
SOLUTION TO PROBLEM OF STRONG EVAPORATION OF A MONATOMIC GAS BY THE MONTE CARLO METHOD

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The Monte Carlo method has been used to obtain a numerical solution to the problem of strong evaporation of a monatomic gas in which the molecules are modeled by pseudo-Maxwellian and hard spheres. A comparison with the results of other authors is made. The results agree well with the solution of the problem obtained on the basis of the model Bhatnagar-Gross-Krook kinetic equation.

1. The aim of the present work is to solve the problem of strong evaporation of a monatomic gas on the basis of Boltzmann's equation. The problems associated with the formulation of the problem have been considered in [1-8], and we therefore give the formulation of the mathematical problem as it applies to Boltzmann's equation.

It is necessary to solve the time-independent Boltzmann equation (1.1) in a semi-infinite space over an evaporating surface with the boundary condition (1.2) on the surface and the boundary condition (1.3) on the outer edge of the Knudsen layer:

\[
\frac{df}{dx} = \int (f'f-f) gb db de \delta \lambda = J(f,f); \quad \delta = |v_1-v|
\]

\[
f(x=0, v_0>0) = (n_e n_r + n_r) / h_w \exp(-h_w v^2)
\]

\[
f(x=\infty) = n_e / h_w \exp(-h_w [(v_0 - \alpha \omega)^2 + v_0^2 + v_e^2])
\]

Here, \( f \) is the distribution function of the molecules, \( v \) is the velocity of a molecule, \( b \) is the impact parameter, \( \varepsilon \) is the azimuthal angle; \( h_w = m / 2kT_w \), where \( m \) is the mass of a molecule, \( k \) is Boltzmann's constant, \( T_w \) is the temperature of the surface, \( n_{ev} \) is the density of the saturated vapor of the material of the surface at the temperature \( T_w \), \( n_r \) is the density of the reflected molecules, and \( a_w \) is the coefficient of evaporation [9]. The \( x \) axis is along the normal to the surface on the side of the gas.

The surface parameters \( n_{ev}, T_w, \) and \( a_w \) are assumed given. It is necessary to find the hydrodynamic parameters \( n_\infty, T_\infty, \) and \( u_\infty \) on the outer edge of the Knudsen layer as a function of the flow rate of the evaporating material.

In such a formulation, the problem has been considered in a number of studies. Three approaches were used: 1) approximate solution based on approximation of the distribution function [1-4]; 2) numerical solution of the problem, the collision integral \( J(f, f) \) being taken in the Bhatnagar-Gross-Krook form [5-7]; 3) numerical solution of Boltzmann's equation by Bird's method of statistical simulation [10].

In the first approach, one writes down the conservation equations for the mass, momentum, and energy fluxes for control surfaces near the evaporating surface and at...
the outer edge of the Knudsen layer. There are differences here in the choice of the approximating function for the distribution function of the molecules incident on the surface. In [1], this function is taken to be a Maxwellian distribution function with parameters corresponding to the density, velocity, and temperature of the gas at the surface. In [2-3], the approximating function is taken to be the Maxwellian distribution function at the outer edge of the Knudsen layer (1.3) multiplied by some constant, which characterizes the knocking out of molecules moving toward the surface from the outer edge of the Knudsen layer. In [4], the system of moment conservation equations was closed by means of an approximate expression for the change in the entropy of the gas across the Knudsen layer.

The second approach is based on numerical solution of the Bhatnagar–Gross–Krook model kinetic equation with the boundary conditions (1.2)-(1.3). Such an attempt was first made in [5]. However, it was subsequently shown [7] that the employed method of iteration has a slow convergence comparable with the errors of the calculations, which led to incorrect results of the calculations. To obtain correct results, it is necessary either to improve the rate of convergence of the iterative process [7, 11], or to take an initial approximation sufficiently close to the exact solution, as was done in [6], in which the results of the approximate solution of the problem obtained in [4] were taken as initial approximation.

The third approach consists of statistical simulation of the problem (1.1)-(1.3). In [10], this problem was solved numerically by Bird’s method of statistical simulation. For this, a surface in equilibrium with its vapor at temperature $T_0$ was considered. Then the temperature of the surface was abruptly increased to $T_L$ and the development of the flow in time was considered. To calculate the complete picture of the flow for given attachment coefficient $a_w$, two quantities were specified in [10]: $n_0/n_L$ and $eta = \frac{(n_L - n_0)/n_0}{(T_L - T_0)/T_0}$, where $n_0$ and $n_L$ are the vapor densities at the temperatures $T_0$ and $T_L$. A compression wave and a contact discontinuity travel away from the surface, and behind them a region of gas flow develops. The formation of the flow in the Knudsen layer after the compression wave and contact discontinuity have traveled sufficiently far from the evaporating surface was considered in [10]. The calculations established a dependence of the hydrodynamic parameters at the outer edge of the Knudsen layer for given flow rate $m_*$ of the evaporating material on the value of the parameter $\beta$. However, it is known that the problem is a one-parameter problem [5]. The two parameters evidently arise because the restrictions in [10] on the computer memory and the calculation time did not make it possible to follow completely the establishment of the flow in the Knudsen layer.

2. We assume that a monatomic gas consisting of $N$ molecules is between two parallel surfaces with finite separation $L$ between them. The distribution function of the molecules on the lower surface $(x = 0)$ has the form (1.2); on the upper $(x = L)$, the form (1.3). We considered molecules with interaction cross section of the form $\sigma = \sigma_0/g$, corresponding to pseudo-Maxwellian spheres ($\sigma_0 = $ const), and $\sigma = \text{const}$, corresponding to hard-sphere molecules. The velocity of the molecules after collision is determined by

$$v' = 0.5(v + v_n + gn), \quad v_n' = 0.5(v + v_n - gn)$$

where $n$ is a random vector uniformly distributed over the surface of the unit sphere.

The complete space is divided into $M$ strips of width $H = L/M$, within which the gas parameters $n$, $u$, and $T$ are assumed constant, the width $H$ of the strip being assumed less than the mean free path of the molecules. The process is simulated in accordance with the scheme proposed in [12].

The solution of the problem on the basis of the model BGK kinetic equation [7] showed that it is convenient to solve the problem in the inverse formulation, when the parameters $n_*$, $T_*$, $u_*$ are assumed given and the ratios $n_*/n_{ev}$, $T_*/T_{w}$ are found from the conservation laws for the mass and energy fluxes across the Knudsen layer. In the solution by the Monte Carlo method it is convenient to assume that the parameters $n_*$, $T_*$, $u_*$, where $n_*$ is the mean density of the gas, are given. The ratios $n_*/n_*, n_{ev}/n_*, T_*/T_{w}$ are also found from the conservation laws for the mass and energy fluxes written down in the sections $x = 0$ and $x = L$. The mass and energy fluxes are calculated in the process of the numerical simulation on the basis of the number of molecule impacts...