Calculation of the expansion dynamics of evaporated tungsten under the action of a laser pulse

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Abstract. The paper is devoted to the numerical implementation of a model of the dynamics of the tungsten vapors flow evaporating from the sample surface. To calculate the speed and mass flow rate of the substance evaporating from the sample surface, a system of gas dynamics equations is numerically solved. The boundary conditions for the gas velocity and density on the heated surface have a great influence on the solution of the problem. Boundary conditions for temperature are obtained as a result of solving the two-phase Stefan problem in a cross-section of the sample. The aim of the study is to model the erosion of the sample surface and penetration of heat flow into the material.

1. Introduction

Mathematical modeling of evaporation problems is in the focus of research already for a longer period. On the experimental stand Beam of Electrons for materials Test Applications (BETA) created in the INP SB RAS, the results of heating the tungsten plate by the action of a high-speed electron beam on it were obtained [1]. The work is devoted to calculating the gas flow from the sample surface at the beginning of the evaporation process, when the temperature of the heated surface rises to 4000K. The calculation of the gas flow from the sample surface is based on the solution of a system of gas dynamics equations in an axially symmetric formulation. An important component of the problem statement is the statement of adequate boundary conditions for the density and velocity of gas escape on the heated surface. Comparison of the calculation results for different variants of boundary conditions with existing estimates for the dependence of the density and velocity of the escaping gas on the temperature was carried out in [2]. To determine the temperature on the heated surface, the temperature distribution in the sample is calculated based on the solution of the Stefan problem [3]. The position and speed of the phase boundary depends on nonlinear coefficients. The condition at the
free melt-solid boundary consists in the continuity of temperature and discontinuity of the heat flow
due to the absorption or release of a known amount of heat. The known results cannot be used due to
the specificity of the problem statement (temperature and pressure range, spatial and time scale). The
novelty and complexity of solving the problem is mainly due to the need for a correct description of
nonlinear boundary conditions describing the heating and evaporation of the material on its surface.

2. Problem definition
The tungsten plate is heated by a powerful laser pulse. The plate is located in a vacuum. The power
density \( W(r) \) has a radius distribution close to normal (Fig. 1 a). At a temperature above 3000 K,
significant metal evaporation begins (Fig. 1 b).

![Figure 1. Radial distribution of heat flux power (a) and graph of surface temperature dependences of gas density (b)](image)

The temperature on the surface of the heated area in the center of the plate is significantly higher
than at its edges (Fig. 2 a). As shown in [3], the loss of energy for evaporation in the center of the plate
is about 20 % of the energy of pulsed heating. Numerical modeling is necessary to determine the
velocity and density distribution of the outgoing flow of vaporized tungsten. The mathematical model
of gas flow from the sample surface is based on the solution of a system of gas dynamics equations (1):

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \text{div}(\rho \vec{v}) &= 0, \\
\frac{\partial (\rho \vec{v})}{\partial t} + \text{div}(\vec{v}(\rho \vec{v}) + P) &= 0, \\
\frac{\partial (\rho E)}{\partial t} + \text{div}(\vec{v}((\rho E) + P)) &= 0, \\
(\rho T) &= \frac{2 M}{3 R} \left((\rho E) - \rho \vec{v}^2/2\right), \\
\vec{v} &= \frac{(\rho \vec{v})}{\rho}, \quad T = \frac{(\rho T)}{\rho}, \quad P = \frac{R}{M}(\rho T),
\end{align*}
\]

where \( \rho \) is the gas density, \( \vec{v} = (v_r, v_z) \) is the gas velocity, \( P \) is the gas pressure, \( T(r, z, t) \) is the
temperature, \( R = 8.31 \cdot 10^{
-3} \text{W} \cdot \text{m/s} \cdot \text{mol} \cdot \text{K} \) is the gas constant, \( M \) is the molar mass. The ratio for an ideal gas
is chosen as the equation of state.

Dirichlet conditions are set on the heated surface of the sample [2]:

\[
\begin{align*}
\end{align*}
\]
\[ \rho|_v = \frac{1}{2} \left( \frac{R}{M} \right)^{-1} \frac{1}{T|_v} \exp \left( a_1 - a_2 / T|_v \right), \quad v|_v = \frac{5}{3} \sqrt{\frac{R}{M} T|_v}. \]  

where \( T^*(r,t) \) is the temperature on the surface \( \gamma \) obtained from the calculation of Stefan problem [3]. The symmetry boundary conditions are set on the axis and homogeneous Neumann boundary conditions are set on the other borders. The surface temperature has an angle-symmetric distribution (Fig. 2 a) and increases non-linearly over time (Fig. 2 b) in accordance with the power of the heat flux \( W \).

![Figure 2](image)

**Figure 2.** Surface temperature 105 μs (a) and graph of time dependences of surface temperature highest value (b) obtained from calculation for shot 680.

Stefan problem used to calculate the temperature in the tungsten plate surface:

\[
\begin{aligned}
&c(T) \rho^*(T) \dot{\rho} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \lambda(T) \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left( \lambda(T) \frac{\partial T}{\partial z} \right), \\
&(n, \nabla T)|_v = \frac{W(t, r)}{\lambda(T)}, \quad W(t, r) = W_{\text{max}}(t) \cdot \exp(-A \cdot r^2), \\
&(n, \nabla T) = 0 \quad \text{at other boundaries,} \\
&T = T_0 \quad \text{at} \quad t = 0,
\end{aligned}
\]  

where \( T(r, z, t) \) is the temperature, \( c(T) \) is the specific heat, \( \rho^*(T) \) is the density, \( \lambda(T) \) is the thermal conductivity, \( W(t, r) \) is the power of the heat flux on the surface \( \gamma \), \( n \) is the normal to the surface, and \( T_0 \) is the initial temperature. In the experiments on the BETA facility, samples of rolled tungsten were exposed to an axisymmetric electron beam. Electrons with an energy of 80–90 keV heat the material in a layer thin as compared with the characteristic depth of heating of the material. At each time step in the numerical simulation, the variable \( W_{\text{max}}(t) \) is taken from the experimental data file, individual for each experiment. The distribution of the heating power density over the surface was measured using X-ray visualization [4]. The heat absorbed by the surface propagates into the material. A sample has dimensions of 25 mm × 25 mm and typical thickness of 4 mm. Since in such a short time the sample is heated to a depth of several hundred microns, the simulation region was a transverse section of the sample, a region of 12 mm × 3 mm. As for the time, the numerical simulation continued until the moment at which the last measurement of the surface temperature was made.

The phase transitions inherent of the problem under consideration are included in the coefficients of temperature Eq. (3). The density, thermal conductivity, specific heat, and power loss are given as...
dependencies on the temperature of the material in the range of $300K \leq T \leq 8000K$. These functions have discontinuities or lose smoothness at the melting point $T_m = 3695K$. It is necessary to choose the function $\lambda(T)$ at large temperature values such that there is no division by zero. The thermal conductivity and heat capacity of solid tungsten are taken from [5]. The estimates for the thermal conductivity of liquid tungsten are taken from [6, 7].

| Parameter | Typical value | Units |
|-----------|--------------|-------|
| $r_0$     | 10           | mm    |
| $t_0$     | 10           | μs    |
| $v_0$     | 1            | mm/μs |
| $T_0$     | $10^4$       | K     |
| $\rho_0$  | $10^{-9}$    | kg/mm$^3$ |
| $R$       | $8.31 \cdot 10^{-6}$ | mm$^2 \cdot$kg/μs$^2 \cdot$mol·K |
| $M$       | 0.18384      | kg/mol |
| $R/M$     | $0.454 \cdot 10^{-4}$ | mm$^2$/μs$^2 \cdot$K |
| $a_1$     | 26.191       |       |
| $a_2$     | 8.39713      | K     |
| $P_0$     | $10^{-9}$    | kg/mm·μs$^2$ |

3. Numerical simulation

Eq. (1, 3) have a divergent form. We use a uniform rectangular grid on spatial variables $(r_i, z_j)$. Grid analogs of the form:

$$f^n_{ik} = f\left(r_i, z_j, v^n_t, \ldots\right): \rho^n_{ij}, (\rho v^n_r)_{ij}, (\rho v^n_z)_{ij}, (v^n_j)_{ij}, (v^n_t)_{ij}, (\rho E)^n_{ij}, (\rho T)^n_{ij}, P^n_{ij}, T^n_{ij}$$

are compared to the required flow parameters $\rho, \rho \vec{v} = (\rho v_r, \rho v_z), \vec{v} = (v_r, v_z), \rho E, \rho T, P, T$. At the initial time, we assume that the sample is at room temperature in a technical vacuum with the following parameters:

$$P^0_{ij} = 10^{-4}, T^0_{ij} = 0.3, \rho^0_{ij} = \frac{R^0 P^0_{ij}}{M T^0_{ij}}, (\rho E)^0_{ij} = \frac{3}{2} \frac{R^2}{M} P^0_{ij}, (\rho T)^0_{ij} = \frac{R}{M} P^0_{ij},$$

$$(\rho v_r)^0_{ij} = 0, (\rho v_z)^0_{ij} = 0, (v_r)^0_{ij} = 0, (v_z)^0_{ij} = 0.$$

The system of equations of gas dynamics (1) is realized by the finite-difference “coarse particle” method [8]. The method consists of two stages, which are based on splitting by physical processes. At the first Euler stage the gas is considered stationary:

$$\begin{align*}
\frac{\partial \rho}{\partial t} &= 0, \\
\frac{\partial (\rho \vec{v})}{\partial t} + \text{grad} P &= 0, \\
\frac{\partial (\rho E)}{\partial t} + \text{div}(P \vec{v}) &= 0.
\end{align*}$$

The system of Euler stage equations is obtained from the original system of equations, if they omit the divergent terms of the density of mass flows, the component of momentum and total energy. The system of equations (4) describes the process of changing the gas parameters in an arbitrary flow.
region due to the work of pressure forces, as well as due to the potential difference. To write the finite-difference scheme of the Euler stage, one can use the central differences or perform linearization of the Euler stage equations [9] and approximate the derivatives using the pressure and velocity values obtained from the exact solution of the linearized problem.

The system of Lagrangian stage equations contains divergent terms and is responsible for the process of advective transfer of gas-dynamic quantities. At the second Lagrangian stage of the scheme, transfer effects are calculated, taking into account the exchange between cells when they are rebuilt to the previous Euler grid. At each time step, the solution of the continuity, motion, and total energy equations is reduced to a sequential implementation of the Euler and Lagrangian stages. As the initial conditions for the Eulerian phase (4) takes the value functions from the previous time step for the Lagrangian initial condition is the solution of the Euler stage. Over time \( \tau \), the mass flows \( \Delta M^a \) pass through the boundaries of Euler cells, determined by the grid step \( h \). In this case, it is assumed that the entire mass is transferred only due to the normal velocity component to the boundary. At this stage, the unknown values density, momentum, and specific total energy \( f^a_{i,j} = f^a_{i,j} \), \( (\rho v)^a_{i,j} \), \( (\rho E)^a_{i,j} \) are determined as:

\[
f^a_{i,j} h^2 = f^a_{i,j} - \Delta M^a_{i+1/2,j} + \Delta M^a_{i-1/2,j} - \Delta M^a_{i,j+1/2} + \Delta M^a_{i,j-1/2}.
\]

Gas-dynamic values are transferred to two neighboring cells, and some of them remain in the original one. When adding flows, the laws of conservation of mass, energy, momentum, and momentum moments are not violated. A part moved in one of the directions \((r,z)\) of a physical quantity can be written as \( \frac{\Delta v}{\Delta x} \) or \( \frac{\Delta v}{\Delta y} \). The flow in the radial direction is determined by first-order precision:

\[
\Delta M^a_{i+1/2,j} = \begin{cases} 
\frac{f^a_{i,j} (v_r)_{i,j}^n + (v_r)_{i+1,j}^n}{2} \Delta r, & (v_r)_{i,j}^n > 0, \\
\frac{f^a_{i+1,j} (v_r)_{i,j}^n + (v_r)_{i+1,j}^n}{2} \Delta r, & (v_r)_{i,j}^n < 0.
\end{cases}
\]

The axial flow is defined in the same way. Modification of this method allows to accurately describe the expansion of gas into vacuum [9,10]. The gas-dynamic model is verified on a series of Toro analytical tests [11].

To accurately reproduce the flow of vaporized gas, a joint solution of the system of equations (1) and the Stefan problem (3) is necessary. The numerical implementation of Eq. (3) is based on the Douglas-Rachford scheme. Homogeneous Neumann boundary conditions and boundary conditions describing the heating and evaporation of the material are used. The solution of Eq. (3) with variable coefficients is tested on experimental data [3]. Equation (3) can be implemented with a rough time step, since the method used for the solution is unconditionally stable. The system of equations (1) requires a much more detailed grid in both space and time. This is not only due to the use of an explicit schema. Since the mass flow at low temperatures is very small (Fig. 1 b), it is necessary to accurately transmit the density flow from the plate surface during evaporation (2).

4. Simulation results
The isolines in figure 3 show the propagation of the velocity components, temperature, and density of the gas at three points in time in the plane \((r,z)\), where the values of the coordinates \( r \) and \( z \) are given in centimeters. Over time, the temperature of the heated surface increases. As the temperature increases, the density of the gas on the surface increases in accordance with the boundary condition (2). The evaporation of tungsten vapor begins at 2000 K. At a surface temperature of 4000 K, the density of the generated vapors reaches 0.01 kg/m\(^3\). The axial velocity component grows in the high temperature zone (Fig. 3 a). The radial component of the velocity increases over the entire heated area.
surface, but in the high temperature zone it takes its greatest values (Fig. 3 b). The rate of gas departure at the beginning of the evaporation process is approximately 1 mm/μs, which is consistent with the theoretical estimate. The gas departure front has a pronounced spherical shape with a normal distribution of the incident power of the heat flow over the space (Fig. 3 c). As the temperature increases, the shock wave begins to form. The gas temperature smoothly propagates into the vacuum along with the mass of gas (Fig. 3 d).

Figure 3. Isolines of axial velocity (a), radial velocity (b), density (c), temperature (d) at three moments 6.4 μs, 7.04 μs, 7.68 μs obtained from calculation for shot 680.
Experimental data obtained from the use of long-duration laser pulses show that the sample is heated to very high temperatures. For example, shot 680 (Fig. 2 b) has a duration of 125 μs. The surface temperature as a result of this impulse action reaches 8000 K. A higher temperature cannot be reached due to a large loss of energy for evaporation. The share of energy consumed by evaporation raises with the increase of the surface temperature. Since the temperature increases linearly and the evaporation rate increases exponentially, the surface temperature cannot rise above a certain limit.

The gas temperature calculation is necessary for further development of the model by including Maxwell’s equations. For comparison with experimental data, it is necessary to obtain distributions of density and temperature of tungsten vapors at significantly higher temperatures. Electrical resistance can be calculated based on the temperature of tungsten vapors. Unfortunately, it was not possible to perform calculations on a personal computer for long periods of time to reach high temperature 8000 K. For further work, it is necessary to perform calculations on a supercomputer.

5. Conclusion
Calculations have shown that the rate of gas departure at the beginning of the evaporation process is approximately 1 mm/μs, which is consistent with the theoretical estimate. The gas departure front has a pronounced spherical shape with a normal distribution of the incident power of the heat flow over the space. The calculation was performed for temperature growth on the heated surface up to 4000 K. The data obtained do not contradict the ideas about the physics of the process. For comparison with experimental data, it is necessary to obtain distributions of density and temperature of tungsten vapors at significantly higher temperatures. To calculate the temperature increase on the heated surface to 8000 K, it is necessary to perform calculations on a supercomputer. The aim of the study is to model the erosion of the sample surface as a result of evaporation and penetration of heat flow into the material. The calculation of the density and temperature of tungsten vapors over the sample is necessary for modeling the contribution of Lorentz forces to the melt dynamics.

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