Journal of Applied Mechanics and Technical Physics, Vol. 46, No. 5, pp. 658–663, 2005

DIRECT STATISTICAL SIMULATION OF A SUPERSONIC FLOW OF A BINARY MIXTURE OF RAREFIED GASES AROUND A TRANSVERSELY POSITIONED CYLINDER

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UDC 533.7:532.546

A supersonic flow of a binary mixture of gases in a wide range of rarefaction (from a flow with a Knudsen number Kn = 0.1 *to a free-molecular flow) around a cylinder is studied by means of direct statistical Monte Carlo simulations* (DSMC *method). The influence of a small fraction of heavy particles in a light gas flow on the region of significant nonequilibrium near the cylinder and on the heat flux is considered.*

Key words: *binary mixture, rarefied gas, supersonic flow, flow around a cylinder,* DSMC *simulation.*

The study of a supersonic rarefied gas flow around a cylinder has attracted attention of researchers since 1950s [1, 2]. The possibilities of the numerical solution of this problem have been recently expanded by the development of numerical methods of gas dynamics on one hand and by the evolution of computational engineering on the other hand. The flow around a cylinder was numerically studied by solving the Navier–Stokes equations in [3–5] and the Reynolds equations in [6]. The Variable Soft Sphere (VSS) model was tested in [7] in the case of Direct Statistical Monte Carlo (DSMC) simulations [8] of a nitrogen flow around a cylinder. The solutions obtained by modeling the flow around a cylinder on the basis of the Navier–Stokes equations and by the DSMC method were compared in [9]. The influence of internal degrees of freedom of molecules on the flow field and heat transfer in a hypersonic rarefied gas flow around a cylinder was considered in [10]. A supersonic rarefied gas flow on a transversely positioned infinite cylinder was examined in [11] to study the influence of rarefaction on the flow structure and heat transfer. In particular, this work was initiated by the development of a technique for determining the accommodation coefficient in a supersonic free-molecular flow around a thin-wire probe [12]. Various aspects of only a uniform gas flow around a cylinder were analyzed in these activities.

The effect of vibrational relaxation and chemical reactions on the shock-wave structure for a flow around a cylinder by a mixture of gases whose composition corresponds to the Martian atmosphere was considered in [13] for low Knudsen numbers. The heat transfer between the cylinder and the ambient gas in a wide range of rarefaction values for a binary mixture of gases is studied in the present paper.

Formulation of the Problem and Solution by the DSMC Method. The gas flow impinges on a cylinder of infinite length. The cylinder centerline is perpendicular to the flow direction. A rectangular coordinate system is used: the flow passes along the x axis, the y and z axes are perpendicular to the flow, and the z axis coincides with the cylinder centerline.

It is implied that the plane of the source of an undisturbed supersonic flow is located in the cross section $x = x_1 < 0$, the cylinder centerline passes through the origin of the coordinate system, and a completely absorbing surface is located in the cross section $x = x_e$. The cylinder diameter is d. By virtue of symmetry of the problem, we pass to the following formulation: the plane $y = 0$ is assumed to be specular, and the free-stream boundary conditions are set on the plane $y = y_e$. If a particle returns to the source plane, it is absorbed.

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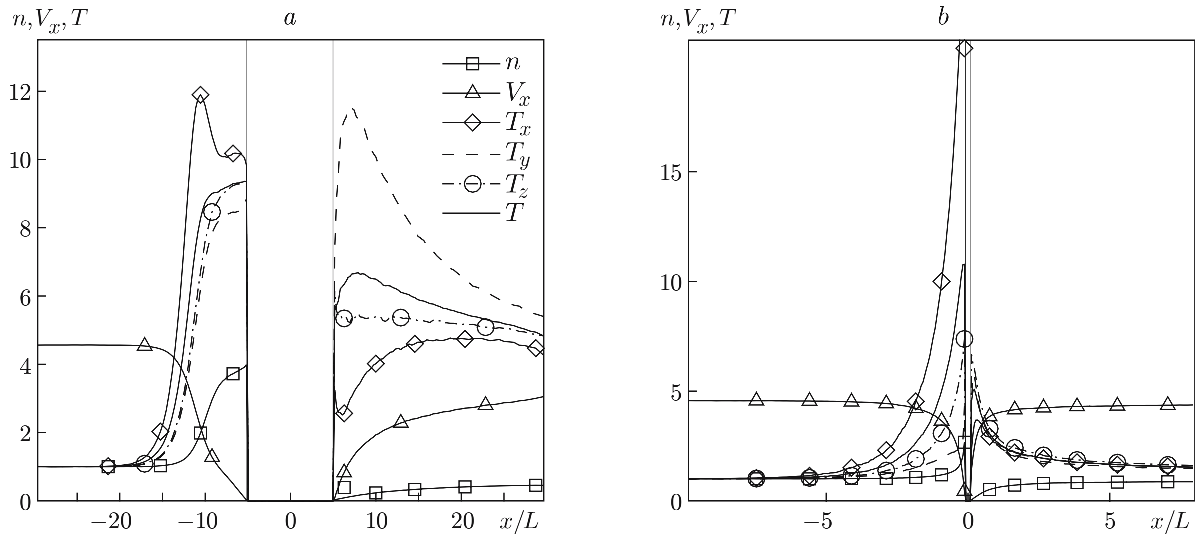

Fig. 1. Distribution of flow macroparameters along the plane of symmetry for a helium flow around a cylinder with $T_w/T_s = 9.33$ and Kn $= 0.1$ (a) and 5 (b).

The following boundary conditions are set for the flow of the gas mixture in the source plane: translational temperature T_s, velocity V_s, and number density n_s. The temperature of the cylinder surface T_w is constant.

Specific features of the flow around a cylinder by a binary mixture of gases with disparate molecular weights were considered. Models of molecules corresponding to helium and xenon (the ratio of molecular weights was 32.78) were used in numerical experiments. The law of interaction of particles with each other involved the VSS model [8] with parameters corresponding to helium and xenon. The interaction of particles with the cylinder surface was described by a diffuse model corresponding to particle reflection at the surface temperature T_w. It was assumed that helium was always reflected from the cylinder surface in a diffuse manner, whereas xenon was absorbed by the cylinder surface with a probability α and was diffusely reflected from the cylinder surface with a probability $1 - \alpha$. In the source plane, helium and xenon were assumed to have identical temperatures and velocities. Their concentration in the mixture is determined by the ratio of their number densities $\theta = n_s^{\rm Xe}/n_s^{\rm He}$. Hereinafter, the superscripts Xe and He refer to parameters for xenon and helium, respectively.

To write the problem in a dimensionless form, we used the following characteristic quantities: the temperature T_s, the density n_s, the most probable thermal velocity of helium particles at the temperature T_s $[c_m = (2kT_s/m^{\rm He})^{1/2}]$, and the mean free path L. The mean free path L was determined from helium macroparameters in the free stream. Rarefaction was characterized by the Knudsen number Kn $= L/d$. As a result, the problem was defined by the following parameters: Mach number $\mathrm{M}_s^{\rm He}$, ratio of temperatures T_w/T_s, Knudsen number Kn, and concentration θ. Obviously, the size of the computational domain (in particular, the positions of the planes $x = x_e$ and $y = y_e$) affects flow formation. Beginning from certain values of x_e and y_e, the flow in the vicinity of the cylinder is almost independent of the computational domain size. These were the distances used in computations. A steady-state solution of the problem was of prime interest.

The following macroparameters of the flow were computed for each component of the mixture: density, Mach number, temperatures (velocities) in the directions along the flow T_x (V_x) and perpendicular to the flow T_y (V_y) and T_z (V_z), mean temperature $T = (T_x + T_y + T_z)/3$, heat flux Q between the gas and the cylinder, and drag coefficient of the cylinder C_x.

Numerical experiments showed that the accuracy of heat-flux computations strongly depends on the grid step, time step, and number of simulated molecules. Therefore, 1 million to 2.5 million of particles were used at each time step to ensure acceptable accuracy. The steady-state solution was constructed on the basis of a large number of timer steps. Several million of particles were actually used in each cell to estimate flow macroparameters for the light component. The accuracy of results was monitored by varying the grid step and the time interval of the DSMC algorithm. The solution was assumed to be "precise" if a further decrease in the grid step and time interval did not lead to changes in computed parameters greater than the statistical error.

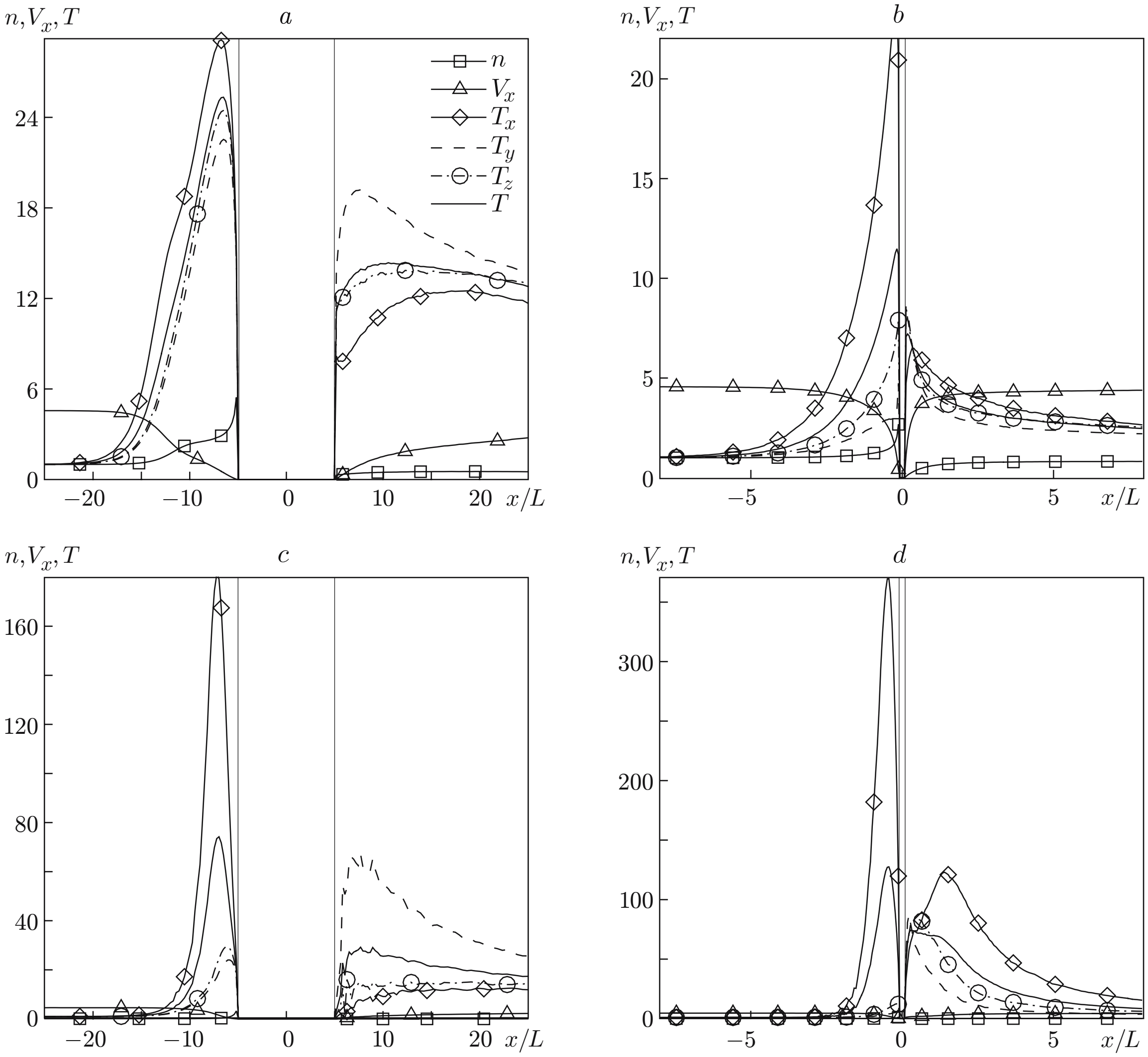

Fig. 2. Distribution of flow macroparameters along the plane of symmetry for a cylinder exposed to a mixture of gases with $\theta = 10\%$, $T_w/T_s = 9.33$, and $\alpha = 0$: the parameters of helium (a and b) and xenon (c and d) are plotted for Kn $= 0.1$ (a and c) and 5 (b and d).

Computation Results. The numerical experiments were performed for the following set of parameters: Kn $\in [0.1, \infty)$, $\theta = 1$, 5, and 10%, $\alpha \in [0, 1]$, the Mach number for helium $\mathrm{M}_s = 5$, and the temperature ratio varied within $T_w/T_s = 6.2$–15.5. The stagnation temperature for helium was $T_0 = 9.33T_s$. The free-stream Mach number for the mixture with concentrations considered was $\mathrm{M} = 5.73$, 7.92, and 9.86.

The pattern observed in a supersonic flow around a cylinder has the following specific features. A disturbed flow region characterized by strong nonequilibrium is formed around the cylinder. The density substantially increases ahead of the cylinder, and a rarefaction zone is observed behind the cylinder. A significant increase in temperature in a certain vicinity of the cylinder is noted. Behind the cylinder, there is a subsonic flow region, which rapidly become supersonic.

To have a more clear idea about the flow in the vicinity of the cylinder, we give the distributions of flow macroparameters (density n, velocity V_x, temperatures in the directions T_x, T_y, and T_z, and mean temperature T) along the plane of symmetry for a helium flow around a cylinder (Fig. 1). The cylinder position is indicated by two vertical lines around the point $x = 0$. In the vicinity of the cylinder, there is a region with significant nonequilibrium characterized by a substantial difference in temperatures in different directions. The greatest increase in temperature T_x is observed in the region ahead of the cylinder. For Kn $= 5$, the behavior of T_x approaches

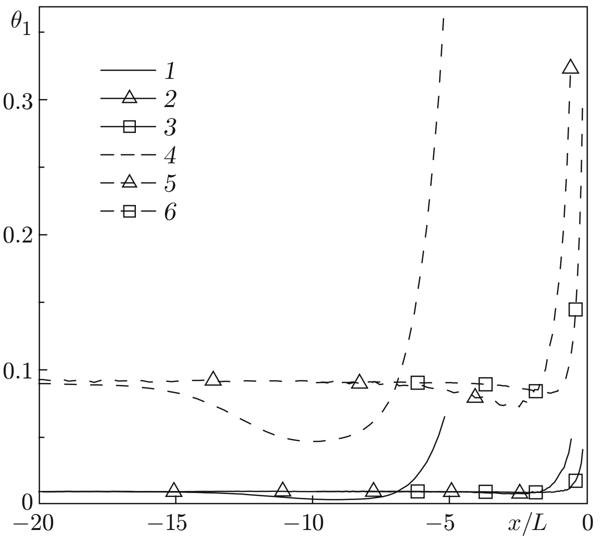

Fig. 3. Distribution of xenon concentration along the plane of symmetry for $\alpha = 0$: the solid and dashed curves refer to $\theta = 1$ and 10%, respectively; Kn $= 0.1$ (1 and 4), 1 (2 and 5), and 5 (3 and 6).

the case of a free-molecular flow. As the Knudsen number decreases, collisions between the incident and reflected molecules lead to a decrease in T_x and to an increase in T_y and T_z. For Kn $= 0.1$, there are two maximums in the distribution of T_x, which can indicate the beginning of formation of a detached shock wave. An increase in density and a decrease in the mean temperature with decreasing Kn are noted. The greatest increase in temperature T_y is observed in the region behind the cylinder, which seems to be related to collisions of particles from almost opposite fluxes directed toward the plane of symmetry. The behavior of T_x in the region behind the cylinder is qualitatively similar to the case of evaporation from the cylinder surface into vacuum [14] and is determined by the behavior of molecules reflected from the cylinder surface. Comparing Figs. 1a and 1b, we can see an increase in the disturbed flow region (in terms of the local mean free paths) with decreasing Knudsen number.

Particular attention in the present work is focused on nonequilibrium processes in the disturbed flow region and their effect on gas–cylinder heat transfer. The numerical experiments conducted in [11] revealed a weak effect of the ratio T_w/T_s on the disturbance region. Simulations for a mixture of gases confirmed this conclusion; hence, the basic computations were performed for $T_w/T_s = 9.33$. The influence of the Knudsen number, concentration of heavy particles in the mixture, and probability of absorption of heavy particles by the cylinder surface is much more significant.

Analyzing the results obtained, we should note that the length of the disturbed flow region determined in terms of helium is greater in the case of a mixture of gases than in pure helium; for xenon, the length of this region is smaller than for helium.

Let us also note some other features of the structure of the disturbed layer in the vicinity of the cylinder:

— the presence of a 1% admixture of heavy particles exerts a weak effect on the helium flow; this effect decreases with increasing Knudsen number;

— the distribution of macroparameters starts to change with increasing concentration of heavy particles, in particular, the temperature and density of helium in the vicinity of the cylinder increase;

— the difference between the flows with $\alpha = 0$ and $\alpha = 1$ decreases with increasing Knudsen number.

To illustrate the changes in the flow pattern for a cylinder exposed to a mixture of gases, the distributions of flow macroparameters along the plane of symmetry for helium and xenon for $\theta = 10\%$ are plotted in Fig. 2. Figure 3 shows the distribution of the concentration $\theta_1 = n^{\mathrm{Xe}}/(n^{\mathrm{He}} + n^{\mathrm{Xe}})$ along the plane of symmetry for $\alpha = 0$ and different values of the Knudsen number. The presence of a minimum in the vicinity of the cylinder surface is explained by a more extended region with elevated density for helium than that for xenon.

Figure 4 shows the heat flux Q as a function of the Knudsen number for xenon and helium. The expected decrease in the heat flux for xenon with decreasing Kn is visible; the value of Q in the case of complete absorption is higher, in particular, because of deceleration of heavy particles on particles reflected from the cylinder surface.

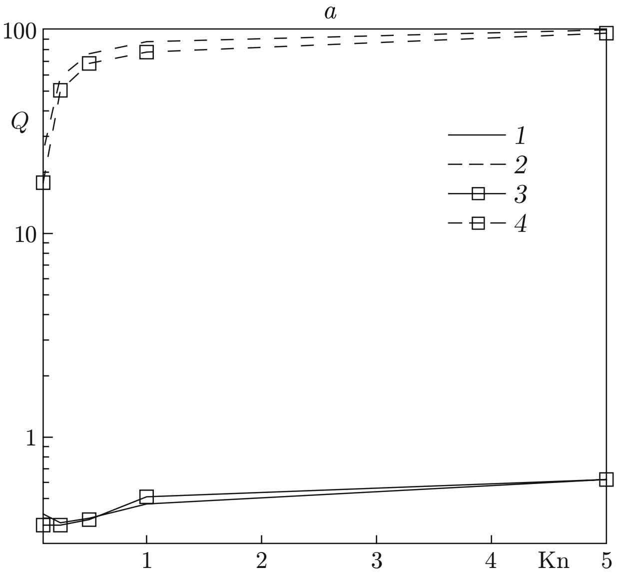

Fig. 4. Heat flux versus the Knudsen number for xenon (dashed curves) and helium (solid curves) for $\theta = 1$ (a) and 10% (b): $\alpha = 1$ (1 and 2) and 0 (3 and 4).

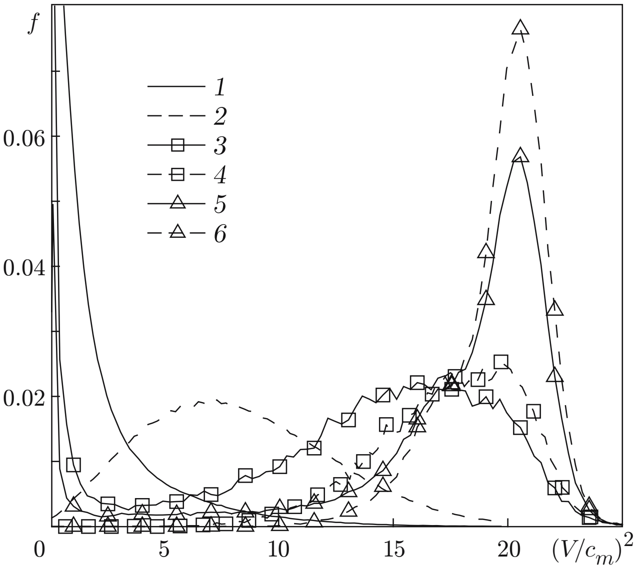

Fig. 5. Distribution function of the squared velocity of xenon atoms interacting with the cylinder surface for $\theta = 10\%$: 1) Kn $= 0.1$ and $\alpha = 0$; 2) Kn $= 0.1$ and $\alpha = 1$; 3) Kn $= 1$ and $\alpha = 0$; 4) Kn $= 1$ and $\alpha = 1$; 5) Kn $= 5$ and $\alpha = 0$; 6) Kn $= 5$ and $\alpha = 1$.

The behavior of the heat flux for helium with different concentrations is qualitatively different: as the Knudsen number decreases, the value of Q^{He} decreases in the case of low concentrations and increases in the case of high concentrations. Apparently, this can be associated with acceleration of helium atoms by heavy particles in the disturbed flow region.

To obtain a more detailed idea about the energy of particles colliding with the frontal part of the cylinder, we plotted the distributions of the squared velocity both for helium and for xenon. Of major interest is the behavior of the distribution function for xenon with decreasing Kn. Figure 5 shows the distribution function for xenon atoms interacting with the cylinder surface for different values of the Knudsen number and values of α. For $\alpha = 0$, the single-peak distribution function with the peak at $V^2 \approx 21$ and $\mathrm{Kn} = 5$ gradually transforms to a double-peak function at $\mathrm{Kn} \approx 1$ and then to an actually single-peak function at $\mathrm{Kn} = 0.1$ with the peak at zero. For $\alpha = 1$, no double-peak distribution function was observed. The double-peak distribution function was not observed for helium either.

Conclusions. In studying a supersonic flow of a gas mixture around a cylinder, versatile gas-dynamic structures and nonequilibrium states of the gas in the disturbed region near the cylinder were found in the range of transitional regimes from the free-molecular to near-continuum flow. The flow under consideration cannot be characterized by macroscopic values of the Mach, Reynolds, and Knudsen numbers and dimensionless concentration. It should involve the longitudinal (along the streamline) and transverse separation of gases with different (normally, non-Maxwellian) velocity distribution functions. This eliminates the mere possibility of using continuum approaches.

Manifestation of nonequilibrium effects, such as a high temperature of the heavy gas in the vicinity of the cylinder surface and an anomalously high energy of collisions of heavy particles with the surface, indicates the expediency of further studies aimed at creating the basis of new technologies for separation of gases, deposition of films, processing of cylindrical surfaces in vacuum, organization of specific chemical processes, and controlling the latter.

This work was supported by the Russian Foundation for Basic Research (Grant No. 03-01-00213), Foundation “Leading Scientific Schools of Russia” (Grant No. NSh-910.2003.1), and Integration Project No. 2 of the Siberian Division of the Russian Academy of Sciences.

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