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AERO- AND GAS-DYNAMICS OF FLIGHT VEHICLES AND THEIR ENGINES

Calculation of High-Altitude Jets of the Rocket Engine Based on Quasi-Gasdynamic Equations

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Abstract—A method based on the use of quasi-gasdynamic equations is developed for calculating the high-altitude jets flowing into a rarefied gas. The equations of continuity of the gas mixture components and the transport equations for vibrational energies in a quasi-gasdynamic formulation are obtained from the Boltzmann equation. It was shown that when calculating with the use of quasi-gasdynamic equations, the radiation intensity of high-altitude jets is significantly lower than when calculating based on the standard system of Navier–Stokes equations. The calculation results are compared with the available experimental data.

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Studying the molecular aspects of hypersonic flow, shock waves, interstellar media, planetary atmospheres, comets and many other scientific and technical problems requires a deep understanding of the problem of thermal nonequilibrium in the rarefied gas dynamics. Supersonic free jets are often used as a reference system for studying relaxation effects associated with thermal nonequilibrium.

The main parameter that characterizes the degree of rarefaction in the flow is the Knudsen number

$$\mathrm{Kn} = \frac{l}{L}\ , \tag{1}$$

where l is the mean free path of molecules; L is the characteristic linear size of the flow region under consideration. The gas is usually considered continuous if $\mathrm{Kn} < 0.01$. The condition $\mathrm{Kn} > 10$ is typical of free molecular flows, almost without collisions between particles.

For intermediate numbers ($0.01 < \mathrm{Kn} < 10$), gas is considered rarefied. The calculation of such flows is more complicated since, on the one hand, the Navier–Stokes (NS) equations obtained in the approximation $\mathrm{Kn} \to 0$ lose their accuracy in analyzing the indicated regimes; on the other hand, the calculation of such flows by the kinetic theory methods requires unreasonably large computational resources, which is due to the relatively high gas density.

Numerical analysis of such flows can be carried out on the basis of direct simulation methods, namely, Monte Carlo or DSMC methods [1–6]. However, these methods also require huge computational resources.

Therefore, for flows within the range of Knudsen numbers of 0.01 – 10, it is desirable to use simpler models.

The Institute of Applied Mathematics has developed a model that is called the quasi-gasdynamic (QGD) equations [7–9].

This approach is based on the use of a mathematical model that generalizes the system of Navier–Stokes equations, being different from it by an additional dissipative term with a small parameter as a coefficient. The principal and significant difference of the QGD approach from the Navier–Stokes

theory is the use of a space-time averaging procedure for determining the main gas-dynamic values, namely, density, velocity, temperature, etc. The additional time smoothing caused the appearance of additional dissipative terms in the equations, which formally distinguishes the QGD system from the Navier–Stokes system.

The basic conservation equations (quasi-gasdynamic equations written for a rarefied gas mixture) include a continuity equation, an equation of momentum, an equation of energy, equations of vibrational energy, equations of continuity of the gas mixture fractions [10]:

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_i}\left(\rho u_i\right)=\frac{\partial g_i}{\partial x_i}; \tag{2}$$

$$\frac{\partial}{\partial t}\left(\rho u_j\right)+\frac{\partial}{\partial x_i}\left(\rho u_i u_j+p\delta_{ij}\right)=\frac{\partial}{\partial x_i}\left\{\tau\left[\frac{\partial}{\partial x_k}\left(\rho u_k u_i u_j\right)+\frac{\partial}{\partial x_i}\left(u_j p\right)+\frac{\partial}{\partial x_j}\left(u_i p\right)\right]\right\}+\frac{\partial}{\partial x_j}\left[\tau\frac{\partial}{\partial x_i}\left(u_i p\right)\right]; \tag{3}$$

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\rho E\right)+\frac{\partial}{\partial x_i}\left(\rho u_i H\right)=\frac{\partial}{\partial x_i}\left\{\tau\frac{\partial}{\partial x_j}\left[\rho u_j u_i\left(H+\frac{p}{\rho}\right)\right]\right\}\\&+\frac{\partial}{\partial x_i}\left[\tau\frac{\partial}{\partial x_i}\left(\frac{1}{2}u_k^2 p\right)\right]+\frac{\partial}{\partial x_i}\left(\tau h\frac{\partial p}{\partial x_i}\right)+\frac{\partial}{\partial x_i}\left(\frac{1}{\mathrm{Pr}}\tau p\frac{\partial h}{\partial x_i}\right);\end{aligned} \tag{4}$$

$$\frac{\partial}{\partial t}\left(E_{V,m}\right)+\frac{\partial}{\partial x_i}\left(E_{V,m}u_i\right)=\frac{\partial F_{m,i}}{\partial x_i}+\dot{E}_{V,m},\quad m=1,2,...,N_M; \tag{5}$$

$$\frac{\partial \rho_s}{\partial t}+\frac{\partial}{\partial x_i}\left(\rho_s u_i\right)=\frac{\partial g_{s,i}}{\partial x_i}+\dot{w}_s,\quad s=1,2,...,N_C-1. \tag{6}$$

Here u_j is the velocity component in the jth direction; p is the pressure; Pr is the Prandtl number; $E=e+\frac{1}{2}u_k^{\,2}$ is the total energy; e is the specific internal energy; $E_{V,m}$ is the vibrational energy of the mth vibrational mode contained in a unit volume of gas; τ is the relaxation parameter that has the meaning of the Maxwell relaxation time $\tau=\mu/p$; μ is the coefficient of dynamic viscosity; ρ_s is the mass (partial) density of the fraction s; $\dot{w}_s$ is the rate of the fraction s formation as a result of chemical reactions; N_C is the number of fractions in the gas mixture; N_M is the number of oscillatory modes; $\dot{E}_{V,m}$ is the vibrational energy source.

The internal energy of each fraction s consists of translational $e_{T,s}$, rotational $e_{R,s}$, vibrational $e_{V,m}$ and chemical h_s^0 energies and their contribution is proportional to the mass share:

$$e=\sum_{s=1}^{Nc}C_s e_{T,s}+\sum_{s=1}^{Nc}C_s e_{R,s}+\sum_{m=1}^{N_M}C_{s(m)}e_{V,m}+\sum_{s=1}^{Nc}C_s h_s^0, \tag{7}$$

where $C_{s(m)}$ is the mass share of the fraction s, to which the mth vibrational mode belongs.

When using the harmonic oscillator model, the following formula is valid for the vibrational energy

$$e_{V,m}=\frac{r_m R\theta_m}{\exp\left(\theta_m/T_{V,m}\right)-1},\quad m=1,2,...,N_M, \tag{8}$$

where θ_m is the characteristic vibrational temperature of the mth vibrational mode; $T_{V,m}$ is the appropriate vibrational temperature; r_m is the degeneracy order of the mth mode of the molecule; R is the gas constant of the substance. It is obvious that $E_{V,m}=\rho_{s(m)}e_{V,m}$.

The exchange term $\dot{E}_{V,m}$ in Eq. (5) has a physical meaning of exciting or deactivating the vibrational degrees of freedom of molecules in inelastic collisions. This process can occur in several ways, namely, first, by direct transition of the kinetic energy of the colliding molecules into vibrational energy and vice versa (the process of direct excitation or deactivation denoted as T–V (V–T) transition); second, through the exchange of energy between the vibrational degrees of freedom of the colliding molecules (the process of vibrational-vibrational exchange denoted as the V–V transition; V–V transitions can be both intramolecular and intermolecular); and third, due to spontaneous radiative deactivation.

The energy transitions considered in this paper are described in detail in [11].

Basic equations (2)–(6) are obtained on the basis of the theory of quasi-gasdynamic equations [4–6] from the Boltzmann equation.

Mass and vibrational energy fluxes are determined as [10]:

$$g_i = \tau\left[\frac{\partial}{\partial x_j}\left(\rho u_j u_i\right) + \frac{\partial p}{\partial x_i}\right] = \tau\frac{\partial}{\partial x_j}\left(\rho u_j u_i + \delta_{ji} p\right); \tag{9}$$

$$g_{s,i} = C_s g_i + \tau\left(\rho u_j u_i + \frac{1}{\mathrm{Sc}}\delta_{ij} p\right)\frac{\partial C_s}{\partial x_j}; \tag{10}$$

$$F_{m,i} = \frac{\mathrm{E}_{V,m}}{\rho} g_i + \tau\left(\rho u_j u_i + \frac{1}{\mathrm{Pr}}\delta_{ji} p\right)\frac{\partial}{\partial x_j}\left(\frac{\mathrm{E}_{V,m}}{\rho}\right), \tag{11}$$

where Sc is the Schmidt number.

The system is closed by the equation of state

$$p = \rho R T. \tag{12}$$

In terms of numerical solution, the basic system of equations is not much different from the system of Navier–Stokes equations describing a dense gas flow; therefore, the method described in [12,13] and the Universe CFD program developed in Moscow Aviation Institute were used for numerical solution of the basic quasi-gasdynamic equations. To effectively solve the "stiff" equations of vibrational energy transfer, we used the technique described in [14]. When forming the methodology, the ideas presented in [15–18] were applied.

Based on the solution of quasi-gasdynamic equations, spatial distributions of gas-dynamic flow parameters can be obtained. Further, these distributions are used to calculate the jet radiation in the infrared wavelength range.

The physical and mathematical model for calculating the optical characteristics of gas flows with regard to vibrational nonequilibrium is described in detail in [11, 19]. They developed a method for calculating thermal radiation of a vibrationally nonequilibrium gas based on the *k*-distribution method, then obtained formulas for calculating the average bandwidth and the effective Planck function for a vibrationally nonequilibrium gas mixture, and created a database for each fraction, in which the dependence of the absorption coefficient was obtained for different values of wave numbers, temperatures (of all energy modes) and partial pressures of gas fractions.

The most important wavelength ranges for us are the following: in a region of 2.7 μm, the radiation of H_2O with transitions from the upper level of the third mode v_3. The vibrational temperature $T_{\mathrm{H_2O}}\left(v_2\right)$ is the most important for radiation in a region of 6 μm. In a region of 2.7 μm (3400–3800 cm^{-1}), the radiation of CO_2 is associated with transitions from the upper levels $2v_2 + v_3, v_1 + v_3$. A very strong CO_2 radiation line is in a region of 4.3 μm, being associated with transitions from the upper level of the third mode v_3. The CO_2 radiation line is in the region of 4.7 μm.

Since CO_2 and H_2O are usually present in the objects under consideration, a special attention is paid to a range of 2.7–2.9 μm.

To analyze the proposed technique, a jet of liquid-rocket engine of the second stage of the Titan 3B rocket (USA) was considered at altitudes from 110 to 180 km [20].

The analysis presented in [21] shows that in the considered range of altitudes a continuum model can be hardly used for calculation.

The initial data are taken from [20]. Fuel is N_2O_4/A-50. The ratio of oxidizer/fuel (O/F) is 1.880. The nozzle expansion ratio is 49.2.

Here are the parameters at the nozzle exit (in mole fractions): H_2 = 0.0185; H_2O = 0.4652; CO = 0.0141; CO_2 = 0.1051; N_2 = 0.3563; H = 0.0089; NO = 0.0141; OH = 0.0021; sum (O_2, O, N) = 0.0167. The temperature, velocity and pressure at the nozzle exit are respectively equal to: T_a = 1318 K; U_a = 3200 m/s; P_a = 9900 Pa. The nozzle exit angle is 10 deg. The diameter of one nozzle is 1.63 m.

The second stage of the Titan 3B has two nozzles, so the equivalent nozzle radius $R_a = 1.63/2\times2^{0.5} = 1.153$ m was used in the calculations.

The dependence of the flight velocity on altitude, according to [20, p.112], is as follows:

Parameter	Altitude, km							
	100	110	120	130	140	150	160	168
Time after launch, s	220	237	253	275	300	334	368	421
Velocity, m/s	2730	2905	3139	3438	3920	4673	5405	5523

When obtaining the results of calculations, both the Navier–Stokes and quasi-gasdynamic equations are used as basic equations.

For each type of equations, three types of calculations are performed using various combinations of gas dynamics models and methods for calculating radiation.

1. Gas dynamics (taking into account vibrational nonequilibrium), radiation (taking into account vibrational nonequilibrium).

2. Gas dynamics (taking into account vibrational nonequilibrium), radiation (equilibrium calculation using the translational temperature as the determining one).

3. Thermally equilibrium calculation of gas dynamics and radiation.

A comparison was made with the experimental data [20, p. 261].

The wavelength range is 2.65–2.95 μm; jet length is 5 km.

Figures 1, 2, and 3 show the results of calculations using various methods and the comparison with the experimental data (denoted by circles).

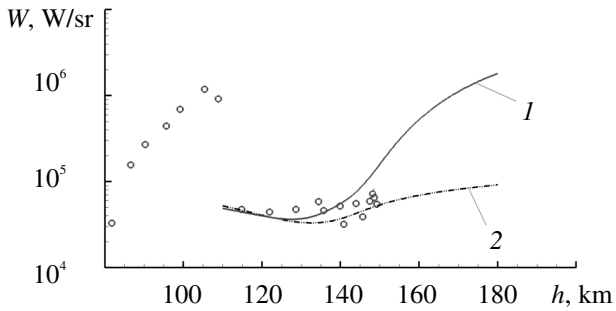

Fig. 1.

Figure 1 presents a plot of radiation intensity versus altitude in the case of thermal nonequilibrium. Here (*1*) the calculation using the Navier–Stokes equations; (*2*) the calculation using the quasi-gasdynamic equations. Model 1 was used.

Figure 2 shows a plot of radiation intensity versus altitude for the calculation using the Navier–Stokes equations. Figure 3 shows a plot of radiation intensity versus altitude in the calculation using quasi-gasdynamic equations. Here: (*1*) model 1; (*2*) model 3; (*3*) model 2.

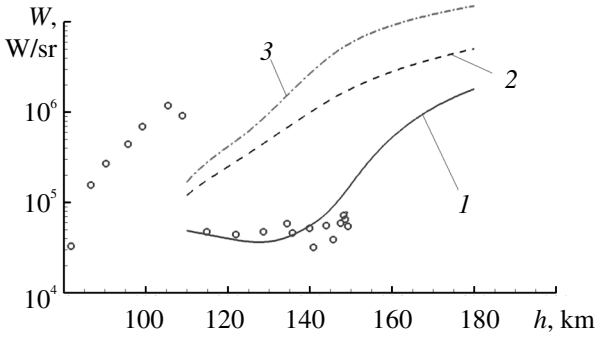

Fig. 2.

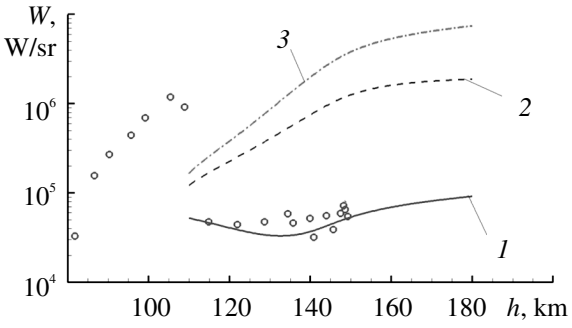

Fig. 3.

Note that Figs. 1–3 do not show the calculation results at the altitudes from 80 to 110 km. This is due to the fact that in the experiment [20] the separation of stages occurs in this part of the flight, which leads to a sharp peak of radiation. This effect is not taken into account in the presented technique.

Analyzing the results, we can come to the following conclusions.

When calculating with the use of QGD equations, the radiation intensity is significantly lower than when calculating with the use of the standard Navier–Stokes equations. This difference begins approximately from an altitude of 125 km, and at an altitude of 180 km it is more than 10 times.

In using the QGD equations, the radiation intensity in the considered range is practically independent of the flight altitude. Lower radiation intensity obtained using the QGD equations, in comparison with NS, is due to the fact that the temperatures (translational, rotational, and vibrational) in the layer of jet mixing with the surrounding air have a lower value. This effect is the most important within the wavelength range around 2.7 μm, since the use of the QGD equations leads to a significant decrease in the vibrational temperatures corresponding to radiation in this range.

The calculation using the assumption of thermal equilibrium (i.e., equilibrium between all energy modes) leads to completely non-physical results, namely, the radiation is overestimated by one–two orders of magnitude.

It is noteworthy that a strong increase in radiation observed during the experiments at altitudes of 90–110 km is associated with the separation of the first and second stages of the rocket.

In conclusion, it should be noted that in terms of computational resources, the calculation using the QGD equations is comparable to the solution of the standard Navier–Stokes equations and much more economical than the direct numerical simulation methods—the Monte Carlo methods.

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