CALCULATION OF NONEQUILIBRIUM FLOWS IN NOZZLES

V. N. Kamzolov and U. G. Pirumov

This paper studies in the one-dimensional formulation the flow of a reacting gas with account for the nonequilibrium behavior of the chemical reactions; the pressure distribution along the stream filament is given. Viscosity, heat conduction, diffusion, and ionization are not taken into account. It is assumed that there is equilibrium excitation of the translational, rotational, and vibrational degrees of freedom.

Several studies have already been made of nonequilibrium flows in nozzles [1–5]. It is known that in the calculation of nonequilibrium flows considerable difficulty arises in selecting the integration step in those regions where the flow is nearly equilibrium. It is found that with the use for numerical integration of the explicit difference schemes of the type of the Euler, Runge-Kutta, etc., the method of integration step for carrying out a stable calculation must be so small that the calculation becomes practically impossible. The present study proposes a method for calculating nonequilibrium flows using a single implicit difference scheme to calculate with a high degree of accuracy and a quite large step (exceeding the step in the explicit schemes by several orders) both those flow regions which are close to equilibrium and those regions where the flow deviates markedly from equilibrium.

A program was compiled using this method for the M-20 electronic digital computer which permitted calculating in the one-dimensional approximation of flows in nozzles with account for the nonequilibrium behavior of the chemical reactions for mixtures containing H, O, C, and N atoms.

Some qualitative peculiarities of the nonequilibrium flows are demonstrated using as an example nonequilibrium air discharge. A comparison is made with experimental and theoretical results of other authors.

The authors wish to thank L. F. Kuz’mina for her assistance in carrying out the present study.

1. Let us consider the system of gasdynamic equations together with the equations of chemical kinetics in the one-dimensional approximation; namely, the equations of motion, energy, continuity, state, and the m equations of chemical kinetics for the m components of the mixture,

\[ \frac{dp}{dz} = -pu \frac{ds}{dz}, \quad h + \frac{u^2}{2} = h_0, \]

\[ pu F = Q = \text{const}, \quad p = \frac{R_0 T}{\mu}, \]

\[ \frac{ds_i}{dz} = \frac{1}{\mu} (D_i - R_i). \]  \hspace{1cm} (1.1)

Here the pressure p, density \( \rho \), gas velocity \( u \), gas enthalpy \( h \), and total gas enthalpy \( h_0 \) are functions of the mixture temperature and the molar fractions of the mixture components; \( h = \frac{1}{\mu} \sum h_i n_i \), \( h_i \) denotes the enthalpies of the individual components, which are functions of the temperature, \( r_i \) denotes the molar fractions of the mixture components, \( \mu \) is the molecular weight of the mixture, \( F \) is the filament area, \( Q \) is the flow rate, \( T \) is gas temperature, \( R \) is the universal gas constant, \( \alpha_i \) is the weight fraction of the components, \( D_i \) and \( R_i \) are the rates of formation and disappearance, respectively, of the \( i \)-th component, which in the general case are functions of \( T \) and of all \( \alpha_i \).

System (1.1) contains \( 5 + m \) unknowns \( p, \rho, T, u, F, \alpha_1, \ldots, \alpha_m \) and \( 4 + m \) equations for their determination. In order to close the system of equations it is necessary to specify some one of the \( 5 + m \) parameters or a connection between them.

The majority of the investigators specify the variation of the jet area with distance along the nozzle. However, for the calculation of the nonequilibrium flows which begin in the subsonic region the specification of the nozzle contour form is inconvenient. As a matter of fact, specifying the initial conditions in the subsonic stream and thereby specifying the flow rate, we cannot be certain that the given dimension of the critical section will pass the specified flow rate, nor can we be certain that if this flow does pass through the nozzle supersonic flow will be realized. In addition, some difficulties arise in the calculation in the vicinity of the singular point in the region of the critical section.

In the present study the pressure distribution \( p \equiv p(x) \) along the nozzle length was specified. This approach is more advantageous for the following reasons. First, no difficulties arise in integrating the system directly from the subsonic portion of the nozzle. Second, the pressure is the parameter which is most easily measured experimentally and the knowledge of which from experiment along a given stream filament permits, integrating system (1.1), determining all the remaining parameters. Third, flow in real nozzles deviates strongly from one-dimensional, and the shapes of the stream filaments differ strongly in the real nozzle. Therefore, when specifying the area \( F = F(x) \) corresponding to the "iron" contour of the nozzle, we do not know whether in the actual two-dimensional flow even one of the stream filaments has the specified shape.

In this connection it is more natural, after calculating by the method of characteristics the equilibrium flow in the given nozzle contour (see, for example, [6]) and the parameters on the various streamlines, and also the pressure distribution on these streamlines, to substitute the pressure distribution thus obtained into the one-dimensional relations (1.1) and, integrating this system along several streamlines, determine approximately the parameters of the new nonequilibrium flow in the given real nozzle. After the pressure distribution along the nozzle length, including the subsonic part, is specified, we can carry out, beginning with some section in the subsonic part, the numerical integration of system (1.1). It is assumed that the flow is equilibrium in the initial section. As a result of the integration all the flow parameters are determined, and the filament area is found from the continuity equation (1.1).

Let us examine the method of calculating the system of equations of chemical kinetics and gasdynamics presented above. It is known that when calculating those regions of nonequilibrium flows in which the parameters are near equilibrium using the popular explicit difference schemes (Euler method, Runge-Kutta method, etc.) it is necessary to reduce considerably the integration step in order to be able, in general, to construct a solution at all, even with low accuracy, which is physically reasonable [2, 3]. The necessity for reducing the step considerably in regions which are near equilibrium is not associated with any physical peculiarity of the flow, rather it arises from the difference schemes used.

The use of linearization near equilibrium [2] to eliminate this difficulty is inconvenient, first because of the need to carry out tedious computations, particularly for complex chemical systems, and second because of the difficulties related with determining the region of convergence of such linearized solutions. Therefore it is desirable to construct a difference scheme for integrating the kinetic equations which
will permit calculating the entire flow field with an adequately large step without any loss of accuracy. Such a difference scheme was constructed in [3]. The present paper suggests a somewhat different scheme, to obtain which we consider a "model" equation corresponding to the kinetic equations.

The equation of chemical kinetics for the i-th component may be represented in the form

$$\frac{d\alpha_i}{dx} = \Phi_i(\alpha_i^* - \alpha_i).$$

(1.2)

Here $\Phi_i$ is a quantity which is the inverse of the length of the relaxation zone and, in the general case, is a function of $p$, $T$, and all $\alpha_i$, $\alpha_i^*$ is the conditional equilibrium value of $\alpha_i$, a function of $p$, $T$, and all $\alpha_i$ and equal to $\alpha_i^*$ for equilibrium flow with constant entropy. From this equation, making the natural assumption on boundedness of the derivative $d\alpha_i/dx$, we find that as $\Phi_i \to \infty$ the flow approaches equilibrium, i.e., $\alpha_i \to \alpha_i^*$. Let us consider in place of Eq. (1.2) the "model" equation obtained from (1.2) if $\Phi$ and $\alpha_i^*$ are considered constants. The general solution of this "model" equation is written in the form

$$\alpha = (\alpha_0 - \alpha^*) e^{\Phi x} + \alpha^*.$$  

(1.3)

Here $\alpha_0$ is the initial value of $\alpha$ for $x = 0$.

We recall that the exact solution of the differential equation has the form

$$\alpha_{n+1} = (\alpha_0 - \alpha^*) e^{-\Phi h (n+1)} + \alpha^*,$$

(1.7)

since $x = h(n + 1)$.

It follows from (1.7) that as $\Phi h \to 0$, for all $s$ such that $0 < s < 1$ the solution of the difference equation (1.6) approaches the exact solution. However, depending on the magnitude of the parameter $s$, the solution of the difference equation (1.6) has a varying order of accuracy, and the stability of the solution for $\Phi h \gg 1$ also depends on the value of this parameter.

Let us consider three cases: $s = 1$, $s = 0$, $s = 1/2$.

For $s = 1$ the solution of the difference equation has an accuracy of first order. However, for $\Phi h > 1$ calculation using this scheme gives a solution differing quite strongly from the exact solution, and the maximal step with which we can integrate numerically Eq. (1.2) using this scheme, in order to obtain a solution close to the exact solution, is equal to $h \approx 2/\Phi$.

For $s = 1$ the difference scheme (1.4) will be a scheme of the type which is used in the Euler, Runge-Kutta, and similar methods. Therefore these methods permit integrating the equations of chemical kinetics in regions which are near equilibrium, where $\Phi h$ is large, only with a small step $h \approx 2/\Phi$.

In many problems of practical interest in internal gasdynamics the quantity $\Phi$ has the order $10^6-10^9$ m$^{-1}$ and, consequently, $h \approx 1/\Phi \approx 10^{-6}-10^{-8}$ m for $s = 1$.