CALCULATION OF VISCOUS FLOW OF A VIBRATIONALLY NONEQUILIBRIUM GAS MIXTURE IN A HYPERSONIC NOZZLE

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UDC 532.516+541.24

The flow in a two-dimensional nozzle of specified geometry is modeled using simplified Navier–Stokes equations. In contrast to [1], where a single-component gas was studied, we consider here an N_2–CO–Ar–He mixture. We take into account vibrational-translational relaxation and intermolecular transfer of vibrational energy (VT and VV' exchange processes). The mixture transport properties are determined using a series of transformations, which ultimately reduce to a problem only of calculating the viscosity coefficients of the components.

The physical flow model is based on the following assumptions: 1) the gas mixture is thermally perfect and uniformly homogeneous in composition; 2) chemical reactions and dissociation do not occur; 3) rotational degrees of freedom of molecules are in equilibrium with translation; 4) each vibrational mode is a harmonic oscillator with a Boltzmann distribution of energy level populations characterized by its own temperature; and 5) viscosity and thermal conductivity are taken into account, while pressure and thermal diffusion and radiative losses of vibrational energy are neglected.

This model was used in [2] to analyze a CO_2 gasdynamic laser using the "narrow tube" method. The analysis of [2] is based on the equations derived in [3]. In the present work, the mixture transport properties are given in a more sequential form than in [2] and [3]. For this, we use the results of [4], excluding those which arise from the physical model assumed here.

We write the initial system of equations:

$$\frac{\partial (r^{\nu}\rho u)}{\partial x} + \frac{\partial (r^{\nu}\rho v)}{\partial r} = 0, \quad \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} = -\frac{\partial p}{\partial x} + \frac{1}{r^{\nu}}\frac{\partial}{\partial r}\left(r^{\nu}\mu\frac{\partial u}{\partial r}\right),$$

$$\rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial r} = -\frac{\partial p}{\partial r} + \frac{4}{3}\frac{1}{r^{\nu}}\frac{\partial}{\partial r}\left(r^{\nu}\mu\frac{\partial v}{\partial r}\right),$$

$$\rho u c_{p_{\rm a}}\frac{\partial T}{\partial x} + \rho v c_{p_{\rm a}}\frac{\partial T}{\partial r} = u\frac{\partial p}{\partial x} + v\frac{\partial p}{\partial r} + \frac{1}{r^{\nu}}\frac{\partial}{\partial r}\left(r^{\nu}\lambda_{\rm a}\frac{\partial T}{\partial r}\right) + \mu\left(\frac{\partial u}{\partial r}\right)^2 - \rho(\Phi_1 + \Phi_2),$$

$$\rho u \frac{\partial E_i}{\partial x} + \rho v \frac{\partial E_i}{\partial r} = \frac{1}{r^{\nu}}\frac{\partial}{\partial r}\left(r^{\nu}\rho D_i\frac{\partial E_i}{\partial r}\right) + \rho\Phi_i \quad (i = 1, 2), \quad p = \rho\frac{R}{M_{\Sigma}}T.$$

Here

$$\Phi_i = \frac{E_i^0 - E_i}{\tau_i} - (-1)^i\xi_1\xi_2 N\gamma\frac{R\theta_i}{M_{\Sigma}} \ (i=1,2); \ N = \frac{\rho}{M_{\Sigma}}N_{\rm A}; \quad \gamma = K\varphi\exp\left(-\frac{\theta_1}{T}\right);$$

$$\varphi = \frac{E_2}{R\theta_2}\left(1 + \frac{E_1}{R\theta_1}\right)\exp\left(\frac{\theta_2}{T}\right) - \frac{E_1}{R\theta_1}\left(1 + \frac{E_2}{R\theta_2}\right)\exp\left(\frac{\theta_1}{T}\right);$$

where $\nu = 0$ corresponds to planar flow and $\nu = 1$ to axisymmetric; x and r are the longitudinal and lateral coordinates with respect to the nozzle axis; u and v are the longitudinal and lateral velocity components; ρ, p, and T are the density, pressure, and temperature; E_i is the vibrational energy of the i-th component per unit mixture mass; $E_i{}^0$ corresponds to thermal equilibrium; E_i is connected with the mean quantum number e_i of the given vibrational mode and with the vibrational temperature T_i by the relations

$$E_i = \xi_i\frac{R}{M_{\Sigma}}e_i = \xi_i\frac{R}{M_{\Sigma}}\frac{1}{\exp(\theta_i/T_i) - 1};$$

where μ is the kinematic viscosity of the mixture; λ_a is the mixture thermal conductivity; c_p is the mixture specific heat; the index a indicates that a quantity gives the contribution

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Novosibirsk. Translated from Prikladnaya Mekhanika i Tekhnicheskaya Fizika, No. 5, pp. 51-56, September-October, 1992. Original article submitted August 1, 1991.

of the active (translational and rotational) degrees of freedom; $D_i^{-1} = \sum_{k=1}^{I} \xi_k D_{ik}^{-1}$ [4] (D_{ik} are the binary diffusion coefficients and I is the number of mixture components, 4 in the present case); τ_i is the vibrational relaxation time of the i-th molecular species; ξ_i is the molar concentration of the i-th component; θ_i is the characteristic vibrational temperature of the i-th component; R is the universal gas constant; $M_\Sigma = \sum_{i=1}^{I} \xi_i M_i$ is the molecular weight of the mixture; M_i is the molecular weight of the i-th component; i = 1, 2, 3, 4 corresponds to N_2, CO, Ar, He; N_A is Avogadro's number; and K is the rate constant for VV' exchange in the reaction

$$N_2(V = 1) + CO(V = 0) \rightarrow N_2(V = 0) + CO(V = 1).$$

The expression for Φ_i, which includes the rates of VT and VV' exchange, is obtained from the theory of vibrational relaxation of binary mixtures of harmonic oscillators [5]. It is derived from equations giving the rate of change of the mean vibrational quantum number for the N_2 or CO molecule.

The dynamic viscosity of the mixture, in accordance with [6], takes the form

$$\mu = \sum_{i=1}^{I} \mu_i \left(1 + \sum_{\substack{k=1 \\ k \neq i}}^{I} G_{ik} \frac{\xi_k}{\xi_i}\right)^{-1},$$

where

$$G_{ik} = \frac{[1 + (\mu_i/\mu_k)^{1/2} (M_k/M_i)^{1/4}]^2}{(2)^{3/2} [1 + (M_i/M_k)]^{1/2}}.$$

The expression for the mixture thermal conductivity for active degrees of freedom is also taken from [6]:

$$\lambda_a = \sum_{i=1}^{I} \lambda_{a_i} \left(1 + 1{,}065 \sum_{\substack{k=1 \\ k \neq i}}^{I} G'_{ik} \frac{\xi_k}{\xi_i}\right)^{-1}.$$

Here

$$G'_{ik} = \frac{[1 + (\lambda_{t_i}/\lambda_{t_k})^{1/2} (M_i/M_k)^{1/4}]^2}{(2)^{3/2} [1 + (M_i/M_k)]^{1/2}};$$

λ_t is the thermal conductivity with only translation excited. For this we use the relation [7] $\lambda_{t_i} = (15/4)(R/M_i)\mu_i$. Substituting this into the preceding equation, we obtain

$$G'_{ik} = G_{ik}, \quad \lambda_a = \sum_{i=1}^{I} \lambda_{a_i} \left(1 + 1{,}065 \sum_{\substack{k=1 \\ k \neq i}}^{I} G_{ik} \frac{\xi_k}{\xi_i}\right)^{-1}.$$

For the monatomic gases Ar and He, $\lambda_{a_i} = \lambda_{t_i}$ (i = 3, 4). When rotation is excited, the Eucken correction [7] is applied, and for N_2 and CO we have $\lambda_{a_i} \simeq 5(R/M_i)\mu_i$ (i = 1, 2).

Bargaftik [8] arrived at an equation which allowed the calculation of the binary diffusion coefficient from the component self-diffusion coefficients:

$$D_{ik} = \left(\frac{M_i + M_k}{2 (M_i M_k)^{1/2}}\right)^{1/2} (D_{ii} D_{kk})^{1/2}.$$

We use the relation from [7] connecting the self-diffusion and viscosity coefficients:

$$\rho D_{ii} = \frac{6}{5} A^* \mu_i$$

where A* is a very slowly-varying function of temperature, close to unity. Thus, we find that to determine the transport coefficients of the gas mixture, it suffices to know the viscosities of the components. The values of the viscosities used here are taken from tabulation [8].

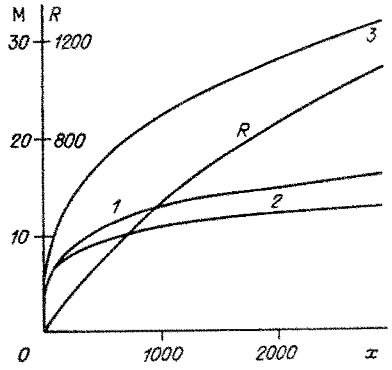

Fig. 1

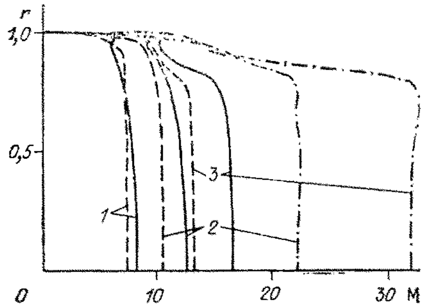

Fig. 2

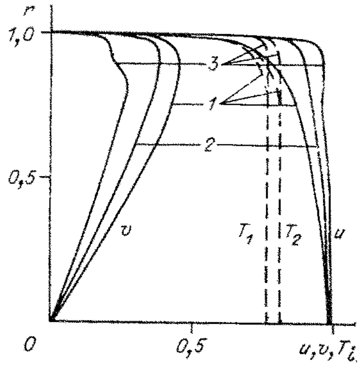

Fig. 3

The mixture specific heat is

$$c_{p_a} = \sum_{i=1}^{I} c_i c_{p_{a_i}},$$

where $c_i = \rho_i/\rho = (M_i/M_\Sigma)\xi_i$; $c_{p_{a_i}} = (5/2)(R/M_i)$ or $(7/2)(R/M_i)$, respectively, for the monatomic molecules He and Ar or the diatomic molecules N_2 and CO with frozen vibrational distributions.

The vibrational relaxation time τ_i for molecules of type i is expressed, in accordance with [9], in terms of the vibrational relaxation time τ_{ik} of gas i when present as a small impurity in gas k:

$$\tau_i^{-1} = \sum_{k=1}^{I} \xi_k \tau_{ik}^{-1} \quad (i = 1, 2).$$

The values of τ_{ik} are approximated by the expression

$$\lg\left[p\tau_{ik}\left(1 - \exp\left(-\frac{\theta_i}{T}\right)\right)\right] = A_1 + A_2 T^{-1/3} + A_3 T^{-2/3}.$$

This equation, as well as the coefficients in it, is taken from [10]. The rate constant for VV' exchange $K = 0.136 \cdot 10^{-15.2+0.0865(T^{-1/3}-0.01)^2}$ cm²/sec and the characteristic temperatures $\theta_1 = 3352$ K, $\theta_2 = 3084$ K are taken from [11].

In this formulation, the system of equations is solved in exactly the same way as in [1]. In the established program, written in FORTRAN, two flows were computed in a conical nozzle with 10° half-angle, both with stagnation conditions $p_0 = 15 \cdot 10^6$ Pa and $T_0 = 1500$ K. In the first flow, the relative mass concentrations of the mixture components were: N_2 0.95, CO 0.01, Ar 0.03, and He 0.01. The computation was performed to validate the modification of the program from the initial program which calculated a single-component gas flow. The computed results for both cases will be presented shortly. In the second flow, the composition was the following: N_2 0.25, CO 0.25, Ar 0.25, and He 0.25. The results are fully realistic, i.e., allow a clear qualitative interpretation. For example, the temperature drop

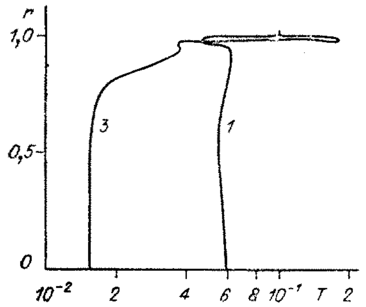

Fig. 4

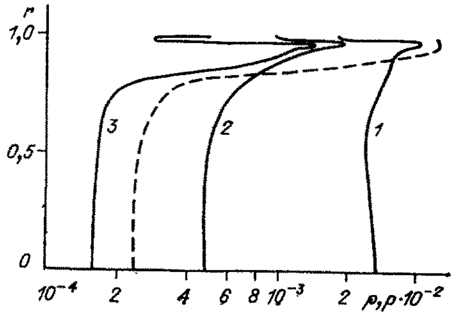

Fig. 5

and the increase in the Mach number M along the nozzle axis occur much faster in the second flow than in the first, which may be explained by the higher concentration of monatomic components in the mixture, and consequently, by the large value of the specific heat ratio $k = c_p/c_V$.

We give results of a computation for a planar nozzle, whose contour is described by the logarithmic function shown as line R in Fig. 1. The flow is composed as follows: N_2 0.1, CO 0.4, Ar 0.5, He 0. The stagnation conditions are $p_0 = 15 \cdot 10^6$ Pa and $T_0 = 3500$ K, with relative wall temperature $T_W/T_0 = 0.1$. In Fig. 1 is shown the variation of M on the axis for the mixture (line 1), and also for flows of N_2 and Ar in this nozzle (lines 2 and 3). In computing the latter flows, the mass concentrations of the other components were set to zero in the program. The distance x is measured from the throat and is nondimensionalized by the throat half-height.

In Fig. 2 are shown the profiles of M in three nozzle sections: x = 200, 1000, and 3000 (lines 1-3, respectively). The lateral distance r is nondimensionalized by the local half-height r_W, so that r = 0 corresponds to the nozzle axis and r = 1 to the nozzle wall. The profiles of M are shown as solid lines for the mixture flow, dashed for the N_2 flow, and dot–dashed for the Ar flow. It may be seen that the three flows, while significantly different quantitatively, have a qualitative similarity. This consists of, first, the presence of a uniform inviscid core, occupying the greater part of the flow area, and second, an overshoot in the boundary layer. We consider the pattern in more detail for the example of the mixture flow; the behavior of the parameters for the pure gases is analogous.

Figure 3 gives profiles of the longitudinal and lateral velocity components, nondimensionalized by the speed $\sqrt{2c_{p_0}T_0}$. The other quantities shown are relative to the stagnation values. The longitudinal velocity profiles are very filled-out, with thin boundary layers. The displacement thickness obtained by the program does not exceed 2% of the half-height along the entire nozzle length. The lateral velocity component is of the same order as the longitudinal. Its maximum is located closer to the wall at distance $0.1r_W$ for x = 200 and 1000 (lines 1 and 2) and shifts to $0.2r_W$ from the wall for x = 3000 (line 3). The largest value of v is obtained at the first section of the nozzle, where the half-angle is 34°, and gradually decreases toward the exit, where the half-angle is 13°. The dashed curves are the vibrational temperature profiles of nitrogen T_1, and of carbon monoxide T_2, at stations x = 200 and 3000. The vibrational temperatures immediately freeze in the entire nozzle, excluding the region near the wall, where a nonequilibrium process occurs due to the assumed equilibrium conditions at the nozzle wall. At the exit, the frozen flow practically fills the nozzle section.

In Fig. 4 are given translational temperature profiles, while Fig. 5 gives profiles of density (notation as in Figs. 2 and 3) and pressure at the station x = 3000 (dashed line). The temperature boundary layer is larger than that of the velocity, over 20% of the flow at the nozzle exit. The sharp drops inside this layer attest that a structure is formed in it, which we interpret as a hanging step along the entire extent of the nozzle wall.

Analysis of these results leads to a conclusion which concerns the method used for this problem. The simplified Navier–Stokes equations, used in the flow computations here, were obtained from the full equations using the assumption that the ratio v/u is small. However, we have found using the simplified model that this ratio is not so small in a nozzle with large entrance half-angle. Because the displacement thickness is small, it would appear that for such a nozzle, a more acceptable approach would consist of a sequential calculation of the inviscid core and of the boundary layer. But using this traditional method, one cannot obtain the formation of a density jump inside the boundary layer, which, apparently, the present method succeeded in capturing. In our opinion, the model based on the simplified Navier–Stokes equations, although not without error, nevertheless gives an adequate picture of the flow.

In conclusion, we note that the algorithm may be extended to calculations of flows of other mixture compositions within the framework of multitemperature relaxation.

The authors express gratitude to V. N. Vetlutskii for useful discussions.

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