Numerical model of evaporation of tungsten in vacuum under high-power transient heating

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Abstract. On the BETA facility, an electron beam is used for simulation of pulsed thermal loads on ITER-relevant tungsten. Numerical experiments are used for verification of the models. This paper presents extension of the model of electron beam heating, supplemented with dynamics of gas evaporation from a heated surface in vacuum.

1. Introduction

One of the most critical problems in the international experimental thermonuclear reactor (ITER project) is the design of the first wall and the divertor plates, e.g. problems of lifetime of materials exposed to high-power plasma streams relevant for fusion reactors with different geometries of magnetic field. The plasma-facing materials shall meet a number of requirements: high resistance to neutron flux, relative cheapness, high thermal conductivity, high heat capacity, high temperature of destruction (spattering, dust formation, melting, sublimation, etc.). For all these reasons, it is planned to use tungsten. Since ITER has not been launched yet, the conditions of the divertor and the first wall cannot be reproduced exactly. On the BETA facility, an electron beam is used for simulation of pulsed thermal loads on tungsten, potentially the most devastating. It was shown in [1] that no vapor shielding occurs for the electron beam, and thus the simulation results can be used to model the effect of runaway electrons, as well as the plasma flow if, for some reason, the vapor shielding does not occur. Modeling of particle formation and motion is also one of the final objectives of the work because even a few particles ejected to the core plasma may lead to severe damage or tritium accumulation by dust, which is also restricted by safety requirements. The full-scale experiment goes in parallel with computational ones. Melting of tungsten under exposure to a pulsed electron beam was modeled numerically, the evaporation process taken into account [2-5]. The calculation is based on the experimental time dependence of the total beam power. The model of the tungsten heating process is based on solving the two-phase Stefan problem; the position of the phase boundary depends on...
nonlinear coefficients. This expansion of the model involves gas dynamics equations to model the dynamics of the gaseous phases of the metal. The paper presents a new model of gas evaporation in vacuum from a heated surface.

2. Problem definition

**Figure 1.** Scheme of computational domain. Tungsten plate (red), evaporation from whose surface occurs in vacuum (blue).

In the experiments on the BETA facility, tungsten samples are exposed to an axisymmetric electron beam [3]. Electrons with an energy of 80–90 keV heat the material in a layer of thickness comparable with the characteristic depth of heating of the material. The power distribution over the surface of the heat flux is

\[ W(t,r) = W_{\text{max}}(t) \cdot \exp(-A \cdot r^2), \quad A = 0.03088523 \text{ mm}^{-2}. \]  

(1)

A typical pulse duration is 100 µs, with a power flux density of several dozen GW m\(^{-2}\).

Consider the following heat equation with surface heating to calculate the temperature in the tungsten plate (Fig. 1):

\[
\begin{cases}
\rho c(T) \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \lambda(T) \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left( \lambda(T) \frac{\partial T}{\partial z} \right), \\
(n, \nabla T)|_{\Gamma} = \frac{W(t,r)}{\lambda(T)}, \\
(n, \nabla T) = 0 \text{ at other boundaries,} \\
T = T_0 \text{ at } t = 0,
\end{cases}
\]

(2)

where \( T(r,z,t) \) is the temperature, \( c(T) \) is the specific heat, \( \rho^*(T) \) is the density of solid tungsten or tungsten melt, \( \lambda(T) \) is the thermal conductivity, \( W(t,r) \) is the power of the heat flux on the surface, \( n \) is the normal to the surface, and \( T_0 \) is the initial temperature.

For the melting process to be taken into account, the enthalpy of the phase transition \( L_m \) was introduced into Eq. (2) [9]:

\[
(c(T)\rho(T) + L_m \delta(T,\varepsilon)) \frac{\partial T}{\partial t} = \text{div}(\lambda(T)\nabla T),
\]

(3)

where the melting point is \( T_m = 3695 \) K,

\[
\delta(T,\varepsilon) = \begin{cases} 
\frac{1}{2\varepsilon}, & |T - T_m| \leq \varepsilon, \\
0, & |T - T_m| > \varepsilon,
\end{cases}
\]
with the smoothing interval \([-\varepsilon, \varepsilon]\), \(\varepsilon = 5K\), and the heat of fusion \(L_m = 51.1 \cdot 10^4 \frac{W \mu S}{mm^3}\).

The process of evaporation at the boundary is taken into account via setting the resultant energy flux \(W_{(t,r)} = W(t,r) - N(T_b)\), where \(W(t,r)\) is the power of the heat flux (see (1)), \(N(T_b) = L_v \cdot \frac{dm}{S \cdot dt}\) is the power loss, \(T_b\) is the boundary temperature, \(P(T)\) is the saturated vapor pressure, and \(\frac{1}{S \cdot dt}\) is the mass evaporation rate. The power loss is calculated with the following parameter values:

\[
L_v = 4.482 \cdot 10^{12} \frac{W \mu S}{kg}, \quad \frac{1}{S \cdot dt} = P(T_b) \sqrt{\frac{M}{2\pi RT_b}} = \\
\exp \left(26.19104 - \frac{83971.3K}{T_b} \right) \sqrt{\frac{0.184K}{2\pi 8.314T_b}} \cdot 10^{-12} \frac{kg}{mm^2 \cdot \mu S}.
\]

At each time step in the numerical simulation, the variable \(W_{max}(t)\) 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]. A sample has typical dimensions of 25mm x 25mm and thickness of 4mm. 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 x 4 mm. As for the time, the numerical simulation continued until the moment at which the last measurement of the surface temperature was made.

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 \(T_m = 3695K\). There are no available data on tungsten conductivity at higher temperatures, so results can be inaccurate at high loads. The thermal conductivity and heat capacity of solid tungsten are taken from [6]. The estimates for the thermal conductivity of liquid tungsten are taken from [7,8].

Consider the following gas dynamics equations to calculate the evaporation in vacuum (Fig. 1):

\[
\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial (r \rho v_r)}{\partial r} + \frac{\partial (\rho v_z)}{\partial z} = 0, \\
\frac{\partial (\rho v_r)}{\partial t} + \frac{1}{r} \frac{\partial (r \rho v_r v_r)}{\partial r} + \frac{\partial (v_r \rho v_z)}{\partial z} = \frac{\partial P}{\partial r}, \\
\frac{\partial (\rho v_z)}{\partial t} + \frac{1}{r} \frac{\partial (r \rho v_r v_z)}{\partial r} + \frac{\partial (v_z \rho v_z)}{\partial z} = \frac{\partial P}{\partial z}, \\
\frac{\partial T}{\partial t} + v_r \frac{\partial T}{\partial r} + v_z \frac{\partial T}{\partial z} - \frac{2T}{3} \left[ \frac{1}{r} \frac{\partial (r v_r)}{\partial r} + \frac{\partial v_z}{\partial z} \right] = 0 \\
P = \frac{R}{M} \rho T, \\
T_b = T^*(r), \quad (n, \nabla f) = 0 \quad \text{at other boundaries}, \\
T_{b=0} = T(0), \quad (v_r, v_z)_{b=0} = 0, \quad \rho_{b=0} = 0.
\]
where $\rho$ is the gas density, $\mathbf{v} = (v_r, v_z)$ is the gas velocity, $P$ is the gas pressure, $R = 8.31 \cdot 10^6 \text{W} \cdot \text{mol} \cdot \text{K}$ is the gas constant, $M = 0.183 \text{mol}$ is the molar mass, $T'(r)$ is the temperature on the surface of the plate obtained from the calculation of Eq. (2).

It is not easy to specify satisfactory boundary conditions. In transient heating of evaporated surface, there are at least two different regimes. At the first stage, the temperature rises so fast that any previously evaporated material almost does not affect the flow from the surface. So, the properties of the vapor roughly depend only on the surface temperature. However, the pressure increase falls when the cooling by evaporation becomes substantial. That is, now the internal structure of the velocities and pressures matters (gas properties near the surface depend on the previous history of the vapor flow). At the second stage, the flow near the surface is almost stationary. This simulation will be used in future to investigate different variants of boundary conditions to look for proper behavior at both regimes. The current version of boundary conditions corresponding to the steady state evaporation regime is

$$\frac{\partial v_r}{\partial z} \bigg|_{r} = 0, \frac{\partial \rho}{\partial z} \bigg|_{r} = 0. \quad (6)$$

It is more convenient to proceed in non-dimensional variables, for example, as follows:

$$r^* = \frac{r}{r_0}, \quad \lambda^* = \frac{\lambda}{\lambda_0}, \quad \rho^* = \frac{\rho}{\rho_0}, \quad c^* = \frac{c}{c_0},$$

$$t^* = \frac{\lambda_0}{\rho_0 c_0 r_0^2}, \quad T^* = \frac{T}{T_0}, \quad W^* = \frac{\lambda_0 T_0 W}{r_0}. \quad (7)$$

The numerical values of the parameters are given in Table 1.

| Parameter | Typical value | Units |
|-----------|--------------|-------|
| $r_0$     | $10^{-1}$    | mm    |
| $t_0$     | $10^2$       | $\mu$s|
| $\lambda_0$ | $10^{-1}$ | $W/mm \cdot K$ |
| $\rho_0$ | $10^{-5}$ | $kg/mm^3$ |
| $c_0$     | $10^8$       | $W/\mu s/kg \cdot K$ |
| $T_0$     | $10^3$       | $K$   |
| $W_0$     | $10^3$       | $W/mm^2$ |
| $\rho_0$ | $10$         | $kg/m^3$ |
| $v_0$     | $10^3$       | $m/s$ |

3. Numerical simulation

Eq. (2) has a divergent form. We use a uniform rectangular grid on the spatial variables $(r_i, z_i)$. The numerical implementation is based on the Douglas-Rachford scheme [10]. Homogeneous Neumann boundary conditions and boundary conditions describing the heating and evaporation of the material are used. The solution of Eq. (2) with variable coefficients is tested on experimental data [2].

The system of equations of gas dynamics is solved by the finite-difference method of large particles [11]. The modification of this method enables accurate description of gas expansion into vacuum [12,13]. The gas-dynamic model is verified on a series of Toro analytical tests [14].

4. Simulation results
The boundary conditions used can be considered as a flow without disturbance of density to vacuum. If we assume that temperature changes are slow enough, the pressure disturbance can be neglected. Therefore, if we change our reference system so that the vapor is in rest, the velocity of incoming disturbance caused by the interaction with vacuum cannot exceed the speed of sound. So, the estimations for this model predict the velocity at the surface to be the same as the speed of sound:

$$v_r = \sqrt{\frac{5R}{3M}} \sqrt{T}.$$  \hspace{1cm} (8)

On the other hand, any inertia between the vacuum and surface leads to lower speed at the surface because of the pressure drop spent on acceleration of the existing vapor. In Fig. (2), we see good qualitative agreement between the theory and numerical experiment.

![Figure 2. Estimated (red line) and numerical result (black dots) for gas velocity](image)

This setting of boundary conditions has a problem of almost random density and pressure of vapor. As it was mentioned earlier, satisfactory boundary conditions are to be found later.

5. Conclusion

The mathematical model of heating of tungsten plate exposed to a pulsed electron beam was supplemented with calculation of gas distribution in vacuum. The problem of satisfactory boundary conditions was mentioned. Simulation results with boundary conditions corresponding to steady state evaporation are in good agreement with the theory. Further development of the theory can lean on this implementation of the model.

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