do this, the system of difference Eqs. (7), (9) is solved.

Step 4. The value of the temperature in the gaseous medium is determined with the help of an implicit iterative scheme using the known gas-dynamic parameters.

Step 5. In order to increase the accuracy and stability of the calculation, all of the loops which have been considered were united into a common loop which included Eqs. (5)-(11). The number of iterations in this loop was 1-2.

The optimal value of the step size τ was determined by systematic calculations on the basis of which the following method of choosing the integration step size was proposed. The step size remained unchanged if the number of iterations satisfied the conditions $[(5-6)\leqslant k\leqslant(10-12)]\cup[1\leqslant l\leqslant 10]$. If $k<(5-6)$, τ was increased by a factor of 1.1-1.2. If one of the numbers $k, l>(10-12)$, the step size was reduced by a factor of 2. Furthermore, the value of τ had an upper limit set by the Courant parameter $\tau\leqslant\tau_k$.

Let us note the computational features of the proposed algorithm: when $M=1$, the iterative loops converge after a single iteration $k=l=1$, the integration step size increases and is limited solely by considerations of the permissible error; and M deviates from unity ($M<1$), the number of iterations l and k increase, the step size decreases, and $k, l\leqslant 4$ at the optimal value of τ.

6. Analysis of the results of the calculations.

An irregular net, with respect to the spatial coordinate, containing 60 mesh points was used in the calculations: 20 mesh points for the heat transfer equation and 40 mesh points for the gas-dynamic equations. The first five intervals on either side of the boundary of separation $z=0$ were specified with constant step sizes: $h_1=0.2\,\mu$m in the case of the condensed medium and $h_2=25\,\mu$m in the case of the gaseous medium. The following step sizes were increased by a factor of 1.3. The calculations were carried out using the following initial data: $G=5\cdot10^8$ W/cm^2, $\lambda=1.06\,\mu$m, $h=100\,\mu$m, $L=20$ cm, $\rho_1=2.7$ g/cm^3, $T=0.03$ eV, $\rho=10^{-8}$ g/cm^3, $u=v_*=0$.

Numerical modelling using the Knudsen layer vaporization model showed that the back pressure due to the vapour is unimportant at the start of the process during vaporization into a vacuum and when M=1. The formation of a plasma close to the surface brings about a sharp decrease in the parameter M down to the appearance of negative values (see Fig. 2). When this occurs, vaporization takes place in two short intervals of time, where M>0.

The first period of vaporization is due to the laser radiation and finishes when $t\approx16$ n sec as a result of intense absorption of the radiation by the ionized vapours. Vaporization ceases when M=0 in spite of the fact that the temperature of the surface $T_*\approx0.3$ eV is

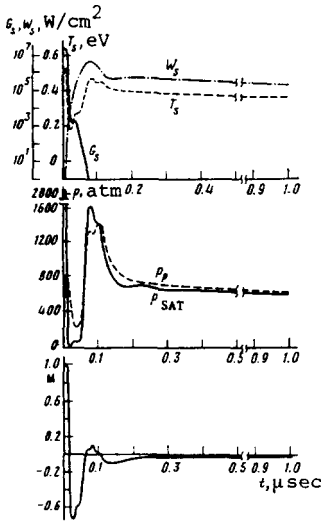

Fig. 2

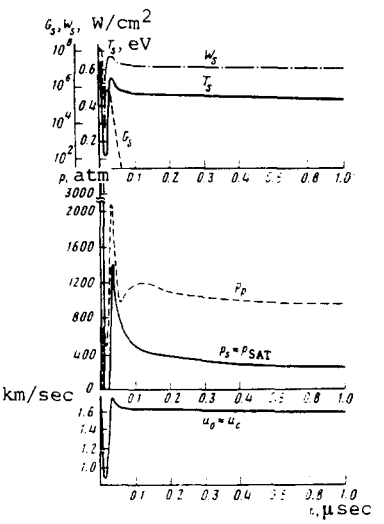

Fig. 3

significantly higher than the temperature at which aluminium boils under normal conditions $T_*=0.24$ eV. The cessation of vaporization is due to the fact that the pressure in the plasma becomes comparable with the pressure of the saturated vapours $p_p\approx p_{SAT}$, i.e. a gas dynamic factor plays a decisive role in this situation. An increase in the pressure in the plasma leads to the inequality $p_p\geqslant p_{SAT}$ and to the occurrence of negative values of M. A change in the initial direction of the gas dynamic flow, which, when M<0, is directed towards the surface of the condensed medium where condensation of the vapour must take place, corresponds to a change in the sign of the parameter M.

Condensation processes are not included in the mathematical model (1)-(3) and it is therefore assumed that the flow from the gaseous medium $\rho_p u_0$ which reaches the surface is completely deposited onto it. For this purpose the quantity $\rho_0 u_0$ in the boundary conditions was replaced by the quantity $\rho_p u_0$, where ρ_p is the density of the substance calculated in the first interval from the surface. The intensive gas dynamic dispersion of the hot vapours leads to their clarification and to an increase in the radiation flux W, which is incident on the surface. An increase in the value of W, leads to an increase in T, and $p_{SAT}(T_*)$. When the inequality $p_{SAT}(T_*)>p_p$ is satisfied, the Mach number again takes positive values, opening up a second period of vaporization $60\leqslant t\leqslant100$ nsec. The appearance of a new portion of cold vapour increases the optical thickness of the medium and attenuates the flux W, which leads to the relationships $p_{SAT}(T_*)<p_p$ and M<0. Under the conditions of a unidimensional formulation of this problem, this situation is maintained up to the end of the input pulse at $t=1$ μsec (Fig. 2). Vaporization ceases, as in the first period, under the action of a gas-dynamic factor. The temperature of the surface in this interval of time is $T_*=0.5-0.4$ eV (Fig. 2).

The calculations which were carried out enable us to note the following features of the vaporization process in the presence of a laser plasma.

1. Vaporization may cease under the influence of a gas dynamic factor which enables us, in particular, to explain the absence of vaporization in the presence of reemission.

2. The vaporization process is of a particularly non-stationary nature.

3. The mathematical model of surface vaporization with a Knudsen layer requires further development. When M<0, the sense of certain interpolation relationships is imparted to the boundary conditions (3). However, their use in the calculations is not completely correct from a physical point of view by virtue of the asymmetry of the vaporization and condensation

processes. The occurrence of negative values $M<0$ needs to be included in the mathematical model describing the condensation kinetics.

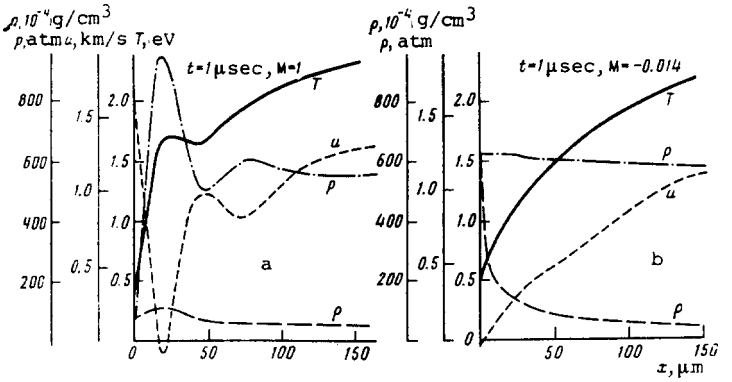

Fig. 4

Calculations using the isothermal discontinuity model in which $M=1$ showed that vaporization takes place over the duration of the whole radiation pulse (Fig. 3) with the exception of a short interval of time when the surface is screened. As a result of this screening, the temperature of the surface T_s falls to 0.1 eV which is significantly below the boiling point of the metal under normal conditions. Resumption of vaporization occurs under the action of the flux of the characteristic plasma radiation W_s. The effect of the gaseous medium is completely excluded when there is a fixed value of M in the boundary conditions. In the final analysis this leads to a contradiction since, after the formation of a laser plasma, the vapour flux, by virtue of the specified boundary conditions, moves from the region with a low pressure into a region where the pressure is several times higher (see Fig. 4a). For comparison, the spatial distributions of the main parameters of the gaseous medium, obtained using the Knudsen layer model, are shown in Fig. 4b.

Hence, the calculations suggest that the vaporization process is characterized by two factors: a temperature factor (the surface temperature T_s) and a gas-dynamic factor (the parameter M). Under certain conditions each of these factors can individually lead to the cessation of the vaporization process which has developed. The fixed value of M in the isothermal discontinuity model leads to a state of affairs where the vaporization is completely controlled by the temperature factor and the effect of the bakc pressure of the gaseous medium is excluded from this treatment. Furthermore, in the isothermal discontinuity model by virtue of the conditions $P_s=p_{SAT}(T_s)$, the temperature factor also completely determines the back pressure P_s which is only true in one case: when $M=0$. In the final analysis this does not enable one to determine quantitatively the true values of m and P_s within the framework of the isothermal discontinuity model. As the calculations showed, rejection of the condition $M=1$ in this model does not completely remove the inadequacies which have been indicated.

A more detailed comparative analysis of this regime of vaporization is presented in /36/.

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