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Preliminary numerical study of three-temperature model investigation of hypersonic oxygen flow under rotational nonequilibrium

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The effect of rotational nonequilibrium on the macroscopic parameters of the flow behind a normal shock wave in oxygen gas flow has been examined. The electron thermal equilibrium was taken into account where the electron temperature was equal to the vibrational temperature according to Park's assumption. Therefore, only the effect of rotational nonequilibrium on the translational and vibrational temperature was analyzed. Rotational and vibrational relaxation time for the O₂-O₂ and O₂-O collisions proposed recently by Andrienko and Boyd are used. Also, the O₂ dissociation rates proposed by Kim and Park are used. The results obtained with the three-temperature model well reproduce the data obtained in shock tube for the shock velocity of 4.44 km/s.

Keywords: hypersonic, nonequilibrium, shock wave, rotation, vibration, oxygen flow.

To date, many authors prefer to use in their hypersonic simulations the Park's two-temperature model which takes into account the approximation of the equilibrium between the translation and rotation modes [1–4]. This brief communication focuses on the effect of the rotational nonequilibrium phenomena behind a normal shock wave for the oxygen flow. To simulate this case, the flow was considered as a reactive mixture of the five species O₂, O, O₂⁺, O⁺, and e⁻ with eight elementary reactions including dissociation, charge exchange, associative ionization, and electron impact ionization reactions. The reaction rates are calculated using the modified Park93 chemical kinetic model [5] including the O₂ dissociation rates proposed by Kim and Park [6]. The 1D Euler equations with rotational and vibrational nonequilibrium source terms are solved just behind the normal shock wave using the finite difference method. The conservation equations of the flow are:

Equation of continuity, momentum, and energy:

$$\frac{d(\rho u)}{dx} = 0, \quad \frac{d(\rho u^2 + p)}{dx} = 0, \quad \frac{d(p + \rho e)u}{dx} = 0 \quad (1)$$

The equation of relaxation of the chemical species, the rotational and vibrational energy continuity:

$$\frac{d(\rho_s u)}{dx} = \omega_{c,s}, \quad \frac{d(\rho_s e_{r,s} u)}{dx} = \omega_{RT,s} + \omega_{CR,s}, \quad \frac{d(\rho_s e_{v,s} u)}{dx} = \omega_{VT,s} + \omega_{CV,s} \quad (2)$$

The pressure of the gas mixture is given by the Dalton's law of partial pressures:

$$p = \sum_{s \neq e}^4 p_s + p_e = \sum_{s \neq e}^4 \rho_s \frac{R}{M_s} T + \rho_e \frac{R}{M_e} T_v, \quad (3)$$

where e is the total energy per unit mass which include translational, rotational, and vibrational energies, the enthalpies of formation of the species, the species electronic energy, the electron energy and the kinetic energy [4]. The model used for calculating the energy exchange between translational-vibrational modes $\omega_{VT,s}$ and translational-rotational modes $\omega_{RT,s}$ have the Landau–Teller form with high-temperature correction of Park [7].

$$\omega_{VT,s} = \rho_s \left((1-f) \frac{e_{v,s}(T) - e_{v,s} \left(\frac{T_{ch} - T_{v,s}}{T_{ch} - T_{v,s, ch}} \right)^{s-1}}{\tau_{MW,s} + \tau_{\rho,s}} + f \frac{e_{v,s}(T_{r,s}) - e_{v,s}}{\tau_{MW,s}} \right), \quad (4)$$

where: $s = 3.5 \exp(-5000/T_{ch})$. T_{ch} and $T_{v,s, ch}$ are the translational and the vibrational temperature evaluated just behind the shock wave.

$$\omega_{RT,s} = \rho_s \left(\frac{e_{r,s}(T) - e_{r,s}}{\tau_{r,s}} + f \frac{e_{v,s} - e_{v,s}(T_{r,s})}{\tau_{MW,s}} \right) \quad (5)$$

The vibration-chemistry $\omega_{CV,s}$ and rotation-chemistry $\omega_{CR,s}$ exchange are employed by the Candler and McCormack formula [8].

$$\omega_{CV,s} = e_{v,s} \omega_{c,s}, \quad \omega_{CR,s} = e_{r,s} \omega_{c,s}, \quad (6)$$

f is the fractional contribution of the rotation-to-vibration energy transfer to the total energy transfer. Kim and Boyd [9] suggested that the value of f is

$$f = \frac{(\xi_{vib,s}/2)RT}{(\xi_{rot,s}/2)RT + 1.5RT}, \quad (7)$$

$\xi_{vib,s} = 2(\theta_{v,s}/T)/(\exp(\theta_{v,s}/T) - 1)$ and $\xi_{rot,s} = 2$ represents the number of degrees of freedom of the vibrational and rotational modes, respectively. Instead of using the Millikan–White relaxation time for the O_2 - O_2 collisions, the relaxation time of Ibragimova et al. [10] was used and is given by:

$$p\tau_{v,O_2-O_2} = 8.8 \times 10^{-14} \exp(172.7T^{-1/3})T^{0.5} / (1 - \exp(\theta_{v,s}/T)), \quad (8)$$

where p must be given in atmospheres. The rotational relaxation time for the O_2 - O_2 collisions proposed by Hanquist and Boyd [11] is given by:

$$p\tau_{r,O_2-O_2} = 3.0173 \times 10^{-10} T^{0.611}. \quad (9)$$

For the O_2 - O collisions, the rotational and vibrational relaxation time proposed by Andrienko and Boyd [12] was used according to the following function:

$$p\tau_{x,O_2-O} = 10^{-8} \left[A \left(\frac{T}{1000} \right)^3 + B \left(\frac{T}{1000} \right)^2 + C \left(\frac{T}{1000} \right) + D \right] \quad (10)$$

Table 1

Coefficients of the vibrational and rotational relaxation time [12]

| x | A | B | C | D |
|-------------------|-------------------------|-------------------------|-------|------------------------|
| $p\tau_{v,O_2-O}$ | 1.576×10^{-4} | -9.543×10^{-3} | 2.232 | 1.385 |
| $p\tau_{r,O_2-O}$ | -3.764×10^{-5} | -6.211×10^{-3} | 1.331 | 2.451×10^{-1} |

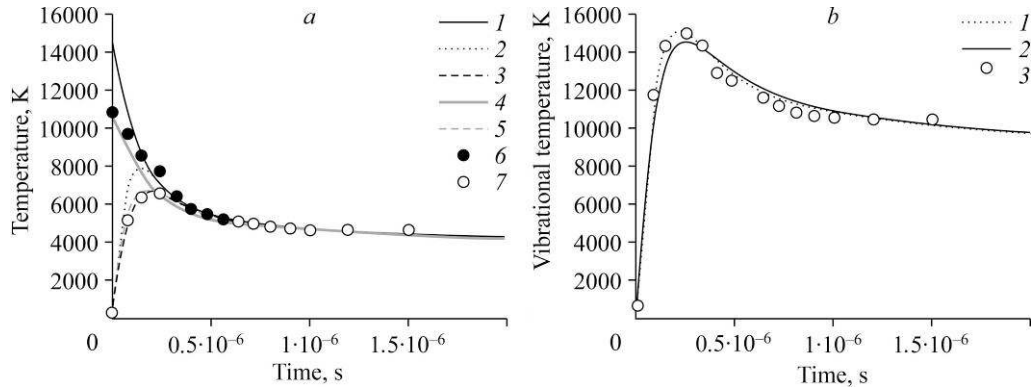


Fig. 1. Evolution of temperature profiles compared to results of [10] (a).

Vibrational temperature profile with different values of the arbitrary parameter s (b).

a — calculations for T according to the 3T (1) and 2T (4) models and for T_r according to the 3T model (2), as well as for T_v according to the 3T (3) and 2T (5) models and experimental data [10] for T (6) and T_v (7);

b — calculation at $s' = 2$ (1) and 3.5 (2) and experimental data [10] for T_v (3).

Figure 1a presents the evolution of the translational, rotational, and vibrational temperature just behind the shock wave using 2T and 3T model. The highest experimental freestream condition of [10] in which shock velocity of 4.44 km/s ($M=13.4$) with ambient pressure of 0.8 torr (106.66 Pa) is selected as a test case. Using the Rankine–Hugoniot relation, the translation temperature reaches 14000 K behind the shock wave then decreases slowly to reach the equilibrium value; in contrast a strong rotational and vibrational nonequilibrium was observed. This decrease is mostly the result of the absorption of the kinetic energy of the molecules due to their molecular rotation and vibration and also by the chemical reactions such as dissociation and ionization which are endothermic reactions. In the nonequilibrium region, the rotational relaxation time is faster than the vibrational relaxation time and, therefore, the rotational temperature is higher than the vibrational temperature. Concerning the comparison of the results, it should be noted that the dissociation rates for the three-temperature model are slower than those of two-temperature model and, therefore, the relaxation zone increases while the translation and vibration temperature becomes much closer to the measured values.

The correction of the vibrational relaxation was proposed by Park to take into account the diffusion nature that occurs at high temperatures (higher than 5000 K for N_2). The bridging formula between the Landau–Teller model ($s = 1$) and the diffusion model ($s = 3.5$ [5]) for the nitrogen flow have the form $s = s' \exp(-5000/T_{ch})$ with $s' = 3.5$. According to this formula, the overall vibrational temperature decreases when s' increases. For example, Fig. 1b shows that change of s' from 3.5 to 2 increases considerably the vibrational temperature peak, leading to a good agreement with the experimental data.

Figure 2 shows the molar-mass concentration of O_2 and density profiles vs time. The initial molar-mass concentration of O_2 in the study of [10] is equal to $(0.0625/2=0.03125 \text{ mol/g})$ equivalent to $(1/0.03125=32 \text{ g/mol})$ which is the molar mass of O_2 and, therefore, the pure oxygen was used as a test case. The results show satisfactory agreement concerning the molar-mass concentration. However, the calculated density deviates from measured values for both 2T and 3T model but the results can be considered acceptable due to the lower density. In the 2T model, the dissociation rate occurs faster than in the 3T model. According to [13], the vibrational and rotational degrees of freedom do not completely equilibrate before dissociation occurs at higher temperatures (above 5000 K). This means that a slow dissociation occurs under rotational and vibrational nonequilibrium (3T model) compared to the 2T model under vibrational nonequilibrium with rotational equilibrium.

Even in this medium hypersonic speed condition, the obtained results show that the rotational nonequilibrium slightly increases the thickness of the relaxation zone and, therefore, the translational and vibrational temperature becomes closer to experimental data. Consequently,

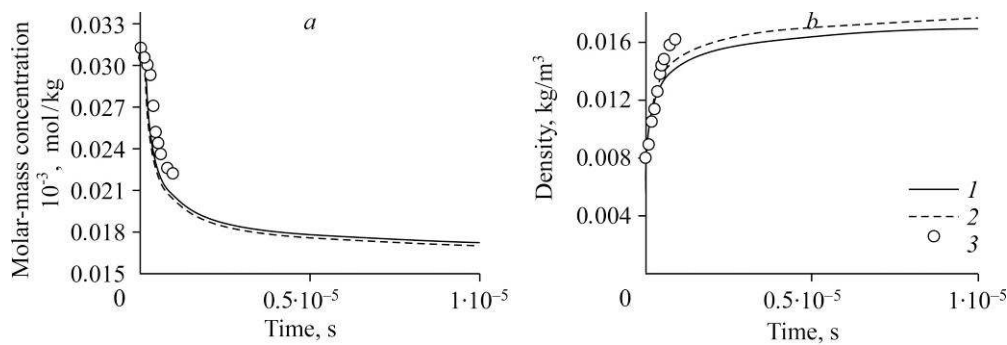


Fig. 2. The molar-mass concentration of O₂ and density profiles.
Calculations using models 3T (1) and 2T (2) and experimental data [10] (3).

rotational nonequilibrium is important for hypersonic flow and must be taken into account whatever the selected flow such as oxygen, nitrogen or air flow. Also, this work uses the three-temperature model assuming Boltzmann distribution of the vibrational level population which is the standard assumption. However, recent papers [14,16] show some deviations of the real vibrational level population from the Boltzmann one. In fact, in these experiments, population of the highest vibrational energy level were not taken into account. A more suitable numerical method using the state-to-state (STS) approach will be the scoop of a future work.

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