DIRECT STATISTICAL SIMULATION OF THE EVAPORATION INTO A VACUUM FROM AN APERTURE WITH AXIAL SYMMETRY

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We discuss a method of calculating the flux of particles and the distribution of density, velocity, and temperature of a gas in the presence of evaporation from the inner surface of an axisymmetric hole.

When materials are subjected to highly concentrated energy fluxes, apertures (holes) can be formed because of melting and evaporation of the material. When the depth of the hole is larger than its diameter, the rupture of the material deviates significantly from the one-dimensional case. In the case of a thermal mechanism of rupture, the velocity of the moving surface of evaporation is much smaller than the velocity of motion of the vapor in the hole and the resulting gas-dynamical problem is quasisteady and can be considered separately from the problem of heat conduction for the walls of the hole [1].

There is a large number of papers in the literature in which the formation of a hole is studied on the basis of a solution of the heat equation inside a region with moving phase transition boundaries (see [2-6], for example). However, the gas dynamics of the dispersion of the vapor and its effect on the rupturing process of the material (and hence on the spreading of the hole) has not been studied extensively. We note that the calculation of the integral characteristics of crater formation upon electron-beam treatment of materials has been discussed in [7] for intermediate flux densities and has been studied in [8] for relativistic electron beams. The one-dimensional flow of an inviscid vapor, with the condensation of the vapor inside a cylindrical hole and on its walls taken into account, has been considered in [1]. It is often assumed that in the quasi-steady evaporation regime the shape of the hole is approximately a paraboloid of revolution and is constant in time, while the temperature of the evaporating surface can be assumed to be constant (see [2], for example).

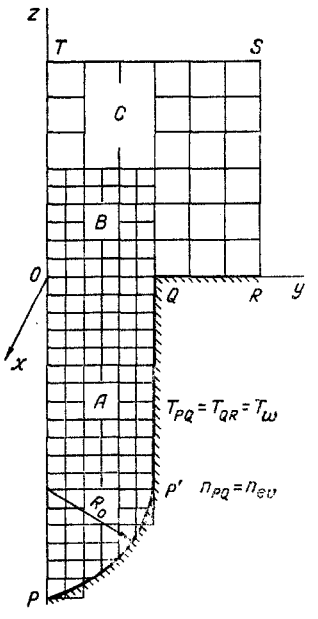

Fig. 1. Aperture region and the layout of the computational grid. The number of cells of the zones A and B along the x and y axes; $N_A \leqslant 15$.

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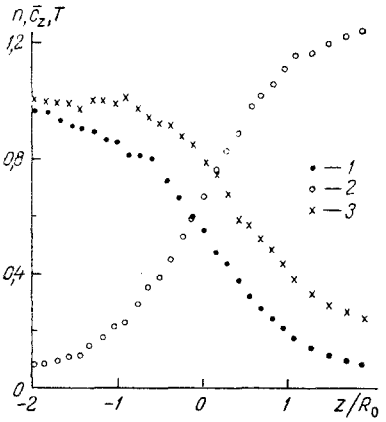

Fig. 2. Variation of the density distribution, z-component of the average velocity, and temperature along the z axis (Kn = 0.2): 1) n; 2) $\bar{c}_z$; 3) T.

In the present paper we solve the steady-state kinetic equation describing the efflux of gas into a vacuum from an axisymmetric hole in the presence of evaporation of material from its inner surface. The aperture region (Fig. 1) is formed by rotating about the z axis the generatrix PQ, consisting of a part of a circle PP' of radius R_0 smoothly joined to the line segment P'Q such that the cross-sectional radius of the hole is also R_0. The temperature along the surface of evaporation is assumed constant and equal to T_w. Motion of the liquid phase is not taken into account, as in [2]. The gas flow is studied by solving numerically the Boltzmann kinetic equation in three-dimensional space:

$$c_x \frac{\partial f}{\partial x} + c_y \frac{\partial f}{\partial y} + c_z \frac{\partial f}{\partial z} = \int (f'f_1' - ff_1)\, g d\sigma dc_1. \tag{1}$$

On the surface of evaporation PQ, a Maxwellian distribution function f^+ is specified for the particles entering the region:

$$f^+_{PQ} = f_{ev}(\mathbf{r}, \mathbf{c}) = n_{ev}\left(\frac{h_w}{\pi}\right)^{3/2} \exp(-h_w c^2),\ \mathbf{c}\cdot\mathbf{n}_{PQ} > 0 \text{ and } r(x, y, z) \in \Gamma_{PQ}, \tag{2}$$

where Γ_{PQ} is the surface of evaporation. The normal vector n_{PQ} is directed inward toward the computational region. All particles incident on the surface PQ are absorbed, which corresponds to an absorption coefficient $\beta = 1$ (this is approximately correct for metals). The density of evaporating particles n_{ev} is given by the saturation curve $n_{ev} = n_{ev}(T_w)$ for the particular material.

On the surface QR we have

$$f^+_{QR} = f_r(\mathbf{r}, \mathbf{c}) = n_r\left(\frac{h_w}{\pi}\right)^{3/2} \exp(-h_w c^2),\ \mathbf{c}\cdot\mathbf{n}_{QR} > 0,\ r(x, y, z) \in \Gamma_{QR}. \tag{3}$$

Thus it is assumed that on the surface QR there is total diffuse reflection of incident particles. We assume that the flux of particles on the surface RS and ST from the vacuum is zero. Then the boundary conditions are

$$f^+_{RS} = f(\mathbf{r}, \mathbf{c}) = 0,\ f^+_{ST} = f(\mathbf{r}, \mathbf{c}) = 0,\ \sqrt{x^2 + y^2 + z^2} \to \infty,\ z > 0,\ \mathbf{n}\cdot\mathbf{c} > 0. \tag{4}$$

Similar boundary conditions at infinity were used in [9] in studying the plane-symmetric problem of the efflux of gas from a straight crack. The problem is assumed to be symmetric with respect to the coordinate surfaces x = 0 and y = 0. It then follows that the entire computational region lies in the first quadrant of the coordinate space.

We chose the following quantities as units of length, density temperature, velocity, and distribution function: R_0, n_{ev}, T_w, $h_w^{-1/2}$, $n_{ev}h^{3/2}$, and so the fundamental parameters of the problem are the Knudsen number $Kn = l_0/R_0$, the number density n_{ev}, the temperature T_w of the surface PQR, the radius of the aperture R_0, and the depth of the hole h. The mean free path l_0 is calculated for saturated vapor in thermal equilibrium with the surface of the hole $l_0 = (\sqrt{2} n_{ev}\sigma)^{-1}$. Here $\sigma = \pi d^2$ is the total collision cross section for a "hard sphere" particle. This model is assumed to represent the interactions between the molecules of the gas. The mean free path can vary from $0.066R_0$ to $50R_0$.

The numerical solution of (1) with the boundary conditions (2) through (4) is obtained using direct statistical simulation. This method is based on a decomposition of the problem

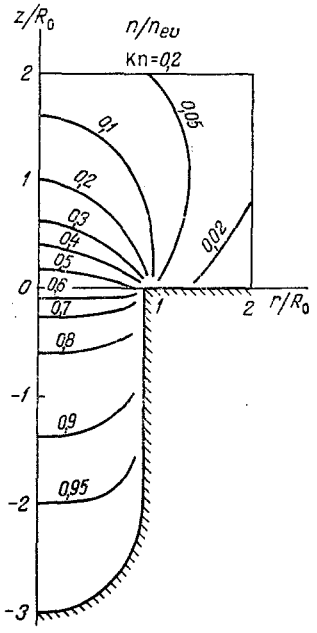

Fig. 3. Equal-density contours inside the hole and in the region above it.

defined by (1) into a succession of simpler problems for each time interval Δt, which is chosen to be sufficiently small. The original idea behind this decomposition was developed by Berd (see [11], for example) in which molecular flow is simulated by following the evolution of a system consisting of several thousand particles, representing the actual gas medium. The method of Berd requires that there be not less than 20-30 particles on average in each cell of the computational grid in order to ensure a physically valid collision frequency [11]. In the present paper we use the Belotserkovskii and Yanitskii modification of the direct statistical simulation method [10], in which the collision of particles is described as a Markov process, thus ensuring a valid collision frequency for a small average number of particles $N_0 \sim 1$. This device significantly widens the possibilities of the method for calculations of two-dimensional and three-dimensional flows.

The Belotserkovskii and Yanitskii scheme for the numerical simulation of a three-dimensional flow can be summarized as follows. The real gas medium is replaced by a set $\{\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, \mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_N\}$ on N coordinates and velocities (representing the particles) which at the initial time are distributed over the cells of the computational grid (see Fig. 1) in correspondence with the initial conditions of the problem. The evolution of the system during the time Δt is split up into two steps.

Step I. Collisions between the particles are followed in each cell assuming that the particle does not leave its own cell during the time Δt. The algorithm consists of the following two-step procedure for each pair of particles $(\mathbf{c}_i, \mathbf{c}_j)$ in a given cell.

(1) The collision of the pair $(\mathbf{c}_i, \mathbf{c}_j)$ occurs with the probability

$$P_{ij} = \frac{\sigma g_{ij}}{\Delta V} \Delta t,$$

where ΔV is the cell volume, and $g_{ij} = |\mathbf{c}_i - \mathbf{c}_j|$.

(2) If a collision takes place the velocities of the particles $(\mathbf{c}_i, \mathbf{c}_j)$ are changed into the post-collision velocities $(\mathbf{c}_i', \mathbf{c}_j')$ using the formulas

$$\mathbf{c}_i' = 0{,}5(\mathbf{c}_i + \mathbf{c}_j + g\mathbf{e}),\ \mathbf{c}_j' = 0{,}5(\mathbf{c}_i + \mathbf{c}_j - g\mathbf{e}),$$

where $\mathbf{e}$ is a random unit vector which has a uniform distribution on the surface of a unit sphere.

If a collision does not take place, the velocities $\mathbf{c}_i$ and $\mathbf{c}_j$ remain unchanged.

Step II. The collisionless displacement (free dispersion) of all particles during the time Δt is followed. The displacement of a given particle is proportional to its velocity. In this step absorption and evaporation of particles on the surfaces are modeled in correspondence with the boundary conditions (2)-(4).

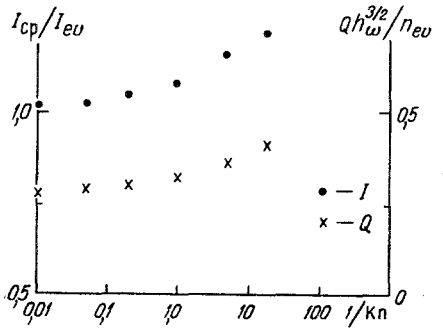

Fig. 4. Dependence of the flux of particles and total energy at the hole outlet on the reciprocal of the Knudsen number.

The macroscopic parameters describing steady flow in the cells are determined by computing the average molecular characteristics for a particular realization of the model process after its transient period. Although macroscopically the problem is axisymmetric, the direct use of axial symmetry (solution in the two-dimensional (r, z) region) in the simulation leads to an artificial density gradient of particles in the radial direction [11] and this decreases the accuracy and efficiency of the simulation. Therefore a three-dimensional quantities were then averaged over all cells whose centers were within a certain interval Δr of the radial coordinate r.

The computational region PQRSTO consists of three zones A, B, and C ($B \subset C$) which are subdivided into cubic cells of volume $\Delta V = \Delta H_\alpha^3$ (α = A, B, or C). In doing this, it is assumed that a given cell belongs to the computational grid if its center lies inside the computational region. In the calculations we took $\Delta H_A = \Delta H_B = (0.2\text{-}0.5)\Delta H_C$. The lengths of the line segments OT and TS forming the outer boundaries of the region C were chosen such that the outflow approximated free-molecular flow in order that the solution inside the computational region be free of perturbations due to insufficient braking of the moacroscopic characteristics of the external flow. In the calculations with holes of different depths h, the total number of cells of the entire region was varied between $2\cdot10^3$ and $1.5\cdot10^4$, and the number of particles was varied from $3\cdot10^3$ to $1.5\cdot10^4$. The total number of particles in the steady regime depends on the rate of evaporation, and therefore is directly related to the density of evaporating particles n_{ev}. Detailed calculations for different values of n_{ev}, in which the average number of particles N_0 per cell was varied from 0.5 to 5, support the stability of the results obtained from the Belotserkovskii—Yanitskii scheme; this agrees with the theoretical conclusions (see the addendum to [11] by Yanistkii). This means that the calculations can be performed using a minimum number $N_0 \sim 1$ of particles per cell. In this way, the execution time for the most time-consuming runs was 8-10 h on a computer of the type ES-1055 for $N_0 \sim 1$ and 4000-5000 statistical samples in a cell.

Figure 2 shows the results for n, $\bar{c}_z$, and T along the z axis for Kn = 0.2 inside the hole and in the region above it. For $z < -2R_0$ the vapor density is practically the same as the equilibrium value. A qualitatively similar result is obtained for the case of slow evaporation from the inner surface of a cylindrical capillary [12]. We note that when $g/kT_w > 3$ the condition for supersaturation of the vapor holds inside the hole.

The density distribution is shown in Fig. 3. Inside the hole the gas density is higher near the surface than on the axis of the hole. But over the cross section of the hole the radical dependence of n depends on the Knudsen number Kn. For example, for large Kn it is found that n is practically constant, while for small Kn the gas density is larger on the axis than near the surface. The gas temperature is practically constant over the cross section of the hole.

It follows from Fig. 4 that the flux of particles at the outlet of the hole increases fairly slowly with increasing 1/Kn; we have $I_{cp}/I_{ev} \approx 1$ for $0 < 1/Kn < 0.1$. We note that $I_{cp} \sim \sqrt{1/Kn}$ for the slow evaporation from an infinite cylindrical capillary in the limit of small Kn. As for the variation of I_{cp} with the depth of the hole h/R_0, we find that for $h_0/R_0 < 0.5$, $I_{cp} \approx I_{ev}$. In the interval $0.5 \leqslant h/R_0 \leqslant 3$, we note that I_{cp} and Q increase, for $h/R_0 > 3$, I_{cp} and Q are practically constant. The effect of surface irregularities was studied in [13] for the case of a fast evaporation of a gas from a two-dimensional periodic surface.

NOTATION

$f(\mathbf{r}, \mathbf{c})$, velocity distribution of gas molecules; $\mathbf{r} = x, y, z$, position vector in Cartesian coordinates; $\mathbf{c} = c_x, c_y, c_z$, molecular velocity vector; $f' = f(\mathbf{r}, \mathbf{c}')$, $f_1' = f(\mathbf{r}, \mathbf{c}_1')$, distribution function of particles with velocities $\mathbf{c}'$ and $\mathbf{c}_1$ after collisions; n_{ev}, density of saturated vapor at temperature T_w; n_r, density of molecules diffusely reflected from the surface of the material; n, vapor density; $\bar{c}_z$, z-component of the average velocity; $h_w = m/2kT_w$; k, Boltzmann constant; m, molecular mass; d, molecular dmaimeter; q, energy required to evaporate an atom; I_{ev}, flux of particles evaporating from a unit area of the inner surface of the hole; I_{cp} and Q, flux of particles and total energy at the hole outlet, respectively; $g = |\mathbf{c} - \mathbf{c}_1|$, magnitude of the relative velocity of the particles.

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CHARACTERISTICS OF A DESCENDING DISPERSED-ANNULAR FLOW

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Experimental data on the loss of liquid from the surface of a film and the resistance of dispersed-annular flow are presented.

Film heat- and mass-transfer apparatus is widely used in different sectors of the economy. In such apparatus descending flow of a film of liquid and gas often occurs. The most common flow regime in heat exchange equipment at nuclear power plants is a descending, comoving regime. The film apparatus with descending direct flow operate at low pressures ($0.05 < P < 1$ MPa). Under these conditions the velocity of the gas flow, as a rule, exceeds 20 m/sec, as a result of which drops are observed to separate from the surface of the film [1, 2]. The dispersed-annular flow regime is characterized by continuous mass transfer between the film and the core of the flow, intensifying heat transfer and simultaneously increasing the hydraulic losses. Systematic studies of dispersed-annular flows concern primarily small-diameter evaporation channels ($d < 20$ mm) with insignificant fluid flow rates in thin films ($Re_1 < 3000$) and ascending motion of the mixture [3-5].

We therefore pose the problem of studying experimentally the characteristics of a descending dispersed-annular flow in pipes 30 mm in diameter under conditions characteristic

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