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GAS-DYNAMIC COLLIDERS: NUMERICAL SIMULATIONS

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A collision of supersonic flows of gas mixtures with disparate molecular weights, which are limited in their cross-sectional size, in vacuum leads to formation of a cloud with an elevated concentration and elevated temperature of the heavy gas. Under certain conditions, the governing factor is the collision of molecules of the heavy gas being compressed at the center of the collision of the flows. The generator of such a flow can be called a collider. Results of studying the flows in jet-type, cylindrical, and mixed two-stage colliders are described. The main attention is paid to separation of gases in terms of energy and composition.

Key words: *supersonic flow, counterflow, nonequilibrium processes, shock layer, jet, temperature, separation, collider, Monte Carlo method.*

Introduction. In mixtures of gases with disparate molecular weights or collision cross sections, gradients of temperature, pressure, or concentration give rise to relative fluxes of mass, energy, and momentum of different components. In a continuous medium, these processes have a diffuse character. For instance, the mass flux is determined by gradients of concentration, pressure, and temperature and by mass forces in accordance with the known diffusion equation. In this case, the thermal effects and molecular energy exchange processes do not lead to a multi-temperature character of the medium. A decrease in pressure may provide conditions for the relaxation times to become commensurable with the characteristic gas-dynamic time. For such a flow, the equations of continuous media are inapplicable in the general case. The processes can be described by the laws of physical kinetics. Under these conditions, it is more correct to consider separation of gases in terms of their masses and energies as an inertial process. Separation effects can be fairly significant (see [1–4]).

Separation effects were studied by analyzing a rarefied gas mixture flow [1–3], by investigating acceleration of heavy molecules with the use of this process for deposition [4–6], and in searching for optimal schemes of gas-dynamic separation [7–9]. In [1–9], the challenge was to collect the accelerated molecules (by means of inertial separation in terms of mass), aimed at separating the gases, or to identify molecules with high energies for research and technological applications.

The objective of this work is to find and analyze gas-dynamic schemes for obtaining hyperthermal gas objects as a result of collisions of flows of gas mixtures. Let us consider the following example. Let a mixture of helium with a small amount of xenon, having a stagnation temperature T_0, be expanded in a free jet to the maximum reachable Mach numbers. The limiting energy of the xenon flow (if the mass of the xenon atom is assumed to be 132) corresponds to a stagnation temperature $33T_0$. Extraction of the flow of individual xenon atoms with energies close to that indicated above is a technically soluble problem. A skimmer with a high inlet Knudsen number is used; behind the skimmer inlet, the flow passes to a collisionless regime. Obtaining a pure flow of accelerated xenon rather than a molecular xenon beam from the gas mixture flow is impossible.

Let us consider a supersonic flow of a certain mixture of gases colliding with an obstacle; the flow around this obstacle is characterized by a Knudsen number $\mathrm{Kn} \gg 0.01$. A shock layer whose thickness equals several mean free paths is formed ahead of the obstacle. Heavy particles may retain their energy; in this case, their velocity is close to the free-stream velocity when they collide with the surface. If the obstacle has a mirror surface, i.e., the

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accommodation coefficients for all forms of energy equal zero, the smaller the number of collisions of particles of the heavy and light gases in the shock layer formed near the obstacle, the higher the recovery temperature of this layer. The concentration of the heavy gas near the surface inevitably increases. These phenomena were previously considered under different conditions with the use of various engineering surfaces [1–3].

A gas-dynamic collider can be schematically presented as a collision of identical counterflows. In contrast to the collider known in nuclear physics, the gas-dynamic collider corresponds to a collective collisional process resulting in formation of a gas object with thermal motion, which can be characterized by temperature.

As is shown below, different schemes of gas-dynamic colliders are possible. The choice of gas mixtures for modeling in the present work is explained by the authors' interest in development of optimal schemes of gas-jet deposition of polytetrafluoroethylene-like (PTFE-like) films or finely disperse particles from a tetrafluoroethylene (C_2F_4) flow (the light gases are used as carrier gases). The main attention, however, is paid to separation of gases in terms of energy and concentration with allowance for the molecular structure of the components.

Modeling Method. Flow analysis was based on the known direct simulation Monte Carlo (DSMC) method [10]. Particle collisions were considered with allowance for energy redistribution between different degrees of freedom. The macroscopic characteristics of the flow (density, velocity, temperatures, etc.) were found by averaging the states of particles over a large number of time steps after the flow reached the steady state.

The scheme of weight factors is constructed so that the particles are eliminated at the transfer stage and duplicated at the collision stage. Collisions are calculated by the majorant frequency scheme [11] modified for a correct allowance of collisions of particles with different masses. The variable soft sphere (VSS) model is used for elastic scattering of molecules, and the Larsen–Borgnakke model is used for energy distribution over the internal degrees of freedom [10]. The parameters of the VSS model were calculated for a stagnation temperature $T_0 = 900$ K (used in all calculations) on the basis of the temperature dependences of viscosity and self-diffusion. They are described by the Lennard-Jones model with parameters taken from [12]. The scattering factor for all colliding pairs of particles is $\alpha = 1.3$. The following values are used for the power exponent ω in the dependence of viscosity on temperature and the particle diameter d_{ref} at a temperature of 900 K: $\omega = 0.645$ and $d_{\text{ref}} = 2.57$ Å for the H_2–H_2 pair, $\omega = 0.679$ and $d_{\text{ref}} = 3.87$ Å for the H_2–C_2F_4 pair, $\omega = 0.713$ and $d_{\text{ref}} = 5.08$ Å for the C_2F_4–C_2F_4 pair.

The number of rotational degrees of freedom was two for H_2 and three for C_2F_4. For H_2, vibrational energy was ignored; for C_2F_4, it was calculated independent of rotational energy: the number of vibrational degrees of freedom ξ_{V} was determined as

$$\xi_{\text{V}}(E_{\text{V}}(T_{\text{V}})) = 2E_{\text{V}}(T_{\text{V}})/(kT_{\text{V}}),$$

where E_{V} is the mean vibrational energy and T_{V} is the vibrational temperature. The value of E_{V} was taken as the time-averaged vibrational energy of molecules in the cell, and T_{V} was calculated by iterations as an inverse function of E_{V}. The dependence $E_{\text{V}}(T_{\text{V}})$ constructed on the basis of data on vibrational frequencies of the C_2F_4 molecule [13] is defined by the polynomial $E_{\text{V}}(T_{\text{V}}) = -10.7T_{\text{V}} + 0.129T_{\text{V}}^2 - 8.77\cdot 10^{-5}T_{\text{V}}^3 + 3.13\cdot 10^{-8}T_{\text{V}}^4 - 4.46\cdot 10^{-12}T_{\text{V}}^5$ in the range of temperatures from 100 to 1000 K [the value of E_{V} is measured in J/(mole·K)]. Only translational–rotational (T–R) and translational–vibrational (T–V) transitions were taken into account.

The number of collisions Z necessary for relaxation is set for all kinds of interaction, except for the T–V transition for H_2: for H_2–H_2, $Z_{\text{T-R}} = 50$; for H_2–C_2F_4, $Z_{\text{T-R}} = 5$ and $Z_{\text{T-V}} = 25$; for C_2F_4–C_2F_4, $Z_{\text{T-R}} = 5$ and $Z_{\text{T-V}} = Z_{\text{V}}(T_t, T_{\text{V}})$. Here T_t is the local translational temperature of C_2F_4 (averaged in time for a cell). Approximate averaging of relaxation times was used for constant values of Z, which did not exert any significant effect on the results.

The value of $Z_{\text{T-V}}$ for C_2F_4 was calculated by the formula [14]

$$Z_{\text{T-V}} = \frac{Z_{10}(T_t)}{1 - \exp(-\Theta_1/T_{\text{V}})}\,\frac{C_{\text{vib}}(T_{\text{V}})}{C_1(T_{\text{V}})}.$$

Here $Z_{10}(T_t)$ is the number of collisions necessary for the occurrence of the vibrational transition, Θ_1 is the quantum of energy of the lower vibrational mode, $C_{\text{vib}}(T_{\text{V}})$ is the total vibrational heat, and $C_1(T_{\text{V}})$ is the heat of the lower mode through which the energy transfer predominantly occurs. For the C_2F_4 molecule, the Landau–Teller dependence [14] has the form $\log Z_{10}(T_t) = 26.4T_t^{-1/3} - 2.76$; the coefficients are found from experimental data on relaxation times τ_{vib}: $\tau_{\text{vib}} = 17$ nsec for $T_t = 300$ K [13] and $\tau_{\text{vib}} = 14$ nsec for $T_t = 373$ K [15].

In constructing the algorithm, we took into account the recommendations of [16], including the recalculation of the "continuum" value of $Z_{\text{T-V}}$ to the corresponding probability of collisions for the Larsen–Borgnakke model.

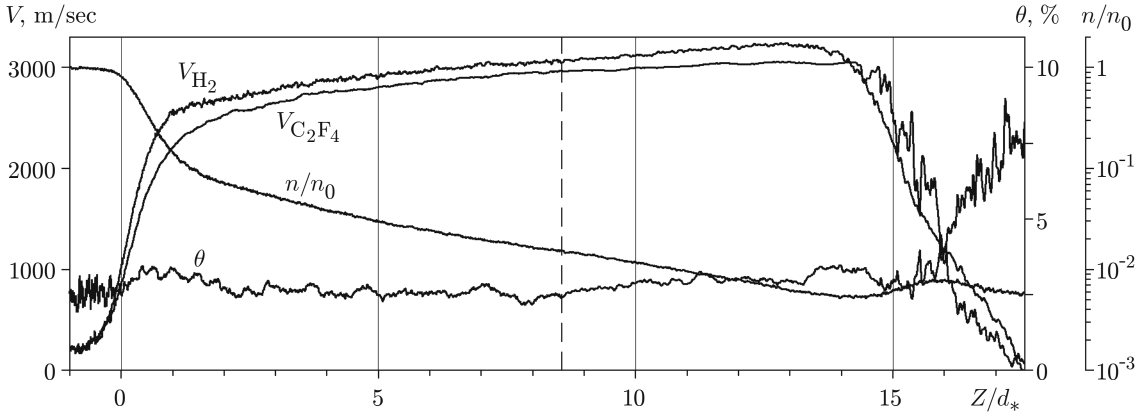

Fig. 1. Variation of parameters along the flow centerline in the jet collider for $\mathrm{Kn}_0 = 1.59 \cdot 10^{-3}$ (the vertical dashed line is the exit plane of the supersonic nozzle; $Z/d_* = 0$ is the position of the throat cross section).

Jet Collider. The jet collider forms a gas-dynamic structure including the region of interaction of two coaxial supersonic counterjets in which the colliding gases are rarefied. An important feature of such a structure is the fan-like expansion of the gas mixture in space surrounding the plane of symmetry of the flow-interaction region. To analyze the flow, it suffices to consider the flow from the stagnation chamber through the nozzle with further expansion to the plane of symmetry, which is subjected to the condition of specular reflection of all particles. On the side of the source, the computational domain is bounded by a fully absorbing surface.

The computed results for the jet collider are presented for two supersonic counterjets of gas mixtures; the initial composition in the stagnation chamber is 97.5% H_2–2.5% C_2F_4, and the initial stagnation temperature is 900 K. We considered the field of interaction of jets issued from supersonic conical nozzles with a ratio of areas at the exit and in the throat equal to 52 and a cone angle 40°. The distance between the nozzle throats was $35d_*$ (d_* is the throat diameter), and the distance between the nozzle exits was $18d_*$. By virtue of symmetry, flow analysis can involve only 1/4 of the axisymmetric flow pattern.

The first computations were performed for interaction of jets of gas mixtures 95% He–5% C_2F_4 with a characteristic Knudsen number calculated by the formula $\mathrm{Kn}_0 = 1/(\sqrt{2}\, n_0 \sigma_0 d_*) = 2.35 \cdot 10^{-3}$ [n_0 is the total number density in the stagnation chamber and σ_0 is the collision cross section of particles of the carrier gas (helium) with each other at the stagnation temperature]. In the stagnation plane, the temperature of gases that reached equilibrium was found to be 250 to 330 K higher than the stagnation temperature.

To find stronger effects of overheating of the heavy gas in the vicinity of the plane of symmetry, the computations were continued only for the mixture of C_2F_4 with hydrogen as a carrier gas. Figure 1 shows the distributions of the dimensionless total number density n/n_0, number fraction of C_2F_4 in the mixture θ, and flow velocities V_{H_2} and $V_{\mathrm{C_2F_4}}$ along the axis of symmetry (along the Z coordinate) for $\mathrm{Kn}_0 = 1.59 \cdot 10^{-3}$. The origin of the coordinate system was assumed to be the nozzle-throat cross section. Flow nonequilibrium turned out to be significant in the entire region up to the plane of symmetry. The slip of components with respect to each other should be noted. Up to the cross section $Z/d_* \approx 14$, we have $V_{\mathrm{H}_2} > V_{\mathrm{C_2F_4}}$, and then the hydrogen jet is decelerated faster. This occurs in the region of shock-layer formation at $Z/d_* > 14$. The shock wave cannot be identified in the shock layer. The conditions of the gas-dynamic collider are satisfied if the shock waves in the counterflows merge together, i.e., if there is no conventional (in the gas-dynamic sense) compressed layer between the shock waves.

Flow nonequilibrium can be estimated by the change in the number fraction of C_2F_4 whose values correlate with the difference between the velocities of the components and drastically increase in the shock layer, exceeding the original values severalfold.

Important information on the flow can be drawn from the dependence $(n/n_0)(Z/d_*)$, which implies that the shock layer starts forming in the vicinity of the cross section $Z/d_* = 14$. Based on this dependence, one can determine the number of the mean free paths of particles in the compressed layer and the shock-layer Knudsen number. If we assume that the shock-layer thickness d_s is the width at the half-height of the shock-layer density

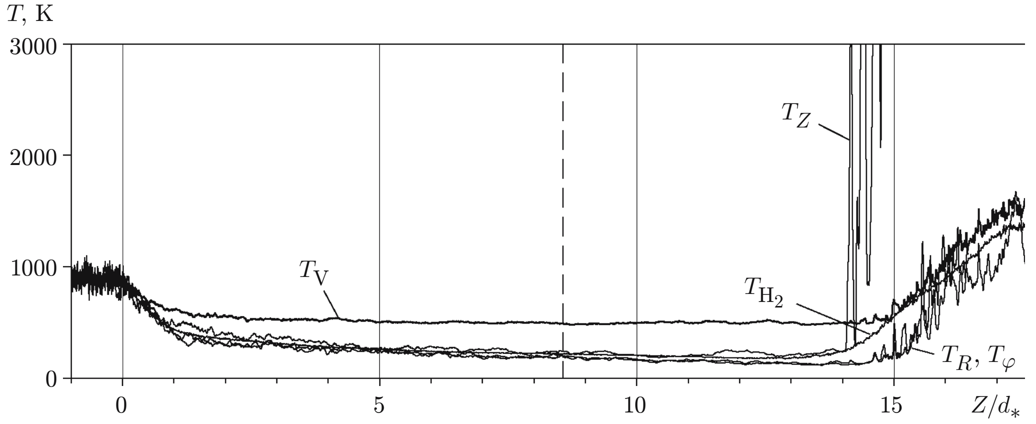

Fig. 2. Variations of temperatures along the flow centerline in the course of its expansion and collision-induced compression (the vertical dashed line is the exit plane of the supersonic nozzle).

profile and use the mean free path in collisions of C_2F_4 molecules with each other, we find the characteristic Knudsen number $\mathrm{Kn}_s = 1/(\sqrt{2}\, n_s \sigma_s d_s) \approx 0.04$ (n_s is the density of C_2F_4 in the shock layer and σ_s is the collision cross section for C_2F_4 molecules at the mean temperature of the shock layer).

Figure 2 shows the temperature distributions along the axis of the colliding flows [mean translational temperature of the carrier gas T_{H_2}, temperature of C_2F_4 in the radial direction T_R, temperature of C_2F_4 in the axial direction (along the streamline) T_Z, temperature of C_2F_4 in the direction normal to the axis T_φ, and vibrational temperature of C_2F_4 T_V]. The region of expansion is characterized by equilibrium in terms of translational degrees of freedom and freezing of vibrational temperature of C_2F_4 at $T_V \approx 485$ K. An increase in longitudinal temperature of C_2F_4 in the compressed layer to T_Z = 20,000–30,000 K seems to be unrealistic. The value of T_Z characterizes the total energy of molecules in the direction of the flow centerline for distributions of longitudinal velocities of molecules of interpenetrating flows significantly different from the Maxwellian distribution. It should be noted that collisions of particles with energies corresponding to the above-mentioned temperatures are possible in the shock layer. Vibrational temperature increases to 1500 K, thus, becoming approximately 600 K higher than the temperature in the stagnation chamber.

At the temperatures found, chemical processes altering the composition of the gases may be initiated (these processes are not considered in the present work). An important fact is that the collision of jets under rarefied conditions forms an almost continuous zone of the heavy gas with a temperature substantially higher than the stagnation temperature. Actually, a high-temperature reactor for a polyatomic gas “suspended” in space not bounded by the walls is formed. The elevated concentration of the heavy gas in the compressed layer, as compared to its initial concentration, is indicative of superposition of the energy separation and separation of the gases of different kinds.

Cylindrical Collider. The drawback of the jet collider is close-to-spherical jet expansion leading to spreading of the gases to a large area with a corresponding increase in the degree of rarefaction. It seems of interest to consider such flows in situations where the decrease in density of the heavy gas during its expansion and interaction with the counterflow becomes less intense. One of the simplest variants of such a flow is an axisymmetric flow of the gas mixture converging toward the centerline. In the present work, we consider convergent flows from sonic and supersonic nozzles in the form of annular sources with the flow directed toward the centerline. Near the nozzle throat, the flow is close to plane–parallel. Toward the axis, the degree of expansion is limited by decreasing flow radius, but it can persist to a certain radius owing to the possibility of expansion in the axial directions. In the vicinity of the axis of the annular source, the convergent flow decomposes into two oppositely directed axisymmetric jet flows. The cylindrical surface where the nozzle exit is located and the side surfaces perpendicular to the collider centerline restrict the computational domain at Mach numbers M > 1 (the flow is assumed to be completely absorbed on these boundaries). The data are presented only for one half of the computational domain, because the plane of symmetry for such a flow may be considered as a specular plane.

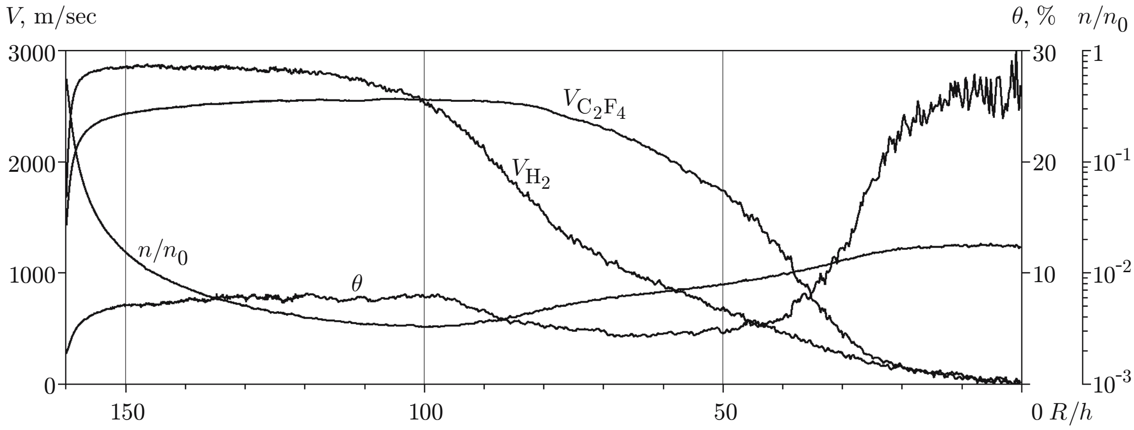

Fig. 3. Variations of flow parameters in the plane of symmetry in the convergent part of the cylindrical collider in the case of flow exhaustion from an annular sonic nozzle toward the collider centerline.

Preliminary calculations for the annular source with a diameter of the supersonic and sonic nozzle exit $D = 6$ mm and with a slot width $h \approx 0.02$ mm ($D/h = 320$) showed that the flow with $\mathrm{Kn}_0 = 1/(\sqrt{2}\, n_0 \sigma_0 h) = 10^{-3}$ is equilibrium everywhere in the plane of symmetry, except for the shock-wave neighborhood, and no influence of the collider is observed. A usual structure with an annular shock wave and a compressed layer inside the latter is formed. In the case of a sonic nozzle and $\mathrm{Kn}_0 = 0.01$, the temperature at the source axis was found to be 300 K higher than the stagnation temperature in the source.

This effect is more substantially manifested in the case of a sonic nozzle at $\mathrm{Kn}_0 = 0.02$. This regime is analyzed below. Figure 3 shows the distribution of flow parameters in the plane of symmetry along the coordinate R/h between the nozzle throat and the axis of symmetry. The origin is the point of intersection of the plane of symmetry and the axis of symmetry of the source.

Flow nonequilibrium is significant in the entire region up to the stagnation region near the axis. The slip of components with respect to each other should be noted: up to the cross section $R/h \approx 100$, we have $V_{H_2} > V_{C_2F_4}$, and then the hydrogen jet is decelerated faster. This occurs in the region of shock-layer formation at $R/h > 100$. A specific feature of this flow is the region with an almost constant velocity of hydrogen (and a constant Mach number of hydrogen) between the cross sections $R/h = 150$ and $R/h = 100$. In this region, hydrogen is weakly decelerated, while C_2F_4 continues to accelerate. The dependence $(n/n_0)(R/h)$ is of interest because it contains information on the beginning of shock-layer formation in terms of density in the vicinity of the cross section $R/h = 100$ and also allows obtaining the average number of mean free paths of molecules in the shock layer and the Knudsen number. In the plane of symmetry of the annular source in the shock layer, we have $\mathrm{Kn}_s \approx 0.02$, i.e., the conditions approach the continuum medium.

The effect of separation of gases is characterized by the quantity θ correlating with the change in velocities of components. It is important that the concentration of C_2F_4 at the axis is more than 10 times greater than the initial value.

Figure 4 shows the changes in temperature between the nozzle throat and the axis [T_R is the translational temperature of C_2F_4 in the radial direction (along the streamline), T_Z is the translational temperature of C_2F_4 in the direction of the collider axis, T_φ is the temperature in the direction perpendicular to the radius in the plane of symmetry of the annular source]. Specific features of the flow under study are its nonequilibrium in terms of translational degrees of freedom and significant temperature anisotropy, especially at the fore front of shock-induced reconstruction of the flow. The peak of the values of T_R on the shock-layer front is typical of shock waves, but it is anomalously high in the present case. High values of T_φ should be noted, which is an apparent consequence of strong compression of the flow in the plane of symmetry of the source. Vice versa, the temperature T_Z acquires the minimum values, because expansion in the direction away from the plane of symmetry of the source is more free. Vibrational temperature rapidly becomes "frozen" and starts increasing inside the shock layer toward the collider centerline. All temperatures in this region approach 1400 K, which 500 K higher than the initial temperature in the stagnation chamber.

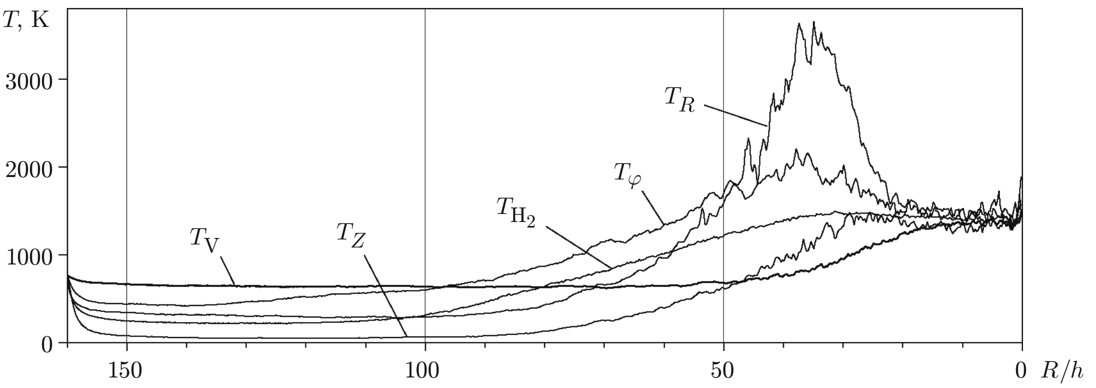

Fig. 4. Temperatures in the plane of symmetry of the cylindrical collider with the flow from the nozzle toward the collider axis ($R/h = 0$).

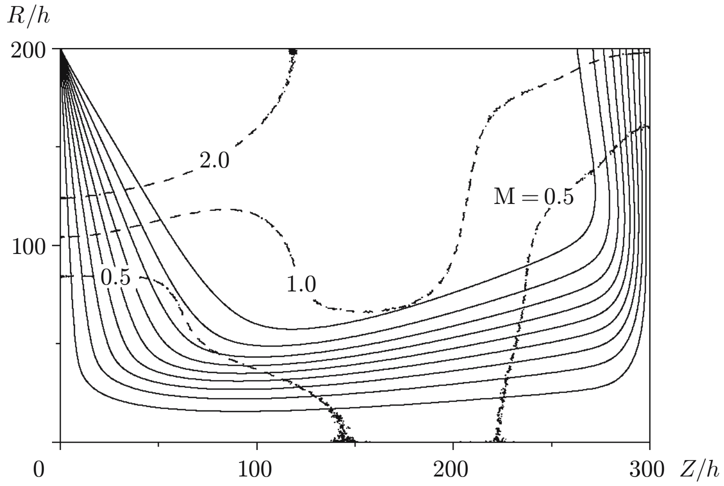

Fig. 5. Flow pattern in a two-stage collider (1/4 of the total pattern): the solid curves are the streamlines of the heavy component; the dashed curves are the Mach number contours for the light component.

A specific feature of the cylindrical collider, which may be important for scientific research and applications, is the character of expansion after the collision. The gas (especially, the heavy gas) flows in both directions in the form of jets collimated to a large extent.

If this flow pattern finds important applications, it will have to be studied more carefully to optimize the parameters of such an unusual reactor.

Two-Stage (Jet-Cylindrical) Collider. The possibility of obtaining a highly concentrated, partly collimated flow of a heavy gas in a heated (hyperthermal) state in the vicinity of the stagnation point of a convergent flow from an annular nozzle determined the direction of further research: collisions of axisymmetric flows from two identical annular colliders. Below, we analyze only the process in the second stage of the collider, with collisions of gas jets axisymmetrically expanding from the cylindrical colliders considered above.

Figure 5 shows the flow pattern in a two-stage collider: the streamlines for C_2F_4 and the Mach number contours for H_2. The left ordinate axis is located in the plane of symmetry of the annular source of the cylindrical collider, normal to the collider centerline, and the right ordinate axis is located in the plane of symmetry of the two-stage collider, normal to the collider centerline. The abscissa axis coincides with the centerline of the two-stage collider. The source diameter is $D/h = 200$, the distance between the colliders is $L/h = 600$, and the Knudsen number of the first stage is $\mathrm{Kn}_0 = 0.02$. Obviously, the streamlines in the left part of Fig. 5 characterize the flow in the cylindrical collider considered above. In the right part of Fig. 5, in the cross section $Z/h = 300$, there is a

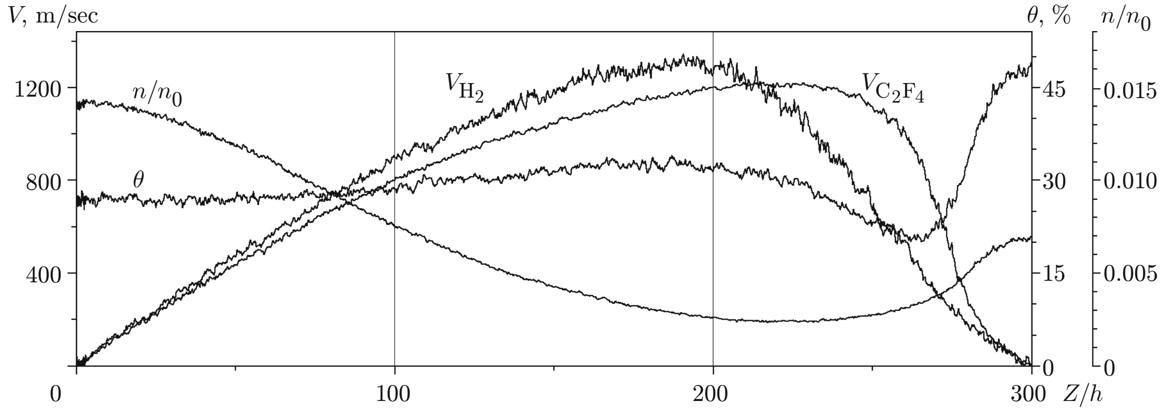

Fig. 6. Parameters of the flow along the centerline of the two-stage collider from the plane of symmetry of the cylindrical collider ($Z/h = 0$) to the plane of symmetry of the two-stage collider ($Z/h = 300$).

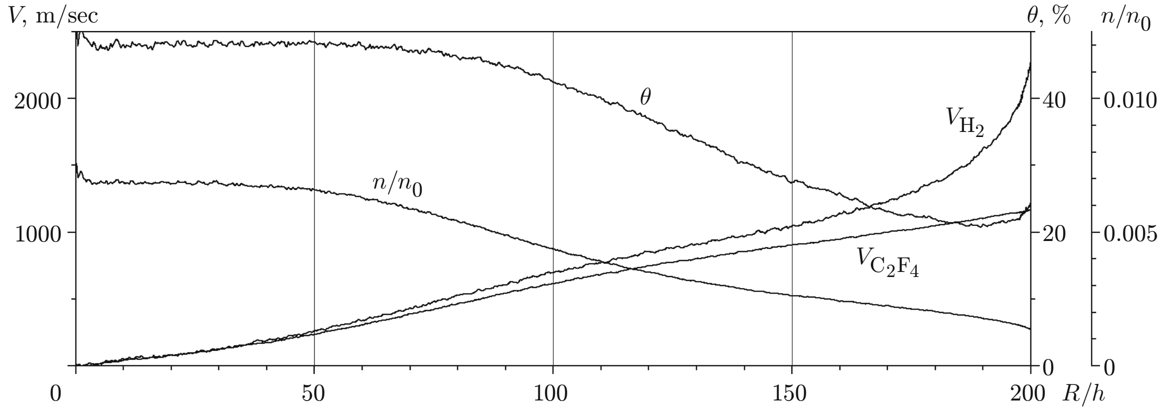

Fig. 7. Parameters of the gas during its radial expansion in from the stagnation point in the plane of symmetry of the two-stage collider.

"mirror" placed in the plane of symmetry of the interaction region of the axial flows from two cylindrical colliders. During its fan-like expansion, the heavy gas is pressed to the plane of symmetry of the two-stage collider. The curve corresponding to $R/h = 200$ and closing the contour of the computational domain is the boundary of the supersonic flow region; therefore, complete absorption boundary conditions set on this contour do not distort the results computed for the flow field considered. Note that the most significant changes in energy and concentrations in the C_2F_4 flow occur in the subsonic region of the H_2 flow.

Let us study the behavior of the parameters of colliding gases issued by two cylindrical colliders. Figure 6 shows that the gases are accelerated with "slipping" relative to each other toward the common plane of symmetry and reach the maximum velocity, approximately half the velocity in the cylindrical collider. The total density in the shock layer in the second stage is approximately twice lower than that in the first stage, but the concentration is approximately twice higher than that in the first stage, i.e., the density of the heavy component remains almost unchanged. The use of two stages increases the relative concentration of the heavy gas almost by a factor of 20, as compared with the stagnation value. The mean translational temperature at the stagnation point of the heavy gas (in the plane of symmetry) reaches 1500 K in the absence of equilibrium of thermal motion with rotational and vibrational energies.

Further fan-like expansion of the gases in the neighborhood of the common plane of symmetry is characterized by the dependences plotted in Fig. 7. At $R/h = 200$, the gases are accelerated to velocities approximately equal to 1000 m/sec; the density and concentration decrease correspondingly.

Conclusions. An analysis of formation of shock layers in collisions of high-velocity flows of gas mixtures, resulting in formation of a gas object surrounded by a rarefied gas medium, seems to be a pioneering study. The calculations reveal unique possibilities of separation of gas mixtures in terms of energies and concentrations. Such objects may be used for physical research. Technological applications are not only possible but also obvious. In particular, colliders considered in the paper may be used as new-type sources for obtaining thin films and ultrafine particles.

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