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:

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

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

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The pressure of the gas mixture is given by the Dalton’s law of partial pressures:
\[
p = \sum_{s \in e} p_s + p_e = \sum_{s \in e} \rho_s \frac{R}{M_s} T + \rho_e \frac{R}{M_e} T_v,
\]
(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 Lnadau–Teller form with high-temperature correction of Park [7].

\[
\omega_{VT,s} = \rho \left( (1 - f) \frac{e_{vs}(T) - e_{vs}}{\tau_{MW,v}} + f \frac{e_{vs}(T_{v,s}) - e_{vs}}{\tau_{MW,v}} \right),
\]
(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.

\[
\omega_{RT,s} = \rho \left( \frac{e_{rs}(T) - e_{rs}}{\tau_{r,s}} + f \frac{e_{rs}(T_{r,s}) - e_{rs}}{\tau_{MW,r}} \right)
\]
(5)

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

\[
\omega_{CV,s} = e_{vs} \omega_{vs}, \quad \omega_{CR,s} = e_{vs} \omega_{rs},
\]
(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

\[
f = \frac{(\xi_{vch,v}^2)}{RT} \left( \frac{\xi_{vch,v}^2}{RT} + 1.5RT \right),
\]
(7)

\( \xi_{vch,v} = 2(\theta_{v,s}/T)^{-1} \) and \( \xi_{vch,v} = 2 \) represents the number of degrees of freedom of the vibrational and rotational modes, respectively. Instead of using the Millikan–White relaxation time for the O₂-O₂ collisions, the relaxation time of Ibragimova et al. [10] was used and is given by:

\[
p_{\tau,v,O_2-O_2} = 8.8 \times 10^{-14} \exp(172.7T^{-1/3}) T^{0.5} / \left( 1 - \exp(\theta_{v,s}/T) \right),
\]
(8)

where \( p \) must be given in atmospheres. The rotational relaxation time for the O₂-O₂ collisions proposed by Hanquist and Boyd [11] is given by:

\[
p_{\tau,r,O_2-O_2} = 3.0173 \times 10^{-10} T^{0.611}.
\]
(9)

For the O₂-O collisions, the rotational and vibrational relaxation time proposed by Andrienko and Boyd [12] was used according to the following function:

\[
p_{\tau,s,O_2-O} = 10^{-8} \left[ A \left( \frac{T}{1000} \right)^3 + B \left( \frac{T}{1000} \right)^2 + C \left( \frac{T}{1000} \right) + D \right]
\]
(10)

| \( X \) | \( A \) | \( B \) | \( C \) | \( D \) |
| --- | --- | --- | --- | --- |
| \( p_{\tau,v,O_2-O_2} \) | 1.576×10^{-4} | -9.543×10^{-3} | 2.232 | 1.385 |
| \( p_{\tau,r,O_2-O_2} \) | -3.764×10^{-3} | -6.211×10^{-3} | 1.331 | 2.451×10^{-1} |
Figure 1 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 translational 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 N2). 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/Tch) 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 O2 and density profiles vs time. The initial molar-mass concentration of O2 in the study of [10] is equal to (0.0625/2=0.03125 mol/g) equivalent to (1/0.03125=32 g/mol) which is the molar mass of O2 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,
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.

References
1. G.V. Shoev, Ye.A. Bondar, G.P. Oblapenko, and E.V. Kustova, Development and testing of a numerical simulation method for thermally nonequilibrium dissociating flows in ANSYS Fluent, Thermophysics and Aeromechanics, 2016, Vol. 23, No. 2, P. 151–163.
2. Ye.A. Bondar, A.A. Shevyrin, Y.S. Chen, A.N. Shumakova, A.V. Kashlovsky, and M.S. Ivanov, Direct Monte Carlo simulation of high-temperature chemical reactions in air, Thermophysics and Aeromechanics, 2013, Vol. 20, No. 5, P. 553–564.
3. O.V. Kovala, G.V. Shoev, and A.N. Kudryavtsev, Numerical simulation of nonequilibrium flows by using the state-to-state approach in commercial software, Thermophysics and Aeromechanics, 2017, Vol. 24, No. 1, P. 7–17.
4. Y. Ghezali, R. Haoui, and A. Chpoun, Study of physico-chemical phenomena in non-equilibrium hypersonic air flow behind strong shock wave, Thermophysics and Aeromechanics, 2019, Vol. 26, No. 5, P. 693–710.
5. C. Park, Review of chemical-kinetic problems of future NASA missions. I-Earth entries, J. Thermophysics and Heat Transfer, 1993, Vol. 7, P. 385–398.
6. J.G. Kim and G. Park, Thermochemical nonequilibrium parameter modification of oxygen for a two-temperature model, Phys. Fluids, 2018, Vol. 30, Iss. 1, P. 016101-1–016101-19.
7. C. Park, Rotational relaxation of N2 behind a strong shock wave, J. Thermophysics and Heat Transfer, 2004, Vol.18, No.4, P. 527–533.
8. G. Candler and R. MacCormack, Computation of weakly ionized hypersonic flows in thermochemical nonequilibrium, J. of Thermophysics and Heat Transfer, 1991, Vol. 5, No. 3, P. 266–273.
9. J. Kim and I. Boyd, Master equation analysis of post normal shock waves of nitrogen, J. of Thermophysics and Heat Transfer, 2015, Vol. 29, No.2, P. 241–252.
10. L.B. Ihragunova, A.L. Sergievskaya, V.Y. Levashov, O.P. Shatalov, Y.V. Tunik, and I.E. Zabelinskii, Investigation of oxygen dissociation and vibrational relaxation at temperatures 4000–10800 K, J. Chem. Phys., 2013, Vol. 139, Iss. 3, P. 034317-1–034317-10.
11. K. Hanquist and I. Boyd, Modeling of excited oxygen in post normal shock waves, in: Joint Thermophysics and Heat Transfer Conference, 2018, AIAA 2018-3769.
12. D. Andrienko and I. Boyd, Rovibrational energy transfer and dissociation in O2-O, J. Chem. Phys., 2016, Vol. 144, Iss. 10, P. 104301-1–104301-19.
13. D. Andrienko and I. Boyd, High fidelity modeling of thermal relaxation and dissociation of oxygen, 54th AIAA Aerospace Sciences Meeting, 2016, AIAA 2016-0736.
14. L.J. Wysong, S.F. Gimelstein, N.E. Bykova, O.P. Shatalov, and I.E. Zabelinski, Impact of flow nonequilibrium in oxygen shock absorption analysis, in: AIP Conference Proceedings, 2019, Vol. 2132. P. 180008-1–180008-8.
15. J. Hao and C.-Y. Wen, Maximum entropy modeling of oxygen vibrational excitation and dissociation, Phys. Rev. Fluids, Vol. 4, Iss. 5, P. 053401-1–053401-17.
16. J. Hao, J. Wang, and C. Lee, State-specific simulation of oxygen vibrational excitation and dissociation behind a normal shock, Chemical Phys. Letters, Vol. 681, P. 69–74.