EFFECT OF NONEQUILIBRIUM PROCESSES IN THE INFRASONIC AND ULTRASONIC REGIONS OF A NOZZLE ON POPULATION INVERSION IN FLOW OF $CO_2 - N - O_2 - H_2O$ GAS MIXTURES

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The processes of oscillatory relaxation in flow through nozzles of CO_2, N_2, O_2, H_2O gas mixtures are studied. The effect of various oscillatory–oscillatory and osciallatory–translational exchange channels between mixture components and CO_2 intermode energy-exchange channels on population inversion is examined. The importance of considering nonequilibrium processes in the infrasonic region of the nozzle is noted. The effect of inclined shock waves on flow characteristics in the supersonic nozzle region and population inversion is studied.

To obtain high temperatures in aerodynamic studies combustion of all possible hydrocarbon fuels is used. The combustion reaction leads to formation of a gas consisting of a mixture of CO_2, N_2, O_2, H_2O, etc., molecules. The mass composition of this mixture depends on the amount of fuel reacted and the completeness of the combustion. Since the combustion product composition differs significantly from that of air, it is necessary to consider this difference in thermodynamic and transfer properties. The combustion process leads to significant increase in gas temperature and excitation of oscillatory degrees of freedom.

In the present study the problem of nonviscous nonequilibrium flow of a gas mixture in a nozzle will be solved in the quasi-one-dimensional formulation for various converger and diffusor configurations. We will use a system of gasdynamic and kinetic equations which consider the contribution of transitions between highly excited oscillatory levels of various modes of CO_2, N_2, and H_2O. These equations were derived in [1].

Initially, we will consider the effect of considering nonequilibrium processes in the infrasonic nozzle region on flow gasdynamic characteristics, degree of inversion, and amplification coefficient. Gasdynamic nozzles described in the literature which produce population inversion have varying converger configurations, which may be classified as follows: a) curved along radius; b) wedge type; c) hyperbolic.

Figures 1 and 2, show the temperature distribution and the coefficient of amplification for one nozzle, with the point at which consideration of nonequilibrium oscillatory relaxation commences to be considered taken at different sections of the infrasonic region of the nozzle. Calculations were performed for a profiled hyperbolic nozzle with minimum radius $r_{min} = 1$ cm and the following initial conditions: $P_0 = 15$ atm; $T_0 = 2000$°K, and $\alpha_{CO_2} = 0.1$; $\alpha_{N_2} = 0.89$; $\alpha_{H_2O} = 0.01$, where α_i are molar fractions.

Commencing from sections in the infrasonic region corresponding to area ratios $F/F_{min} = 1$; 5; 10, calculation was performed with consideration of nonequilibrium, the flow being regarded as in equilibrium up to this section. It developed that at the minimum nozzle section with consideration of the nonequilibrium character of the flow beginning at sections $F/F_{min} = 5$; 10, in the infrasonic region the difference in temperatures T_3, T_4, and T reached the following values: $T_3 - T = 6$°K; $T_4 - T = 29$°K. Such a small difference between oscillatory and translational flow temperatures is a consequence of the almost equilibrium character of the flow. Nevertheless, because of the nonlinear dependence of population inversion on the oscillatory temperature value the small differences in temperatures T_3 and T_1 from their values calculated with the assumption of equilibrium flow in the converger region of the nozzle finally lead to significant changes

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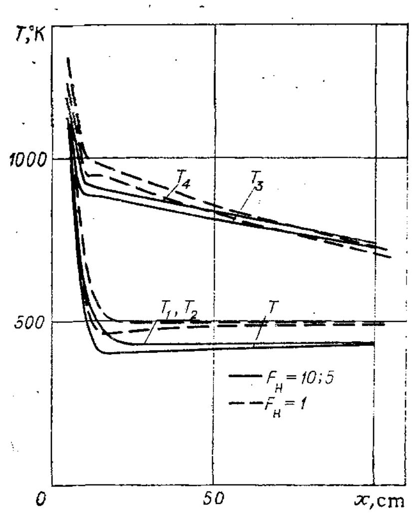

Fig. 1

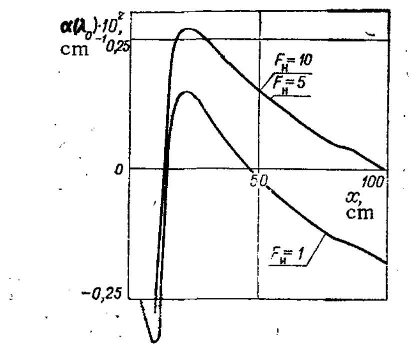

Fig. 2

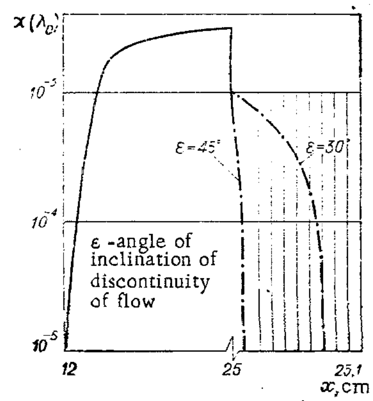

Fig. 3

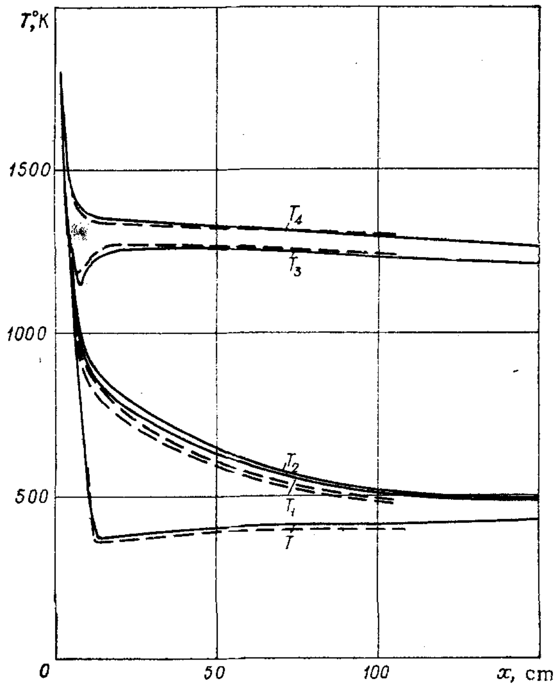

Fig. 4

in inversion. The difference in the case of the variants with consideration of nonequilibrium commencing at $F/F_{min}=5$ or $F/F_{min}=10$ is insignificant (less than 1% for the coefficient of amplification).

Upon consideration of flow nonequilibrium beginning at the minimum section of the nozzle the translational gas temperature proves to be higher, and the entire oscillatory temperature distribution shifts upward (Fig. 1). Then in the working section of the nozzle the temperatures T, T_1, and T_2 are higher than the corresponding temperatures obtained in calculations with consideration of nonequilibrium in the converger. The relaxation rate of the third mode of CO_2 and N_2 is also higher, which leads to more intense exchange between modes and a corresponding drop in population inversion down the flow.

The difference in the maximum value of the coefficient of amplification with consideration of nonequilibrium in the infrasonic nozzle region may reach ~40% of the corresponding value for calculations of a nonequilibrium flow beginning at the nozzle throat (Fig. 2).

In connection with this it must be noted that those systems of kinetic equations which only consider excitation of lower molecular oscillatory levels and on the whole do convey the correct character of physical processes at the low temperatures realized in the working region of the nozzle cease to be valid at the

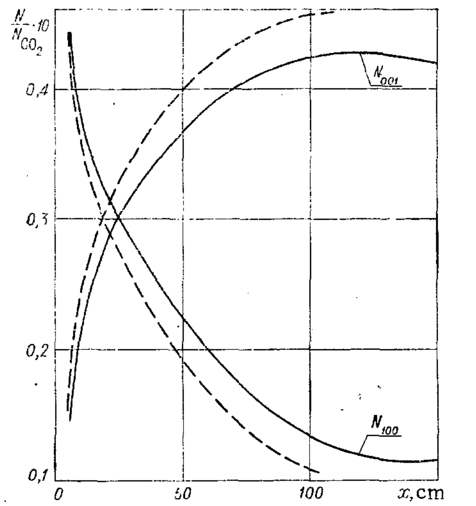

Fig. 5

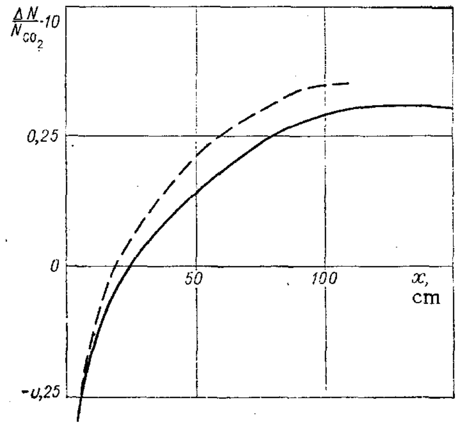

Fig. 6

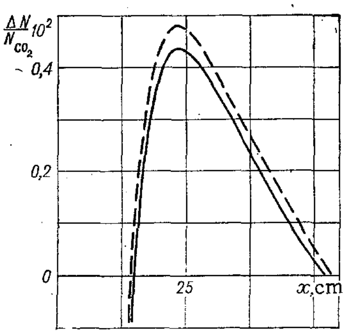

Fig. 7

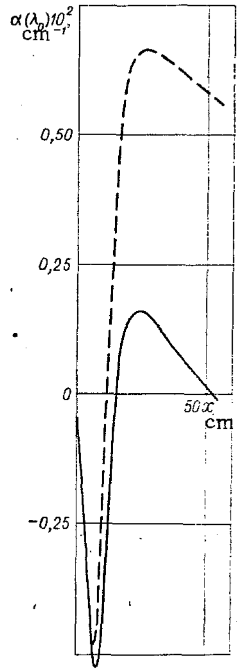

Fig. 8

high temperatures in the infrasonic and transsonic regions of the nozzle. Although simplified kinetic equations do reflect the character of oscillatory temperature behavior (with differences of degrees or tens of degrees), they lead to large discrepancies in the value of the coefficient of amplification (several tens of percent) compared to use of a more complete system of kinetic equations [1].

If the pressure at the nozzle output does not correspond to the calculated value, then we have the appearance of a transverse discontinuity within the nozzle or a transverse or oblique discontinuity at the output. For the case of a profiled nozzle with $T_0 = 2000°K$; $P_0 = 15$ atm; $r_{min} = 1$ cm, and $\alpha_{CO_2} = 0.1$; $\alpha_{N_2} = 0.89$; $\alpha_{H_2O} = 0.01$ the maximum population inversion is reached at a distance of 25 cm from the minimum section. The translational temperature and density at this section are: $T = 427°K$, $\rho = 2 \cdot 10^{-5}$ g/cm^3. Figure 3 shows the change in amplification coefficient at this section upon development of an oblique compression discontinuity. The presence of the discontinuity leads to a decrease in the amplification coefficient. This is because the amplification coefficient behind the discontinuity depends weakly on density and decreases due to the decrease in inversion in the relaxation zone of the shock wave.

We will consider the effect of molecular oxygen on the thermodynamic characteristics of a nonequilibrium flow. Assuming that as a result of fuel combustion there is formed a mixture of molecules CO_2,

N_2, O_2, and H_2O: in addition to the scheme of [2] we will consider the following reactions which describe oscillatory–oscillatory and oscillatory–translational exchange processes between O_2 and other mixture components:

$$O_2(1)+CO_2 \rightleftarrows CO_2(01^10)+O_2,$$
$$N_2(1)+O_2 \rightleftarrows N_2+O_2(1),$$
$$O_2(1)+M \rightleftarrows O_2+M,$$
$$O_2(1)+H_2O \rightleftarrows O_2+H_2O(010),$$

where M is the mass of any of the particles CO_2, N_2, O_2, H_2O.

With the use of [3] and the system of reactions presented, a system of kinetic equations was written, which was then solved simultaneously with the gasdynamic equations. We present below the kinetic equation for oxygen in the notation of [1]:

$$\frac{dy_5}{dx} = \frac{\rho}{um}\Big\{-(1-y_5)\sum_{M}\alpha_M W_{50}(M)\,[y_5 - \exp(-\Delta\varepsilon_{15}/kT)] - \frac{1-y_5}{1-y_2}\alpha_{CO_2}W_{52}\,[y_5 - y_2\exp(-\Delta\varepsilon_{13}/kT)] +$$
$$+\frac{1-y_5}{1-y_4}\alpha_{N_2}W_{45}\,[y_4 - y_5\exp(-\Delta\varepsilon_{11}/kT)] + \frac{1-y_5}{1-y_6}\alpha_{H_2O}W_{65}\,[y_6 - y_5\exp(-\Delta\varepsilon_{16}/kT)]\Big\},$$

where $y_i = \exp(-h\nu_i/kT_i)$; $W_{kl} = P_{kl}Z_{\alpha\beta}$ is the probability of deactivation or energy exchange in one collision ($Z_{\alpha\beta}$, collision frequency); $\Delta\,\varepsilon_j$ is the heat of j-th reaction; u is the velocity; m is the mass; ρ is the density.

The probability of excitation and deactivation processes for oscillatory levels of CO_2, N_2, O_2, H_2O molecules were taken from [2, 4, 5-7], which basically offer values taken from experimental studies. As an example we will present results for the following initial conditions: P_0=15 atm; T_0=2000°K and two mixture compositions: 1) $\alpha_{CO_2}=0.1$; $\alpha_{N_2}=0.89$; $\alpha_{H_2O}=0.01$; 2) $\alpha_{CO_2}=0.1$; $\alpha_{N_2}=0.69$; $\alpha_{O_2}=0.2$; $\alpha_{H_2O}=$ 0.01 for one and the same nozzle with r_{min}=0.1 cm, infrasonic region with hyperboloid profile and asymptotic cone semiangle $\varphi_1=38°$ and profiled diffusor region with area ratio at nozzle end of $F/F_{min}=34$.

Figure 4 shows the temperature distribution. The solid line indicates values for the gas mixture with addition of 20% oxygen and corresponding reduction in nitrogen, while the dashed line is for the mixture without O_2.

It should be noted that in the presence of oxygen the temperatures T_3 and T_4 approach more closely to the translational temperature, while the values T, T_1, T_2 are higher than in the flow without O_2. In other words, oxygen addition creates a flow closer to equilibrium.

The populations of the levels (00°1) and (10°0) of CO_2 molecules for the case considered are shown in Fig. 5. Visible here is a region with population inversion, which is smaller in the presence of the oxygen component. Figure 6 shows corresponding population inversion values, from which it can be concluded that in the given case oxygen reduces the maximum inversion value by 15%.

The probabilities of O_2 deactivation by nitrogen and carbon dioxide gas are 2-3 orders lower than the probability of oxygen exchanges with CO_2, N_2, H_2O, and so in the oxygen kinetic equation only terms considering energy exchange are significant.

It must be noted that the behavior of CO_2 and nitrogen mode temperatures and translational temperature are practically unaffected by consideration of exchange reactions with oxygen, since in the kinetic equations terms describing relaxation of the first and second CO_2 modes and complex exchange ($\nu_3 \rightarrow \nu_1$, ν_2) predominate.

For the case r_{min}=1 cm and identical initial conditions, results are shown in Figs. 7 and 8. From Fig. 7, which shows population inversion, it follows that nonconsideration of exchange reactions leads to an increase in the inversion maximum by 10%.

We note the effect of the exchange reaction between the CO_2 asymmetric mode and the symmetric and deformation modes for mixtures containing oxygen on the value of the weak signal amplification coefficient $\alpha(\lambda_0)$, the expression for which was taken from [8]. It follows from Fig. 8 that without consideration of this reaction the maximum value of the coefficient of amplification proves to be high by a factor of approximately four.

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