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TRANSFORMATION OF ENERGY AND COMPOSITION OF GAS MIXTURES IN A COLLISION OF RAREFIED SUPERSONIC FLOWS

A. K. Rebrov and R. V. Maltsev

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Transformation of energy and composition of gas mixtures in a convergent flow from a strip source on a cylindrical surface toward the axis is systematically studied with the use of the direct simulation Monte Carlo method. Information on the influence of gas-flow rarefaction and system geometry on the temperature and concentration of the heavy gas in a dense cloud formed on the axis is obtained. The use of convergent supersonic flows is demonstrated to offer new possibilities for research in the field of physical gas dynamics.

Key words: *supersonic flow, oppositely directed flows, nonequilibrium processes, shock layer, separation, collider, Monte Carlo method.*

Introduction. Thermal effects that occur in interaction of oppositely directed supersonic flows of a mixture of hydrogen H_2 and tetrafluoroethylene C_2F_4 were found and studied in activities aimed at searching for new gas-dynamic schemes of deposition of polytetrafluoroethylene-like films and ultrafine particles [1]. Results obtained by the Monte Carlo method for an approximate model of collisions of C_2F_4–H_2 flows stimulated a systematic study of transformation of energy and composition of binary mixtures of monatomic gases (He–Xe) for which the collision model does not involve a large number of assumptions.

Separation of gases is known to occur in zones with gradients of macroscopic parameters in flows of mixed gas with different molecular weights. In a continuum flow, the thermal effect of separation is rather weak and can be described by continuum equations with the diffusion equation in the one-temperature approximation.

In transitional regimes from the continuum to the free-molecular flow, where the time of translational relaxation becomes commensurable with the characteristic gas-dynamic time, nonequilibrium effects are manifested: slipping of the species, difference in temperature of the species, anisotropy of temperatures, deviations from the Maxwellian distribution of velocities, and deviations from the Boltzmann distribution over the quantum levels. The present paper deals with these regimes.

Modeling Method. The flow analysis is based on the Direct Simulation Monte Carlo method [2], which is a well-recognized tool for computing low-density flows. The macroscopic characteristics of the flow (density, velocity, temperature, etc.) were obtained by averaging the particle states over a large number of time steps after reaching the steady state.

The scheme of radial weights was constructed so that the number of particles decreased at the transport stage and increased at the collision stage. The collisions were computed by the majorant frequency scheme [3] modified to ensure a sufficient number of collisions of particles with different statistical weights. The variable soft sphere model, which is widely used by many researchers, had the following parameters in the present study: $d_{\rm ref} = 2.14$ Å, $\omega = 0.645$, and $\alpha = 1.34$ for the He–He pair; $d_{\rm ref} = 3.06$ Å, $\omega = 0.646$, and $\alpha = 1.29$ for the He–Xe pair, and $d_{\rm ref} = 4.48$ Å, $\omega = 0.744$, and $\alpha = 1.32$ for the Xe–Xe pair ($d_{\rm ref}$ is the particle diameter at a temperature of 750 K,

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Kutateladze Institute of Thermophysics, Siberian Division, Russian Academy of Sciences, Novosibirsk 630090; rebrov@itp.nsc.ru; roman@itp.nsc.ru. Translated from Prikladnaya Mekhanika i Tekhnicheskaya Fizika, Vol. 50, No. 2, pp. 198–204, March–April, 2009. Original article submitted November 24, 2008.

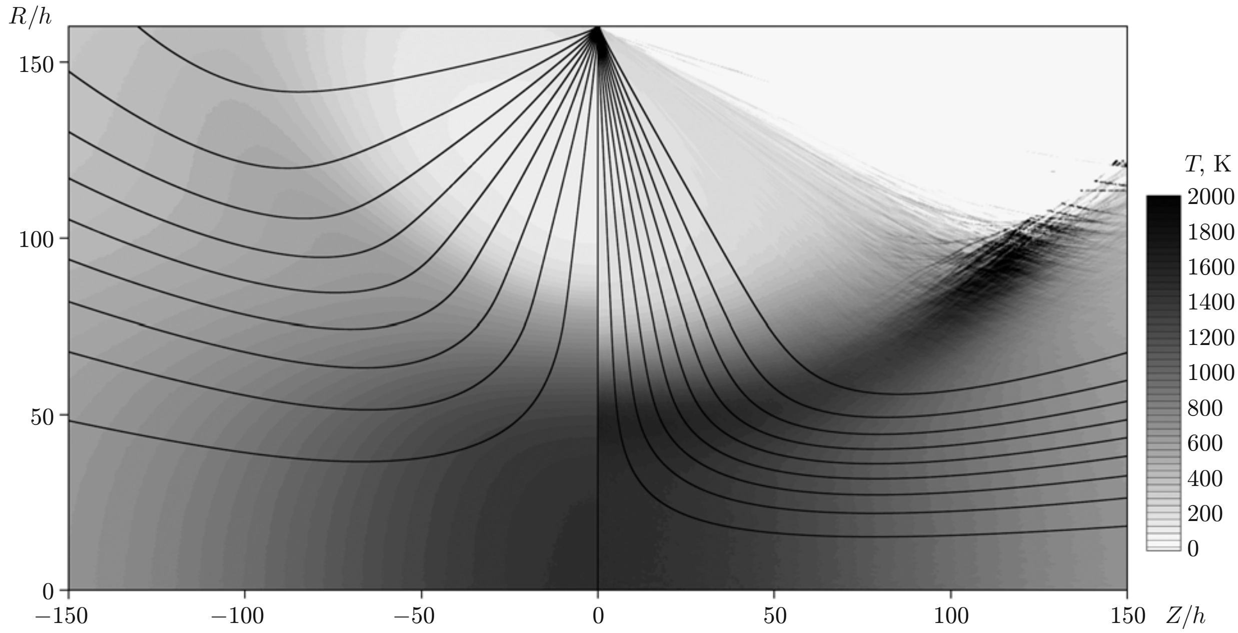

Fig. 1. Streamlines and mean temperature fields in the case of a convergent flow of the mixture of 97.5% He and 2.5% Xe at $\mathrm{Kn}_0 = 0.02$: helium (left) and xenon (right).

ω is the power index in the temperature dependence of viscosity, and α is the factor characterizing the degree of anisotropy of particle scattering over the angles in a collision, which is necessary for balancing the viscosity and diffusion processes).

Analysis of the Convergent Flow Toward the Axis. Apparently, a scheme of an axisymmetric, initially supersonic convergent flow toward the axis with subsequent transition through a subsonic region behind the shock wave and spreading along the axis in the form of two oppositely directed flows was first proposed in [1]. The nonequilibrium flow structure is shown in Fig. 1 (h is the width of the slot on the cylindrical surface and R and Z are the axes of a cylindrical coordinate system). For nonequilibrium flows, the mean temperature is determined via the energy of thermal motion and equals the temperature in the thermodynamic sense under equilibrium conditions.

It should be noted that a dense cloud of the gas in the form of a body of revolution with an oval generatrix, which surrounds the origin of the coordinate system, is an important feature of the flow under study.

Let us compare the computed distributions of parameters in the plane of symmetry of the flow of a mixture containing 97.5% He and 2.5% Xe for the following Knudsen numbers of the flow from the source: $\mathrm{Kn}_0 = 0.002$ and 0.020. The Knudsen number was calculated by the formula

$$\mathrm{Kn}_0 = (\sqrt{2}\, n_0 \sigma_0 h)^{-1},$$

where n_0 is the stagnation density of helium particles and σ_0 is the collision cross section of the carrier gas particles, i.e., He atoms, at a temperature equal to the stagnation temperature. For the case considered, $h = 0.02$ mm, and the slot has a radius of 3.2 mm.

Figure 2 shows the results of flow computations for $\mathrm{Kn}_0 = 0.002$ [V_{He} and V_{Xe} are the velocities of the species, n/n_0 is the density normalized to the stagnation density, T_{He} and T_{Xe} are the mean temperatures of the species, and $\theta = n_{\mathrm{Xe}}/(n_{\mathrm{He}} + n_{\mathrm{Xe}})$ is the relative concentration of xenon]. In this case, the specific features of the flow are the weak nonequilibrium in the course of flow expansion, nonequilibrium in the shock wave, and complete equilibrium in the compressed "layer" (cloud) behind the shock wave. The cloud density on the shock wave increases approximately by a factor of 4.2 and acquires a value close to the classical value at a Mach number $\mathrm{M} = 9$ calculated from the relation between the kinetic and thermal energies of the gas ahead of the shock wave; the temperatures of helium and xenon in the shock wave differ from each other. For the cloud, the Knudsen number Kn_s estimated on the basis of density and thickness of the compressed layer is $7.5 \cdot 10^{-4}$, which is confirmed by the equilibrium state in the compressed layer. By virtue of helium diffusion in the direction away from the plane of symmetry, the

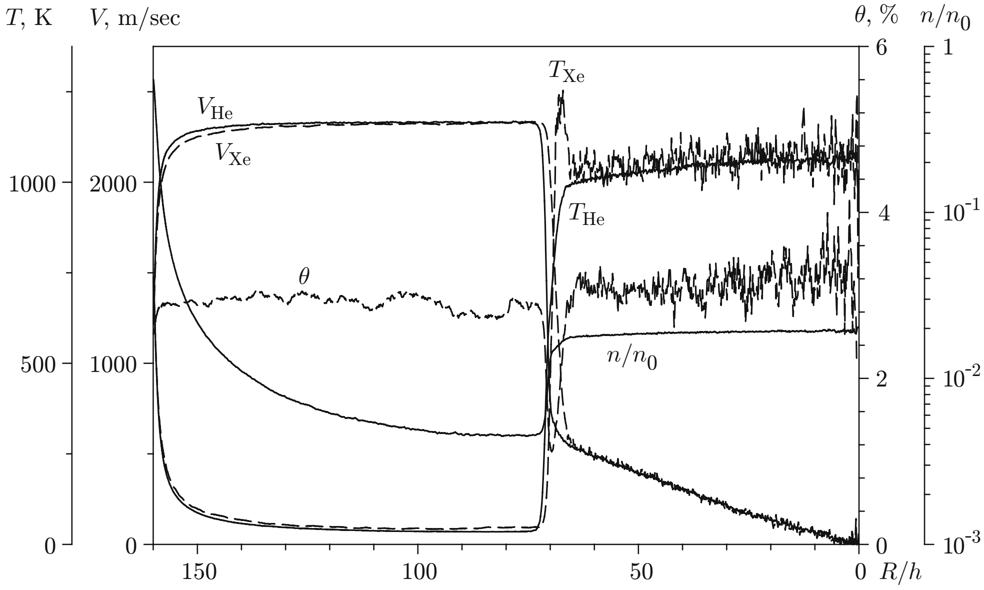

Fig. 2. Radial distribution of flow parameters in the plane of symmetry of the source for $\mathrm{Kn}_0 = 0.002$.

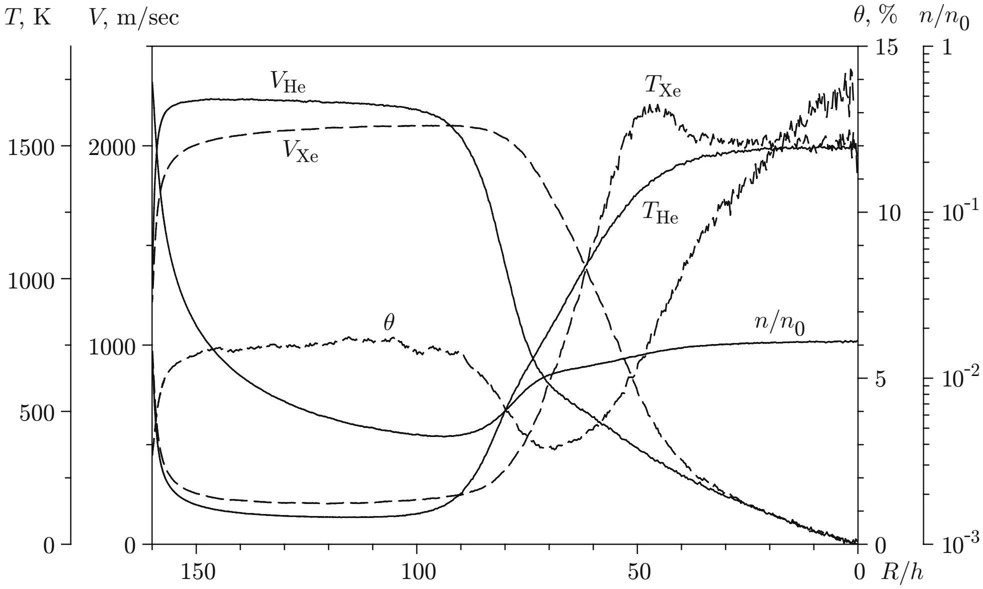

Fig. 3. Radial distributions of flow parameters in the plane of symmetry of the source for $\mathrm{Kn}_0 = 0.02$.

xenon concentration increases from 2.5 to 3.0%. It follows from here that the flow of the mixture of gases with $\mathrm{Kn}_0 = 0.002$ and $R/h = 160$ is practically equilibrium, except for the shock-wave region, and can be described by continuum equations.

For the Knudsen number $\mathrm{Kn}_0 = 0.02$, the flow pattern becomes principally different (Fig. 3). Slipping of the species is observed in the entire radial flow, except for a limited stagnation region near the axis of symmetry: first, helium accelerates xenon, and then, at $R/h < 90$, helium is decelerated on xenon; the temperatures of the species in the flow are considerably different. The xenon concentration increases toward the axis approximately by a factor of 5.6; a hot cloud with a temperature $T \leqslant 1500$ K is formed (the initial stagnation temperature being 1000 K). The classical structure consisting of a shock wave and a compressed layer fails, and a shock layer is formed owing to merging of these elements. The Knudsen number of the compressed layer is $\mathrm{Kn}_s = 0.01$.

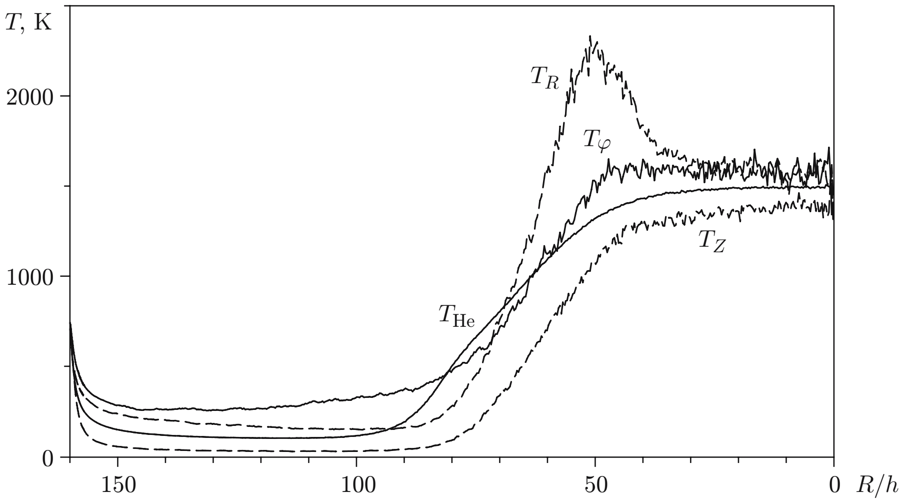

Fig. 4. Temperature anisotropy in the flow for $\mathrm{Kn}_0 = 0.02$.

The tendency of increasing temperature in the shock layer with increasing Knudsen number and a constant value of R/h is inevitable because of changes in the conditions of collisional relaxation in the vicinity of the axis.

The specific feature of the flow under study with $\mathrm{Kn}_0 = 0.02$ and $\mathrm{Kn}_s = 0.01$ is significant three-dimensional temperature anisotropy, which is observed along the flow on its entire path toward the axis. Figure 4 shows the behavior of the mean temperature of helium $T_{\rm He}$, xenon temperature in the radial direction along the central streamline T_R, xenon temperature in the direction parallel to the axis T_Z, and xenon temperature in the direction perpendicular to the radius in the plane of symmetry of the annular source T_φ. Such anisotropy is a typical feature of convergent flows. The temperature T_φ reaches the highest values in the expansion region, the radial temperature T_R has a peak on the shock-layer front, which is typical of shock waves, and the temperature T_Z has the minimum values because of free expansion from the plane of symmetry. We have $T_R > T_\varphi > T_Z$ and $T_\varphi - T_Z > 250$ K ahead of the shock layer. At first glance, this phenomenon (three-dimensional temperature anisotropy in a two-dimensional axisymmetric flow) seems to be unusual. In this case, however, we have a superposition of the transition from an almost plane flow near the source to an axisymmetric flow near the axis. It may be important to take into account the specific features of such flows formed as a result of a "collision" of the flow with the axis for various research activities and applications. It is also important that the gas flows proceed in both directions after the convergent stage is finished, and the heavy gas forms an essentially collimated jet.

Interaction of Oppositely Directed Supersonic Jets of the He–Xe Mixture from Two Convergent Sources. In the case of jet deceleration along the axis from a convergent source, the temperature and concentration of xenon are higher than the corresponding parameters in the convergent source. Figure 5 gives an idea about the collision of such jets where the flow parameters acquire extreme values. Two jets formed by convergent sources with a radius $160h$ at $\mathrm{Kn}_0 = 0.02$ are aligned coaxially, and the distance between the jets is $600h$. The radial coordinate $R/h = 0$ coincides with the axis of the colliding flows, and the line $R/h = 160$ bounds the contour of the computational domain in the supersonic flow. The boundary conditions with complete absorption of the flow on the contour in the supersonic region do not affect the computation results in the domain considered.

Figure 6 shows the axial distribution of flow parameters between the plane of symmetry of the left convergent source and the plane of symmetry of the colliding flows from two convergent sources ($Z/h = 0$ is the plane of symmetry of the convergent source and $Z/h = 300$ is the plane of symmetry of the flow between the sources). Actually, Fig. 6 shows only one half of the flow: axisymmetric jet along the axis. Fan-shaped expansion occurs after the collision, but it is outside the scope of the present work.

It should be noted that the xenon concentration increases by a factor of 13 owing to the collision of the jets at the spreading point. The mean temperature of xenon reaches 2000 K. In the course of shock layer formation, the xenon temperature reaches the maximum value in the subsonic region because of merging of the shock wave with the compressed layer.

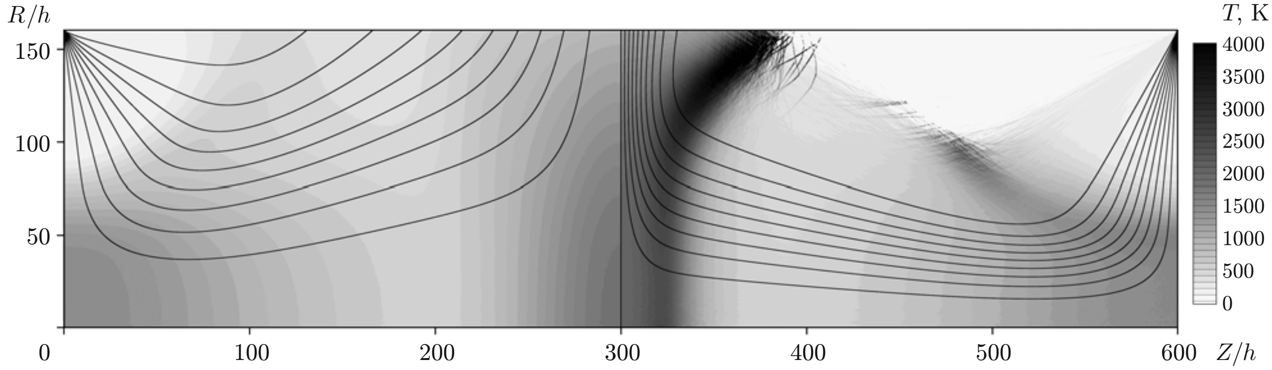

Fig. 5. Streamlines and mean temperature fields computed for the collision of axisymmetric flows of the mixture: helium (left) and xenon (right).

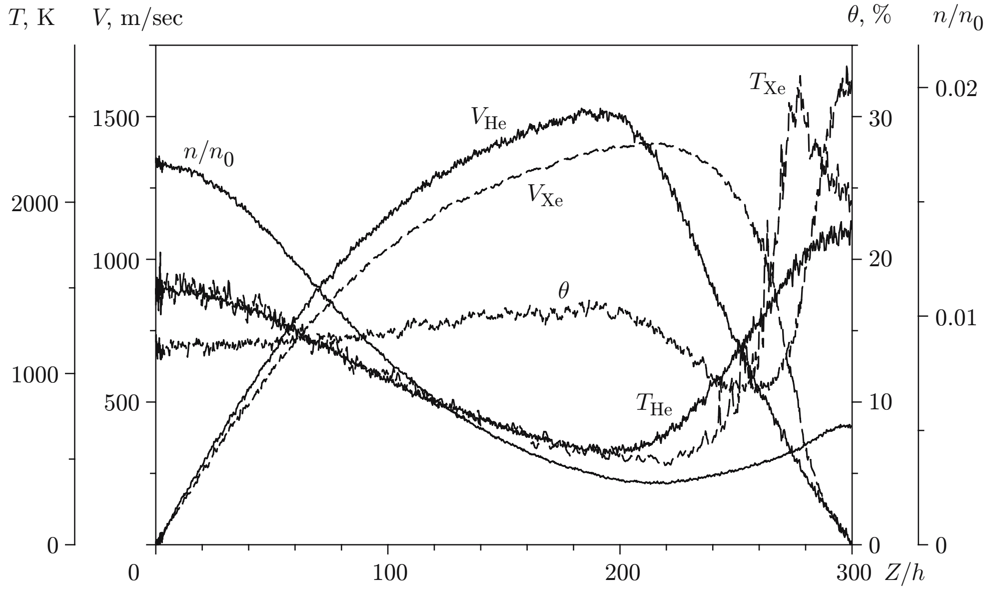

Fig. 6. Variations of axial flow parameters due to the collision of two jets from convergent sources.

Effect of Geometric Parameters on the Flow Structure. An analysis of results computed for equilibrium and nonequilibrium flows from convergent sources revealed the qualitative and quantitative character of the influence of the degree of rarefaction on the distributions of parameters in the plane of symmetry of the source. The effect of geometric parameters, namely, the source diameter D/h cannot be predicted *a priori*.

For a given value of P_0h ($\mathrm{Kn}_0 = 0.01$), which characterizes the degree of rarefaction in the critical cross section, we calculated the maximum values of the flow Mach number and the values of $P_sd_s/(P_0h)$ and d_s/D as functions of D/h (Fig. 7) (P_s is the pressure in the cloud near the axis and d_s is the cloud diameter determined on the basis of the characteristic position of the maximum longitudinal temperature in the shock wave). The quantity P_sd_s is an estimate of the Knudsen (Reynolds) number ahead of gas exhaustion from the cloud in two opposite directions. The ratio $P_sd_s/(P_0h)$ yields a qualitative and a rather informative quantitative estimate of the degree of cloud rarefaction, as compared with the degree of gas rarefaction in the critical cross section. The quantity d_s/D characterizes the cloud size and its position in the cross section coinciding with the plane of symmetry.

At high values of D/h, the quantity P_sd_s is found to reach a horizontal asymptotic line and ceases to depend on D/h; with decreasing D/h, the value of P_sd_s decreases almost monotonically: its value at $D/h = 8$ is 1.5% lower than at $D/h = 100$. The ratio d_s/D reaches an asymptotic line at $D/h \approx 100$, decreasing approximately by 15%. In the examined range of variation of D/h, the Mach number increases in proportion to the logarithm of D/h and

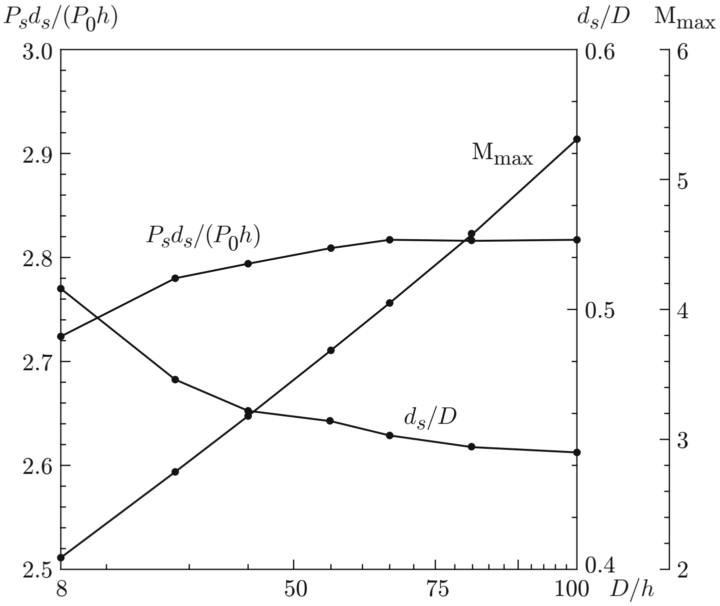

Fig. 7. Cloud diameter d_s/D, degree of rarefaction $P_sd_s/(P_0h)$, and Mach number M ahead of the cloud boundary versus the source diameter D/h.

acquires values from 2.1 to 5.3. It follows from here that the absolute size of the compressed gas cloud increases with comparatively small changes in the degree of rarefaction. An increase in the Mach number to values where an almost limiting velocity is reached shows that the convergent source can be used for maximum possible acceleration of the flow, which is important in the case of gas mixtures with disparate molecular weights. It should also be noted that conservation of the stagnation temperature at the axis in the plane of symmetry was an expected phenomenon in this study.

The analysis of the data obtained shows that the study of collisions of flows, in particular, flows formed by convergent sources, offers new prospects in the field of gas dynamics.

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