MIXING OF HOMOGENEOUS STREAMS OF DISSOCIATING AIR

L. Yu. Artyukh and E. A. Zakarin

UDC 533.601.1: 539.196.6

The influence of nonequilibrium dissociation on the flow field in laminar mixing of homogeneous air flows is investigated by a perturbation method. The Mach, Prandtl, and Schmidt numbers are selected as problem parameters. The solution is obtained taking account of four approximations.

1. The laminar mixing of two reacting streams attracts the attention of researchers firstly by the simple flow geometry, and secondly by the fact that such flows are often encountered in practice as the initial portion of a plane jet, the wake behind a body, etc. Marble and Adamson [1] examined such a problem under the assumption that ignition of a fuel mixture occurs in the mixing zone. Kovitz and Hogland [2] attempted to carry out an analogous investigation with other chemical kinetics, the molecule dissociation and atom recombination kinetics. However, the problem was solved in this paper in a strongly idealized form: the streams move at identical velocities, and the chemical reaction rate depends only on the component concentration.

The problem of laminar mixing of high-speed air streams accompanied by energy dissipation and high-temperature effects such as molecule dissociation and atom recombination is considered below.

The flow under investigation is described by the system of compressible gas boundary layer equations, which in the dimensionless Lees–Dorodnitsyn variables

$$\varphi = \frac{1}{2\sqrt{\xi}} \int_0^{\bar{y}} \bar{\rho} d\bar{y}, \quad \xi = \bar{x} \tag{1.1}$$

has the form

$$(\bar{\rho}\bar{\mu} f'')' + 2ff'' = 0, \tag{1.2}$$

$$\left(\frac{\bar{\rho}\bar{\mu}}{\Pr} \bar{T}'\right)' + 2f\bar{T}' + (\gamma-1) M_I^2 \omega_I f''^2$$
$$= 4\xi f' \frac{\partial \bar{T}}{\partial \xi} + \frac{4Lh_A^0}{\rho_I u_I T_R C_p} \xi \frac{w_A}{\bar{\rho}}, \tag{1.3}$$

$$\left(\frac{\bar{\rho}\bar{\mu}}{S_m} a'\right)' + 2fa' = 4\xi f' \frac{\partial a}{\partial \xi} - \frac{4L}{\rho_I u_I} \xi \frac{w_A}{\bar{\rho}}. \tag{1.4}$$

The prime here denotes the derivative with respect to the coordinate φ; w_A is the rate of atom formation per unit volume in unit time, h_A^0 is the enthalpy of atom formation, L is any characteristic dimension; the subscripts I and II denote the conditions in the upper and lower streams, respectively. All the remaining notation is standard in boundary layer theory. The variable quantities are used in the dimensionless form:

$$\bar{y} = \frac{y}{L}\sqrt{\mathrm{Re}}, \quad \bar{x} = \frac{x}{\mathrm{Re}}, \quad \mathrm{Re} = \frac{u_I L}{\nu_I}, \quad \bar{\rho} = \frac{\rho}{\rho_I},$$

S. M. Kirov Kazakh State University, Alma-Ata. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 20, No. 2, pp. 246-254, February, 1971. Original article submitted December 12, 1969.

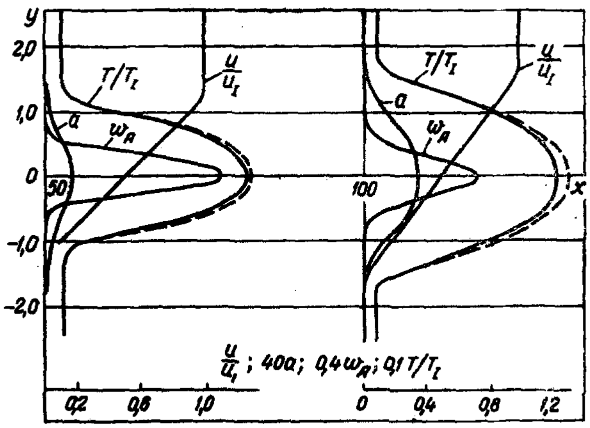

Fig. 1

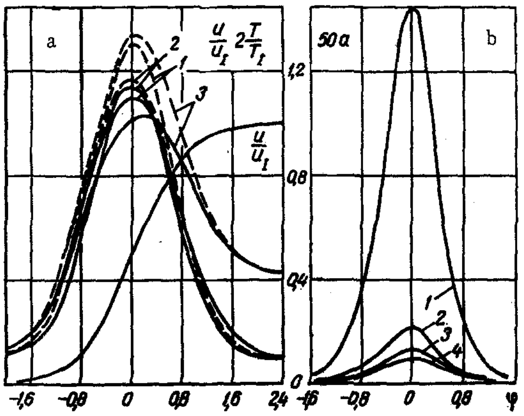

Fig. 2

Fig. 1. Development of velocity u/u_I, temperature T/T_I, atom concentration a, and dissociation rate w_A profiles in the mixing zone of air streams: $u_I = 4500$ m/sec, $u_{II} = 0$, $a_I = a_{II} = 0$, $T_1 = T_{II} = 230$°K, Pr = Sm = 0.72, $M_I = 15.5$.

Fig. 2. Velocity u/u_I, temperature T/T_R (a) and atom concentration a (b) profiles: ——) taking account of dissociation; ----) without taking account of dissociation. $u_I = 4500$ m/sec, $u_{II} = 0$, $T_{II} = 230$°K, $a_I = a_{II} = 0$. For a: 1) Pr = 1, Sm = 1, $T_I = 230$°K, $M_I = 15.5$; 2) Pr = 0.72, Sm = 1, $T_I = 230$°K, $M_I = 15.5$; 3) Pr = 0.72, Sm = 1, $T_I = 1000$°K, $M_I = 7.5$. For b: 1) Pr = 1, Sm = 1; 2) Pr = 0.72, Sm = 1; 3) Pr = 0.72; Sm = 0.5; 4) Pr = 0.72; Sm = 0.36; and for 1-4) $M_I = 15.5$.

$$\bar{\mu} = \frac{\mu}{\mu_I}, \quad f' = \frac{u}{u_I}, \quad \bar{T} = \frac{T}{T_R}, \quad \omega_I = \frac{T_I}{T_R}, \quad \omega_{II} = \frac{T_{II}}{T_R}.$$

The system (1.1)-(1.4) must be solved under the following asymptotic boundary conditions

$$\begin{gathered} \varphi \to +\infty: f' \to 1, \ \bar{T} \to \omega_I, \ a \to a_I, \\ \varphi \to -\infty: f' \to 0, \ \bar{T} \to \omega_{II}, \ a \to a_{II}. \end{gathered} \tag{1.5}$$

The equations of a dissociated boundary layer have been solved in a general formulation only numerically on high-speed electronic computers [3]. The difficulties in such a computation are essentially due to the nonlinear source w_A, the complex form of the dependence of the transfer coefficient on the atom temperature and concentration, and also to the huge amount of computational labor.

2. Complex physicochemical processes associated with the excitation of rotational and vibrational degrees of freedom, molecule dissociation, and atom ionization, occur in air at high temperatures. As is known [4], these processes have different energy potentials, and may hence proceed separately depending on the temperature band.

Let us examine the temperature range within which the oxygen dissociation–recombination reaction occurs

$$O_2 + X \rightleftarrows O + O + X,$$

where the molecules O_2, N_2 or the atom O can play the part of the third particle X. Since the molecular weights of oxygen and nitrogen are sufficiently similar, it can be considered to a sufficient degree of accuracy, that air is a mixture of atoms with the mass concentration a and molecules with the mass concentration $1-a$. This model of an ideally dissociating gas proposed by Lighthill [5] is real for air under the condition that the vibrational and rotational nonequilibrium can be neglected.

The equilibrium properties of the mixture depend on the equilibrium constants

$$K(T) = AT^{-0.5} \exp\left(-\frac{T_D}{T}\right), \tag{2.1}$$

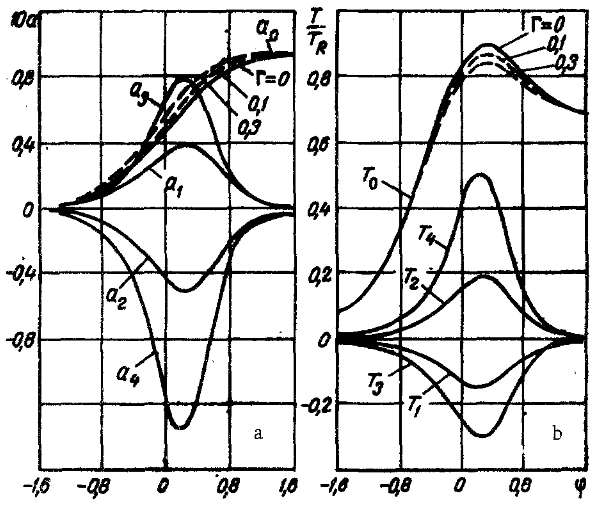

Fig. 3.

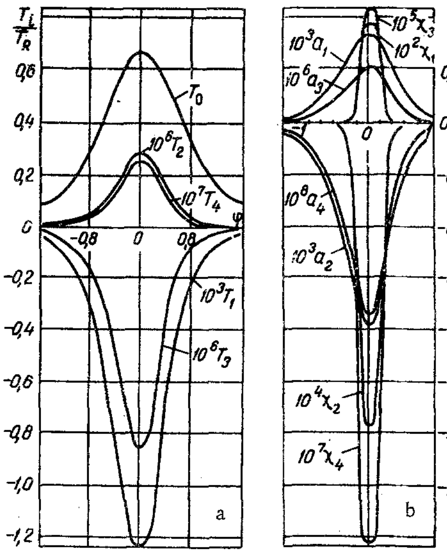

Fig. 4

Fig. 3. Profiles of the expansion functions of the temperature (b) and atom concentration (a); ——) zeroth, first, second, third, and fourth approximations of the functions; ----) the resultant temperature and atom concentration profiles for different sections of the stream mixing zone: $u_I = 4000$ m/sec, $u_{II} = 0$, $T_I = 3000$°K; $T_{II} = 230$°K, $a_I = a_{II} = 0$, Pr = Sm = 0.72.

Fig. 4. Profiles of the expansion functions of the temperature (a), the concentration and reaction rate (b), $u_I = 4500$ m/sec, $u_{II} = 0$, $T_I = T_{II} = 230$°K, $a_I = a_{II} = 0$, Pr = Sm = 0.72.

and the degree of dissociation is defined by the law of effective masses

$$\frac{a_e^2}{1-a_e^2} = \frac{RT_e}{4P} K(T_e). \tag{2.2}$$

In the nonequilibrium state the rate of change of atom concentration is defined by the equation of the chemical reaction rate [6]

$$\frac{w_A}{\rho} = \frac{PC}{RT^2(1+a)}\left[2aBT^{-0,5} + (1-a)\right] \times \left[(1-a)K - \frac{4P}{RT}\,\frac{a^2}{1+a}\right]. \tag{2.3}$$

The following empirical constants were used in (2.1)-(2.3) [6]:

$$A = 1{,}2\cdot 10^6 \text{ kmole}\cdot\text{deg}^{0.5}/\text{m}^3,\quad B = 3.34\cdot 10^2 \text{ deg}^{-0.5},$$

$$C = 1.9\cdot 10^{18} \text{ kmole}\cdot\text{deg}^{0.5}/\text{m}^3,\quad T_D = 5.95\cdot 10^4\,^\circ\text{K},\quad T_R = 4.5\cdot 10^3\,^\circ\text{K}.$$

After the passage to the dimensionless temperature $\overline{T}$ and manipulations associated with the extraction of the characteristic chemical reaction time, we obtain the following expression for the last members in (1.3) and (1.4):

$$\frac{4L\xi}{\rho_I u_I}\cdot\frac{w_A}{\overline{\rho}} = \left\{\frac{L\xi}{u_I}\right\}\left\{\frac{4PC}{RT_R}\exp\left(-\frac{T_D}{T_R}\right)\right\}\chi(a, \overline{T}). \tag{2.4}$$

Here

$$\chi(a, \overline{T}) = \frac{\left[2a\overline{T}^{-0.5}B + (1-a)\right]}{\overline{T}^{2.5}(1+a)}\left\{(1-a)\exp\left[-\frac{T_D}{T_R}\left(\frac{1}{\overline{T}} - 1\right)\right] - \frac{4P}{ART_R}\exp\left(\frac{T_D}{T_R}\right)\overline{T}^{-0.5}\frac{a^2}{1+a}\right\}.$$

The relationship in the first braces in (2.4) characterizes the time that the physical processes proceed τ_{ph}, while the relaxation time $1/\tau_X$ is in the second braces. Let $\Gamma(x)$ denote the relationship between these times:

$$\Gamma(\xi) = \frac{\tau_{ph}}{\tau_x} = \left\{\frac{L\xi}{u_I}\right\}\left\{\frac{4PC}{RT_R} \exp\left(-\frac{T_D}{T_R}\right)\right\}. \tag{2.5}$$

The quantity $\Gamma(\xi)$ is usually called the Dammkeller number and is an important characteristic of physicochemical processes in a flow field. If $\Gamma(\xi)$ is small, then the physical energy and atom transfer processes play a predominant part (in this case it is said that the flow is chemically frozen). For high values of $\Gamma(\xi)$, the process will be in chemical equilibrium, the atom concentration and temperature are determined in this case from (2.1) and (2.2), and hence, there is no longer a need to solve the energy (1.3) and diffusion (1.4) equations. In the general case of a finite value of $\Gamma(\xi)$, when the rates of the physical and chemical processes are commensurate, the problem is solved in a general formulation with (1.2)-(1.4) and (2.4).

The influence of molecule dissociation on the transfer properties of the gas mixture can be taken into account for the ideal dissociating gas model assumed. Computations show [4] that the mixture viscosity is determined well enough by the viscosity of a pure gas consisting only of molecules, say, i.e., $\mu \approx \mu_M \approx \mu_A$ (the symbol M here refers to a molecular gas, and A to an atomic gas). The following relations are obtained for the heat conduction coefficient λ, the specific heat C_p, the numbers Pr and Sm:

$$\lambda = \lambda_M \frac{1 + 1{,}62a}{1 + a}, \tag{2.6}$$

$$C_p = C_{pM} \frac{4 - a'}{4}, \tag{2.7}$$

$$\mathrm{Pr} = \mathrm{Pr}_M \frac{(1 + 0.25a)(1 + a)}{1 + 1.62a}, \tag{2.8}$$

$$\mathrm{Sm} = \mathrm{Sm}_M (1 + a). \tag{2.9}$$

3. Let us examine the flow for which the unperturbed streams are in a chemically frozen state, and a small deviation from this state occurs in the mixing zone because of dissipative heating, i.e., atoms are formed whose local concentration is less than the appropriate equilibrium concentration.

In this case, firstly the physical processes in the whole flow field will proceed more rapidly than the chemical and the Dammkeller number $\Gamma(\xi)$ can be chosen a small parameter, and the problem can be solved by the perturbation method [7]; secondly, because of the low degree of dissociation ($a \ll 1$), the transfer coefficients and their associated quantities (see (2.6)-(2.20)) can be taken equal to the appropriate values of a pure molecular gas.

Let us make still another assumption: $\mu\rho$ = const, which is quite justifiable in the solution of compressible boundary layer problems without chemical reactions, and therefore, should also not introduce rough distortions for slight gas dissociation. A result of such an assumption is the fact that the dynamic equation (1.2) in the Lees–Dorodnitsyn variables is solved independently of the remaining equations in the system. This affords a possibility of using the known solution of (1.2) in [8].

Let us seek the temperature distribution and atom concentration in the form of expansions in the Dammkeller number:

$$\overline{T}(\varphi, \xi) = \sum_{n=0}^{\infty} \Gamma^n(\xi) T_n(\varphi), \tag{3.1}$$

$$a(\varphi, \xi) = \sum_{n=0}^{\infty} \Gamma^n(\xi) a_n(\varphi). \tag{3.2}$$

Substituting the series (3.1) and (3.2) into (1.3) and (1.4) and collecting terms in identical powers of $\Gamma(\xi)$, we obtain the following system of linear ordinary differential equations

$$T_0'' + 2\mathrm{Pr}\, fT_0' + \mathrm{Pr}\,(\gamma - 1)\,\omega_\mathrm{I} M_\mathrm{I}^2 f''^2 = 0, \tag{3.3}$$

$$a_0'' + 2\mathrm{Sm}\, fa_0' = 0, \tag{3.4}$$

$$\cdots\cdots\cdots\cdots\cdots\cdots,$$

$$T_n'' + 2\mathrm{Pr}\, fT_n' - 4\mathrm{Pr}\, nf' T_n$$

$$= \mathrm{Pr}\,\frac{h_A^0}{T_R\,\mathrm{Cp}}\chi_{n-1}(\ldots), (T_0, \ldots, T_{n-1}, a_0, \ldots, a_{n-1}), \tag{3.5}$$

$$a_n'' + 2\mathrm{Sm}\, fa_n' - 4\mathrm{Sm}\, nf' a_n = -\mathrm{Sm}\,\chi_{n-1}(\ldots)(T_0, \ldots, T_{n-1}, a_0, \ldots, a_{n-1}). \tag{3.6}$$

The boundary conditions (1.5) become

$$\begin{aligned} \varphi \to \infty:\ & T_0 \to \omega_\mathrm{I}, \quad a_0 \to a_\mathrm{I}, \\ & T_n \to 0, \quad a_n \to 0, \\ \varphi \to -\infty:\ & T_0 \to \omega_\mathrm{II}, \quad a_0 \to a_\mathrm{II}, \\ & T_n \to 0, \quad a_n \to 0. \end{aligned} \tag{3.7}$$

The source functions χ_n can be obtained by expanding the function $\chi(\Gamma)$ in Taylor series in the neighborhood of the point $\Gamma = 0$. Equations (3.3) and (3.4), with appropriate boundary conditions, describe the frozen flow completely and have an analytical solution [8].

The correction function T_n and a_n which take account of the influence of the chemical dissociation and recombination reactions on the temperature profile and atom concentration, have been obtained by numerical integration of (3.5) and (3.6). The difficulties associated with giving the boundary conditions at infinity, did not permit application of ordinary numerical methods (the method of factorization, the trial and error method, etc.). Hence, the solution is found in the form of quadratures:

$$T_n = \frac{\mathrm{Pr}\, h_A^0}{C_p T_R}\left[I_n(\varphi) - \frac{I_n(\infty)}{Y_n(\infty)}\, Y_n(\varphi)\right] S_n, \tag{3.8}$$

where

$$I_n = \int_{-\infty}^{\varphi} \frac{f''^{\mathrm{Pr}}}{S_n^2}\left(\int_{-\infty}^{\varphi} \frac{S_n \chi_{n-1}}{f''^{\mathrm{Pr}}}\, d\varphi\right) d\varphi,\ Y_n = \int_{-\infty}^{\varphi} \frac{f''^{\mathrm{Pr}}}{S_n^2}\, d\varphi,$$

and S_n are particular solutions of the corresponding homogeneous differential equations

$$S_n'' + 2\mathrm{Pr}\, fS_n' - 4\mathrm{Pr}\, nf' S_n = 0 \tag{3.9}$$

with the boundary conditions $S_n(0) = 1$, $S_n'(0) = 0$. The system of equations (3.8) and (3.9) are solved in combination with an analogous system for the atom concentration to the fourth approximation, inclusive, on an electronic digital computer.

4. Use of a computer permits computation of a set of modifications of this problem depending on the values of the parameters Pr and Sm, as well as on the conditions in the upper and lower streams. The following constraints were hence taken:

1) Stream mixing with a fixed constant-temperature medium was considered, i.e., $u_\mathrm{I} = 0$ and $T_\mathrm{II} = 230$°K;
2) The parameters Pr and Sm varied only during the calculation of the first approximations of T_1 and a_1 and took on the values: Pr = 1; 0.72; Sm = 1; 0.72; 0.5; 0.36. This corresponds to values of the number Le = 0.72; 1; 1.4; 2; 2.8;
3) The number Pr, Sm and Le remained constant, equal to one, in calculations of the remaining higher order (to the fourth, inclusive) approximations.

To estimate the influence of dissociation on the temperature distribution and atom concentration, boundary layer development as a function of removal from the beginning of mixing is shown in Fig. 1 in the physical coordinate plane. Both compressibility and the dependence of Γ on the longitudinal x coordinate were hence taken into account. Temperature profiles without dissociation (dashed lines) are presented for comparison. It is seen from the figure that the exothermal dissociation process results in a diminution of the maximum temperature in the mixing zone, which in turn diminishes the effect of the chemical reaction. When the atom concentration reaches the maximum value, the temperature in the mixing zone probably diminishes so much that further gas dissociation becomes impossible.

The influence of the numbers Pr and Sm on the temperature profile and atom concentration is shown in Fig. 2. A comparison between curves 1 and 2 shows that as the Pr number diminishes, i.e., as the heat elimination from the mixing zone increases, the effect of the chemical reaction on the temperature and especially on the concentration field diminishes (the degree of dissociation drops more than threefold for the small change in Pr from 0.72 to 1). Analogously but no less strong is the influence of the number Sm since a diminution in this parameter will result in more intense elimination of atoms from the mixing domain (Fig. 2b, curves 2, 3 and 4). Additional heating of the stream, as an increase in the number Pr, contributes to dissociation (Fig. 2a, curve 3). An analysis of these results shows that neglecting the change in transfer coefficients even in a domain close to the frozen domain can result in essential distortion of the physical picture of the process.

Four approximations for the temperature and concentration were calculated in order to clarify the higher order effects as well as to determine the radius of convergence of the series (3.1) and (3.2).

Graphs of the temperature and degree of dissociation of the frozen flow and four correction functions are presented in Figs. 3 and 4 for different conditions in the unperturbed stream.

The qualitatively identical behavior of all the approximations strikes the eye. This is evidently due to the nature of the functions, the sources χ_n whose sharp peaks are presented in Fig. 4b. As is seen from this figure, the effect of the chemical reactions is localized in a narrow domain analogous to a diffusion combustion front. This will afford the possibility of using corresponding methods of investigation which have been developed well in flame theory [9].

By comparing Figs. 3 and 4 it can be noted that the correction functions T_n and a_n increase in the first case (Fig. 3) as n increases, while these functions diminish in the second (see Fig. 4). Therefore, the radius of convergence of the series (3.1) and (3.2) depends on the conditions in the unperturbed stream. A numerical "experiment" showed that at the maximum frozen flow temperature $T_{0\max} \leq 3500°K$ the functions T_n and a_n diminish as n grows. This does not mean, however, that the 3500°K temperature is the ultimate possible since the convergence of asymptotic series is not an absolute for obtaining solutions of sufficient accuracy [10]. Compliance with the condition $T_{0\max} \leq 3500°K$ affords the possibility of increasing the number Γ to 0.5 and of hence using just the first approximation.

In conclusion, let us note that dissociation plays a predominant part in all the computed modifications and in order to take account of this effect in this formulation of the problem, it is sufficient to calculate the first approximation. Atom recombination will be felt only for $\Gamma > 1$, i.e., for essentially nonequilibrium flow.

After having completed this research, whose fundamental results were presented to the III All-Union Congress on Theoretical and Applied Mechanics [12], the paper [11] was published in which the influence of nonequilibrium dissociation on laminar stream mixing is also considered. The numerical solution obtained in a quasi-self-similar approximation (the longitudinal coordinate x is taken as the parameter of the problem) qualitatively agrees well with the results herein: atom recombination is felt quite weakly in the whole computed flow domain.

NOTATION

$f' = u/u_I$	dimensionless longitudinal velocity component;
T	temperature;
a	atom concentration;
x, y	longitudinal and transverse coordinates;
ξ, φ	Lees–Dorodnitsyn variables (1.1);
P	pressure;
ρ	density;
μ	kinematic viscosity;
λ	heat conduction coefficient;
$\gamma = C_p/C_v$	ratio of the specific heats;

$\omega_I = T_I/T_R$, $\omega_{II} = T_{II}/T_R$	dimensionless temperatures of the upper and lower streams;
L	characteristic length;
Pr, Sm, Le, M, Re	Prandtl, Schmidt, Lewis, Mach, and Reynolds number;
w_A	rate of atom formation (2.3);
K	equilibrium constant;
χ	function in (2.4);
Γ	Dammkeller number (2.5);
A, B, C, T_D, T_R	empirical constants.

LITERATURE CITED

1. F. E. Marble and T. C. Adamson, Jet Propulsion, 24, 85 (1954).
2. A. A. Kovitz and R. F. Hogland, Physics of Fluids, 3, No. 3 (1960).
3. V. G. Voronkin and L. K. Gerskina, Izv. Akad. Nauk SSSR, Mekh. Zhidk. i Gaza, No. 3 (1969).
4. W. G. Dorrance, Hypersonic Viscous Gas Flow [Russian translation], Mir, Moscow (1966).
5. M. J. Lighthill, J. Fluid Mech., 2, No. 1 (1957).
6. R. J. Conti, J. Fluid Mech., 24, Part 1 (1966).
7. W. Ray, Raket. Tekh. i Kosmon., No. 10 (1963).
8. L. A. Vulis and V. P. Kashkarov, Theory of a Viscous Fluid Jet [in Russian], Nauka, Moscow (1965).
9. L. A. Vulis, Sh. A. Ershin, and L. P. Yarin, Principles of the Theory of a Gas Flame [in Russian], Energiya, Leningrad (1968).
10. M. Van Dyke, Perturbation Methods in Fluid Mechanics [Russian translation], Mir, Moscow (1967).
11. R. Wright and K. Chen, Raket. Tekh. i Kosmon., 7, No. 1 (1969).
12. L. Yu. Artyukh, L. A. Vulis, and E. A. Zakarin, III All-Union Congress on Theoretical and Applied Mechanics [in Russian], Moscow (1968).