Simulation of a two-dimensional binary gas mixture outflow into vacuum through a thin slit on the basis of direct solution of the Boltzmann kinetic equation

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Abstract. Two-dimensional binary gas mixture outflow from a vessel into vacuum through a thin slit is studied on the basis of direct solution of the Boltzmann kinetic equation. For evaluation of collision integrals in the Boltzmann equation a conservative projection method is used. Numerical simulation of a two-dimensional argon-neon gas mixture outflow from a vessel into vacuum was performed. Graphs of mixture components flow rate dependence on time during the flow formation, as well as fields of molecular density and temperature for steady-state regime, were obtained.

1. Introduction

Rarefied gas flow through a thin orifice is of importance in science and technology [1-4]. For one component gas, the problem has been studied rather well [5, 6]. The case of a gas mixture is examined much less [7]. At the same time gas mixture flows are important for engineering applications [8]. In this paper a two-dimensional binary gas mixture outflow into vacuum through a thin slit is considered.

Three regimes of flow are commonly distinguished with respect to gas rarefaction: free molecular, transitional and hydrodynamic. For free-molecular [9] and hydrodynamic [10] gas flow regimes, the solution to the problem is relatively easy to obtain analytically or by numerical simulation. In the case of transitional regime solving the problem is much more complicated. Gas flow in transitional regime can be studied using model kinetic equations, i.e. simplified Boltzmann equation, or direct simulation Monte Carlo (DSMC) technique [11]. Both of the above approaches have known limitations by applicability and accuracy of simulation. For instance, the uncertainty of model kinetic equations is estimated in [7] of about 5%. The DSMC technique is a powerful tool for solving many practical problems of rarefied gas dynamics. However, it is not so efficient for unsteady flows and flows with small Knudsen numbers. In our work an unsteady process of a gas mixture outflow into vacuum through a thin slit in a transitional regime is considered, which requires the direct solution of the Boltzmann kinetic equation to be obtained. The collision integrals are calculated with the conservative projection method [12, 13]. This method is conservative and ensures the exact equality of the collision integral of the Maxwellian distribution function to zero, and is also not affected by statistical noise that makes it possible to analyze the flow not only in a steady state regime, but during the flow formation.
as well. In addition, the implementation of the conservative projection method is relatively simple, and its computational complexity is quite acceptable for numerical simulation even in case of a binary mixture.

Thus, the aim of this work is to perform numerical simulation of a two dimensional problem of the outflow of a binary gas mixture through a slit into vacuum with good accuracy. Also, a study is made of the unsteady process of the flow formation.

2. Statement of the problem
A gas mixture is contained in a large vessel, which is surrounded by vacuum. The mixture consists of argon and neon gases in equal proportions, \( \frac{n_1}{n} = \frac{n_2}{n} = 0.5 \). The gas is in thermodynamic equilibrium with the temperature \( T_0 = 273\, K \) and a given molecular density \( n_0 = 10^{22}\, m^{-3} \). Molecular distribution functions of both components are Maxwellian by momentum variable. For the convenience of calculations, the vacuum space is modeled also by Maxwellian distributions of components with negligibly small densities. At some initial time, gas mixture outflow through the thin slit begins. The problem is two-dimensional in physical space with symmetry along the straight line traced from the middle of the slit width.

The problem setting scheme is shown in Figure 1. Here LPP1L1 is the vessel with binary gas mixture and PRRP1 is the area of vacuum. Due to symmetry with the axis of symmetry MM', counting is performed only in the upper half-plane of MLRM'. Mirror conditions are set on the axis of symmetry MM'. On the walls PD, LP, LM diffuse boundary conditions are posed, and on PR and RM' – the condition for the absence of gas flowing into the region.

3. Mathematical model
To describe a behavior of a binary gas mixture, we introduce distribution functions for each component: \( f_i(t, r, p) \), \( i = 1, 2 \). Macroscopic quantities describing the state of each component of a mixture are expressed in terms of distribution functions as follows: molecular density

\[
n_i(t, r) = \int f_i, \, d^3p.
\]

average gas velocity

\[
u_i(t, r) = \frac{1}{n_i \, m_i} \int p_i f_i, \, d^3p.
\]

temperature

\[
T_i(t, r) = \frac{1}{3 k_B n_i \, m_i} \int (p_i - m_i \, u_i)^2 f_i, \, d^3p.
\]

The evolution of the distribution functions in time is described by the Boltzmann kinetic equation [14]
\[
\frac{\partial f_i}{\partial t} + \frac{p_i}{m_i} \frac{\partial f_i}{\partial r} = \sum_{j=1,2} I_{ij}, \quad i = 1, 2 \quad (4)
\]

where \( I_{ij}(t, \mathbf{r}, \mathbf{p}) = \int_0^{2\pi} d\varphi \int_0^{b_{ij}} db \int_{t_{ij}}^{t_{i+1}} \int_{p_{ij}}^{p_{i+1,j}} d^3 p_j \left( f_i(t, \mathbf{r}, \mathbf{p}_i) f_j(t, \mathbf{r}, \mathbf{p}_j) - f_i(t, \mathbf{r}, \mathbf{p}_i) f_j(t, \mathbf{r}, \mathbf{p}_j) \right) g \) are the collision integrals written for interaction of the \( i \)-th and \( j \)-th gas components.

In this paper, the Lennard-Jones potential is used as an interaction potential of molecules

\[
U(r) = 4\varepsilon \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \quad (5)
\]

Parameters \( \varepsilon, \sigma \) for each component of the gas mixture are given in [15]. Parameters of the potential for interaction of different molecules are found using the combination relations [16]

\[
\sigma_j = \frac{\sigma_i + \sigma_j}{2}, \quad \varepsilon_j = \sqrt{\varepsilon_i \varepsilon_j} \quad (6)
\]

For convenience, dimensionless variables are used. Let the characteristic parameters \( m_0, \sigma_0, \varepsilon_0 \) be equal to those of argon, \( n_0 = n_1 + n_2 \), and \( T_0 = T_1 = T_2 \) be the initial temperature of the mixture. We define the characteristic velocity, time and mean free path of molecules as follows:

\[
v_0 = \sqrt{\frac{kT_0}{m_0}}, \quad \tau = \frac{\lambda}{v_0}, \quad \lambda = \frac{1}{\sqrt{2\pi n_0 \sigma_0^2 \Omega_1^{(2,2)}}}, \quad (7)
\]

where \( \Omega_1^{(2,2)} = \Omega_2^{(2,2)} \left( \frac{kT_0}{\varepsilon_0} \right) \) (see [15]). Let us make the transition to dimensionless variables using the following scheme: \( f \rightarrow \frac{f}{n_0 (m_0 v_0)^{3}}, \quad t \rightarrow \frac{t}{\tau}, \quad \mathbf{p} \rightarrow \frac{\mathbf{p}}{m_0 v_0}, \quad m \rightarrow \frac{m}{m_0}, \quad \mathbf{r} \rightarrow \frac{\mathbf{r}}{\lambda}, \quad b \rightarrow \frac{b}{\sigma_0}, \quad g \rightarrow \frac{g}{v_0} \). In dimensionless variables, system (4) takes the following form:

\[
\frac{\partial f_i}{\partial t} + \frac{p_i}{m_i} \frac{\partial f_i}{\partial r} = \frac{1}{\sqrt{2\pi \sigma_0^2 \Omega_1^{(2,2)}}} \sum_{j=1,2} I_{ij}, \quad i = 1, 2. \quad (8)
\]

Here \( I_{ij} = \int_0^{2\pi} d\varphi \int_0^{b_{ij}} db \int_{t_{ij}}^{t_{i+1}} \int_{p_{ij}}^{p_{i+1,j}} d^3 p_j \left( f_i(p_i') f_j(p_j') - f_i(p_i) f_j(p_j) \right) g \).

4. Transition from mathematical model to numerical simulation

For the numerical solution of system (8), we use the method of splitting by physical processes [17]. The essence of this method lies in the fact that at each iteration in time, the advection equations are first solved

\[
\frac{\partial f_i}{\partial t} + \frac{p_i}{m_i} \frac{\partial f_i}{\partial r} = 0, \quad i = 1, 2, \quad (9)
\]

and then we substitute the obtained intermediate values as initial conditions for the relaxation equations

\[
\frac{\partial f_i}{\partial t} = \frac{1}{\sqrt{2\pi \sigma_i^2 \Omega_i^{(2,2)}}} \sum_{j=1,2} I_{ij}, \quad i = 1, 2. \quad (10)
\]

For the convenience of solving the advection equations, we apply the method of splitting along spatial directions [18], which allows to reduce the solution of the multidimensional advection equation to the sequential solution of one-dimensional advection equations along the coordinate axes.
The main difficulty for carrying out numerical simulation presents the solution of the relaxation equations (10). The conservative projection method [12, 13] is used to calculate the collision integrals on the right-hand side of (10), the calculation of which is resource-intensive.

To perform numerical simulation, we have developed a simulation environment software that uses the Message Passing Interface (MPI) [19] and OpenMP [20] code parallelization technologies. The use of code parallelization made it possible to speed up the computations up to 100 times.

5. Results
Numerical simulation of argon-neon gas mixture outflow for Knudsen numbers equal to $1.27 \cdot 10^{-1}, 5.99 \cdot 10^{-1}, 1.63, 16.6$ has been carried out. The grid step in momentum space was the same in all experiments and equaled 0.2. The radius of the sphere in momentum space, within which the distribution functions are assumed to be nonzero, was 5.7. A non-uniform grid was used in coordinate space to improve the accuracy of numerical simulations. The spatial grid step in the area of the slit was constant for each specific width of the slit and varied depending on geometry of the problem.

The flow establishing process was studied by analyzing the dependence of the output flow on time. Figure 2 represents time dependence of the output flow rate of gas mixture components for various Knudsen numbers. The flow rate is measured in dimensionless units $J_0 = n_0 \cdot v_0 \cdot \lambda^2$, and time is given in $\tau$.

![Figure 2. Output flow rate of gas mixture components on time,](image)

(a) $Kn = 1.27 \cdot 10^{-1}$, (b) $Kn = 5.99 \cdot 10^{-1}$, (c) $Kn = 1.63$, (d) $Kn = 16.6$.

Figures 3-5 represent distributions of molecular density and temperature of gas mixture components near the slit in a steady-state flow for various flow regimes. It can be seen that all the fields substantially depend on the flow regime.
Figure 3. Molecular density and temperature of gas mixture components near the slit in the steady-state flow, $Kn = 1.27 \cdot 10^{-3}$.

Figure 4. Molecular density and temperature of gas mixture components near the slit in the steady-state flow, $Kn = 1.63$. 
Figure 5. Molecular density and temperature of gas mixture components near the slit in the steady-state flow, $Kn = 16.6$.

6. Conclusion

Two-dimensional binary gas mixture outflow from a vessel into vacuum through a thin slit is studied on the basis of direct solution of the Boltzmann kinetic equation. Numerical simulation of a two-dimensional argon-neon gas mixture outflow from a vessel into vacuum in the transitional regime and also near hydrodynamic and near free-molecular ones was performed. Graphs of the gas mixture components flow rate dependence on time during the flow formation, as well as the fields of molecular density and temperature for the steady-state flow, were obtained. The obtained results may serve as a benchmark problem in rarefied gas dynamics [5].

This work was supported by the Russian Foundation for Basic Research, the Government of Krasnoyarsk krai, and Krasnoyarsk Regional Fund for Supporting Scientific and Technologies Activities project nos. 20-48-242918 “Computer modeling and analysis of gas-dynamic processes in multi-element thermoemission energy conversion systems.”

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