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State-to-State Modeling of Non-Equilibrium Air Nozzle Flows

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Abstract. One-dimensional non-equilibrium air flows in nozzles are studied on the basis of the state-to-state description of vibrational-chemical kinetics. Five-component mixture $N_2/O_2/NO/N/O$ is considered taking into account Zeldovich exchange reactions of NO formation, dissociation, recombination and vibrational energy transitions. The equations for vibrational and chemical kinetics in a flow are coupled to the conservation equations of momentum and total energy and solved numerically for different conditions in a nozzle throat. The vibrational distributions of nitrogen and oxygen molecules, number densities of species as well as the gas temperature and flow velocity along a nozzle axis are analysed using the detailed state-to-state flow description and in the frame of the simplified one-temperature thermal equilibrium kinetic model. The comparison of the results showed the influence of non-equilibrium kinetics on macroscopic nozzle flow parameters. In the state-to-state approach, non-Boltzmann vibrational distributions of N_2 and O_2 molecules with a plateau part at intermediate levels are found. The results are found with the use of the complete and simplified schemes of reactions and the impact of exchange reactions, dissociation and recombination on variation of vibrational level populations, mixture composition, gas velocity and temperature along a nozzle axis is shown.

INTRODUCTION

Modeling non-equilibrium kinetics in the flows in nozzles and jets is very important for problems of gas dynamics and laser physics. Rapid expansion in a nozzle of a preliminary heated gas calls strong decrease in the gas temperature and pressure. In this case, the vibrational energy in a flow exceeds significantly the translational energy and strongly non-equilibrium effects should be taken into account while modeling vibrational and chemical kinetics in nozzles. Non-equilibrium vibrational distributions in nozzle flows and their influence on macroscopic flow parameters are studied by many authors in different approaches. The use of the most accurate state-to-state flow description requires the solution of many equations for vibrational level populations of air molecules. The multi-temperature flow models include less equations, however they are also complicate due to the necessity to take into account strongly non-equilibrium vibrational distributions. In the majority of papers, strongly non-equilibrium vibrational-dissociation kinetics in nozzle flows is studied for binary mixtures N_2/N and O_2/O (see for instance [1, 2]). State-to-state and multi-temperature description for nozzle flows of the five-component reacting mixture $N_2/O_2/NO/N/O$ is considered in [3, 4, 5, 6, 7, 8].

In the present paper, quasi-one-dimensional non-equilibrium flows of a 5-component air mixture are studied in the frame of the state-to-state approximation taking into account Zeldovich exchange reactions of NO formation, dissociation, recombination and various vibrational energy transitions. The equations for vibrational level populations of N_2 and O_2 molecules and number densities of species are coupled to the conservation equations of momentum and total energy and solved numerically for different conditions in a nozzle throat. The vibrational distributions, mixture composition, the gas temperature and flow velocity along a nozzle axis are studied.

Formation of non-equilibrium non-Boltzmann distributions of N_2 and O_2 molecules with a plateau part at intermediate vibrational levels is shown for different conditions in a throat. The impact of various vibrational energy transitions and chemical reactions on vibrational distributions and macroscopic mixture parameters is estimated. The results also showed the influence of a noticeable discrepancy in level populations found in the state-to-state and one-temperature approaches on nozzle flow parameters.

KINETIC SCHEME AND GOVERNING EQUATIONS

The flows of five-component air mixture $N_2/O_2/NO/N/O$ are studied under the condition of thermal equilibrium distributions over velocities and rotational energies and taking into account non-equilibrium processes of vibrational and chemical relaxation.

This assumption corresponds to the following relations for the relaxation times of translational τ_{el} , rotational τ_{rot} , vibrational τ_{vibr} degrees of freedom and chemical reactions τ_{react} :

$$\tau_{el} \lesssim \tau_{rot} \ll \tau_{vibr} < \tau_{react} \sim \theta, \quad (1)$$

where θ is the mean time of variation of macroscopic flow parameters.

This relation is well known from experimental results [9] for high temperature flows when translational and rotational equilibration proceeds much faster comparable to vibrational and chemical relaxation.

The considered kinetic scheme includes dissociation and recombination



and Zeldovich exchange reactions



Here i is vibrational state of reagents. In this paper, vibrational excitation of NO molecules is not taken into account. Since these molecules present a small part of the mixture, their vibrational excitation is neglected and NO molecules are considered in the 0-th vibrational state. This assumption is often accepted in calculations, more accurate NO description in shock heated air flows is proposed recently in [10]. We study steady-state and one-dimensional nozzle flow of air mixture, the gas is supposed to be inviscid and non-conductive.

The closed set of equations for vibrational level populations of oxygen and nitrogen molecules $n_{O_2,i}$, $n_{N_2,i}$, number densities of atoms n_O , n_N and NO molecules n_{NO} , gas temperature T and velocity v may be written in the form:

$$\frac{d}{dx}(n_{c,i}vS) = S(R_{c,i}^{vibr} + R_{c,i}^{2 \leftrightarrow 2} + R_{c,i}^{2 \leftrightarrow 3}), \quad c = N_2, O_2, \quad i = 0, 1, \dots, l_c, \quad (8)$$

$$\frac{d}{dx}(n_c v S) = S(R_c^{2 \leftrightarrow 2} + R_c^{2 \leftrightarrow 3}), \quad c = NO, N, O, \quad (9)$$

$$\rho v \frac{dv}{dx} + \frac{dp}{dx} = 0, \quad (10)$$

$$S v \frac{dE}{dx} + (p + E) \frac{d(Sv)}{dx} = 0. \quad (11)$$

Here x is the distance from the throat, v is the flow velocity along the nozzle axis, $S(x)$ is the nozzle cross-section, $\rho = \sum_{c=1}^5 m_c n_c$ is the gas density, m_c is a particle mass, $p = nkT$ is the pressure, $n = \sum_{c=1}^5 n_c$, k is the Boltzmann constant, E is the total energy per unit volume:

$$E = \frac{3}{2}nkT + \sum_{c=N_2, O_2} n_c kT + \sum_{c=N_2, O_2, NO} \sum_{i=0}^{l_c} \varepsilon_i^c n_{c,i} + \varepsilon_0^{NO} n_{NO} + \varepsilon_{NO} n_{NO} + \varepsilon_N n_N + \varepsilon_O n_O,$$

ε_i^c is the vibrational energy of a molecule of species c at the i -th vibrational level, ε_c is the formation energy of a particle of c -th species.

For vibrational energies of N_2 and O_2 molecules, the anharmonic oscillator model is used and the numbers l_c of excited vibrational levels are taken as $l_{N_2}=46$, $l_{O_2}=35$. In this case we have 88 equations in the system (8)–(11).

Source terms $R_{c,i}^{vibr}$ of equations (8), (9) describe the change of vibrational level populations due to vibrational-translational VT energy transitions and VV and VV' vibrational energy exchanges between molecules of the same or different species: $R_{c,i}^{vibr} = R_{c,i}^{VT} + R_{c,i}^{VV} + R_{c,i}^{VV'}$. In the case if only single-quantum energy transitions are considered we have:

$$\begin{aligned} R_{c,i}^{VT} &= \sum_{M=N_2, O_2, NO, N, O} n_M (n_{c,i-1} k_{c,i-1 \rightarrow i}^M - n_{c,i} k_{c,i \rightarrow i-1}^M + n_{c,i+1} k_{c,i+1 \rightarrow i}^M - n_{c,i} k_{c,i \rightarrow i+1}^M), \\ R_{c,i}^{VV} &= \sum_{m=0}^{l_c-1} (n_{c,i-1} n_{c,m+1} k_{c,i-1 \rightarrow i}^{c,m+1 \rightarrow m} - n_{c,i} n_{c,m} k_{c,i \rightarrow i-1}^{c,m \rightarrow m+1}) + \sum_{m=1}^{l_c} (n_{c,i+1} n_{c,m-1} k_{c,i+1 \rightarrow i}^{c,m-1 \rightarrow m} - n_{c,i} n_{c,m} k_{c,i \rightarrow i+1}^{c,m \rightarrow m-1}), \\ R_{c,i}^{VV'} &= \sum_{m=0}^{l_d-1} (n_{c,i-1} n_{d,m+1} k_{c,i-1 \rightarrow i}^{d,m+1 \rightarrow m} - n_{c,i} n_{d,m} k_{c,i \rightarrow i-1}^{d,m \rightarrow m+1}) + \sum_{m=1}^{l_d} (n_{c,i+1} n_{d,m-1} k_{c,i+1 \rightarrow i}^{d,m-1 \rightarrow m} - n_{c,i} n_{d,m} k_{c,i \rightarrow i+1}^{d,m \rightarrow m-1}), \end{aligned}$$

where $k_{c,i+1 \rightarrow i}^M$, $k_{c,i \rightarrow i+1}^M$ and $k_{c,i+1 \rightarrow i}^{d,m+1 \rightarrow m}$, $k_{c,i \rightarrow i+1}^{d,m \rightarrow m+1}$ are the rate coefficients for VT , VV ($d = c$), VV' ($d \neq c$) transitions correspondingly.

Production terms for dissociation-recombination and exchange reactions have the form

$$\begin{aligned} R_{N_2,i}^{2 \leftrightarrow 3} &= \sum_{M=N_2, O_2, NO, N, O} n_M (n_N^2 k_{rec, N_2, i}^M - n_{N_2, i} k_{N_2, i, diss}^M), & R_{N_2,i}^{2 \leftrightarrow 2} &= \sum_{i'=0}^{l_{NO}} (n_{NO, i} n_N k_{NO \rightarrow N_2, i}^{N \rightarrow O} - n_{N_2, i} n_O k_{N_2, i \rightarrow NO}^{O \rightarrow N}), \\ R_{O_2,i}^{2 \leftrightarrow 3} &= \sum_{M=N_2, O_2, NO, N, O} n_M (n_O^2 k_{rec, O_2, i}^M - n_{O_2, i} k_{O_2, i, diss}^M), & R_{O_2,i}^{2 \leftrightarrow 2} &= \sum_{i'=0}^{l_{NO}} (n_{NO, i} n_O k_{NO \rightarrow O_2, i}^{O \rightarrow N} - n_{O_2, i} n_N k_{O_2, i \rightarrow NO}^{N \rightarrow O}), \\ R_{NO}^{2 \leftrightarrow 3} &= \sum_{M=N_2, O_2, NO, N, O} n_M (n_N n_O k_{rec, NO}^M - n_{NO} k_{NO, diss}^M), & R_{NO}^{2 \leftrightarrow 2} &= - \sum_{i=0}^{l_{N_2}} R_{N_2, i}^{2 \leftrightarrow 2} - \sum_{i=0}^{l_{O_2}} R_{O_2, i}^{2 \leftrightarrow 2}, \\ R_N^{2 \leftrightarrow 3} &= -2 \sum_{i=0}^{l_{N_2}} R_{N_2, i}^{2 \leftrightarrow 3} - R_{NO}^{2 \leftrightarrow 3}, & R_N^{2 \leftrightarrow 2} &= - \sum_{i=0}^{l_{N_2}} R_{N_2, i}^{2 \leftrightarrow 2} + \sum_{i=0}^{l_{O_2}} R_{O_2, i}^{2 \leftrightarrow 2}, \\ R_O^{2 \leftrightarrow 3} &= -2 \sum_{i=0}^{l_{O_2}} R_{O_2, i}^{2 \leftrightarrow 3} - R_{NO}^{2 \leftrightarrow 3}, & R_O^{2 \leftrightarrow 2} &= - \sum_{i=0}^{l_{O_2}} R_{O_2, i}^{2 \leftrightarrow 2} + \sum_{i=0}^{l_{N_2}} R_{N_2, i}^{2 \leftrightarrow 2}. \end{aligned}$$

where $k_{c,i, diss}^M$, $k_{rec, c, i}^M$, $k_{NO, diss}^M$, $k_{rec, NO}^M$, $k_{N_2, i \rightarrow NO}^{O \rightarrow N}$, $k_{O_2, i \rightarrow NO}^{N \rightarrow O}$, $k_{NO \rightarrow N_2, i}^{N \rightarrow O}$, $k_{NO \rightarrow O_2, i}^{O \rightarrow N}$ are the rate coefficients of considered processes.

In simulations we used analytical expressions of SSH theory [11] for the vibrational energy transition rate coefficients generalized for anharmonic oscillators [12, 13], the modified Treanor-Marrone model [14] for dissociation in the state-to-state approach [15], and the Warnatz model (see [13]) for exchange reactions. Rate coefficients of forward and backward processes are connected by the detailed balance principle [15].

RESULTS

In this section we present the results of numerical simulations of the 1D air flow in the expanding part of a conic nozzle under the conditions in the throat $T^* = 7000$ K, $p^* = 100$ atm. It is assumed that in the convergent section of a nozzle the flow is in thermal equilibrium. For numerical solution of system (8)–(11) of equations for vibrational level populations and flow parameters, the modification of the Gear method with a variable order based on formulas for backward differentiation was used [16].

First, we consider the results obtained in the frame of the most accurate state-to-state and simplified one-temperature flow description. In the second case level populations of molecules are described by the thermal equilibrium Boltzmann distributions with the gas temperature. The set of macroscopic flow parameters in this case includes number densities of species $n_{N_2}(x)$, $n_{O_2}(x)$, $n_{NO}(x)$, $n_N(x)$, $n_O(x)$, the gas temperature $T(x)$ and velocity $v(x)$. The governing equations contain equations for the mixture composition, temperature and velocity. Reaction rate coefficients in the thermal equilibrium flow are described by the Arrhenius law with parameters taken from [17].

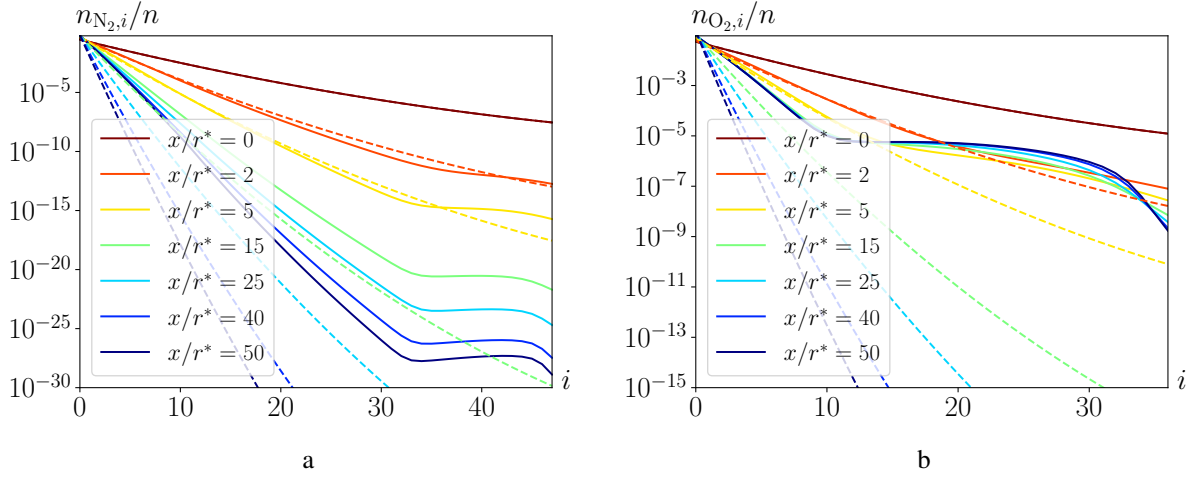


FIGURE 1. The vibrational distributions $n_{N_2,i}/n$ (a) and $n_{O_2,i}/n$ (b) in various cross-sections x/r^* in the state-to-state (solid lines) and one-temperature (dashed lines) approaches.

Figures 1(a,b) present vibrational distributions of N_2 and O_2 molecules as functions of vibrational level numbers for different positions x/r^* (r^* is the radius of the throat) in a nozzle in the state-to-state approach (solid lines) and one-temperature approach (dashed lines). In the state-to-state approach, we can see formation of non-equilibrium vibrational distributions with a plateau part at intermediate levels. This form of distributions was found first on the basis of approximate analytical solutions of master equations in a one-component space-homogenous gas [12], then as a solution of the kinetic equations for distribution functions [15]. In numerical simulations of air nozzle flows, similar distributions were found in [2] for binary mixtures and [6] for air flows.

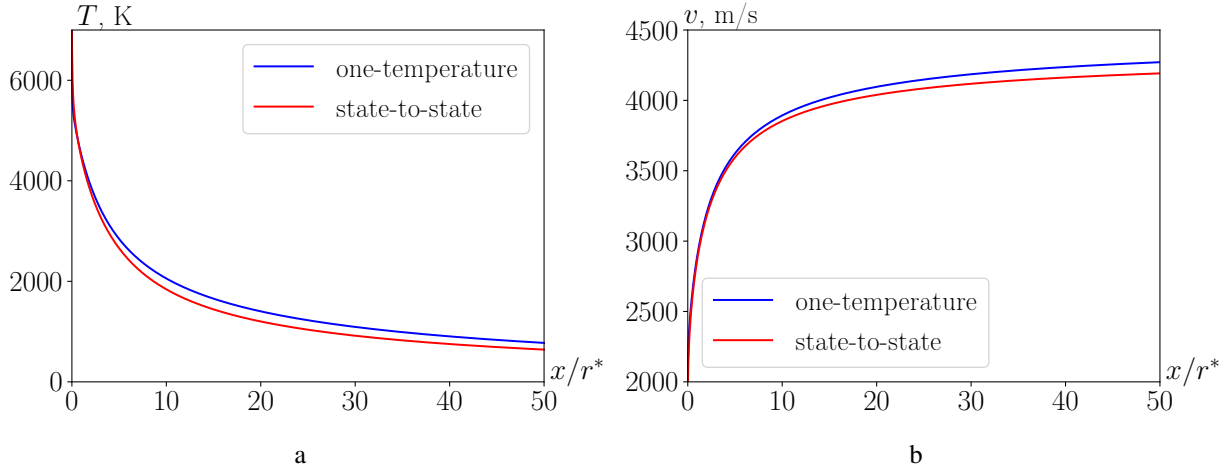


FIGURE 2. The gas temperature T (a) and the flow velocity v (b) in the one-temperature and state-to-state approaches.

It is seen that vibrational level populations found in the state-to-state approach decrease along the nozzle axis considerably slower than those in the one-temperature approach. Therefore in the one-temperature approach we obtain underestimated level populations compared to the accurate state-to-state kinetic description.

It may be also noticed that distributions of N_2 and O_2 molecules presented in Figs. 1(a,b) occur quite different under the considered conditions. More rapid decrease of populations of N_2 than O_2 molecules is defined by differences in corresponding vibrational energy transition probabilities [12].

In Figs. 2(a,b), variation of the gas temperature (a) and velocity (b) along a nozzle axis is shown for the state-to-state and one-temperature approaches. The application of the simplified one-temperature kinetic model leads to

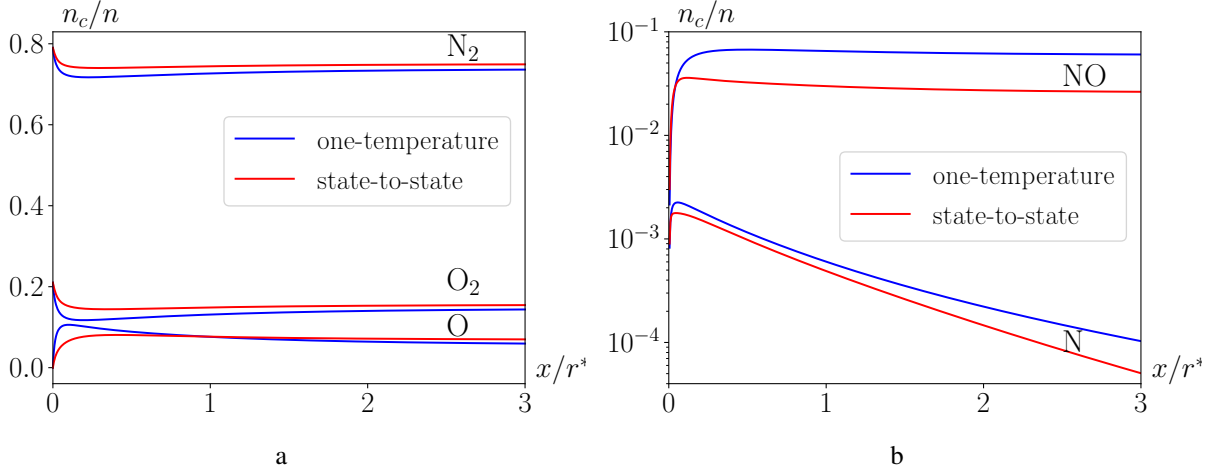


FIGURE 3. Number densities n_{N_2}/n , n_{O_2}/n , n_O/n (a), n_{NO}/n , n_N/n (b) along the nozzle axis in the state-to-state and one-temperature approaches.

overestimated values of the gas temperature and flow velocity in the considered flow. It is explained by the fact that in the thermal equilibrium flow, the gas temperature characterizes not only the translation-rotational energy which decreases fast but also the total vibrational energy which changes due to different vibrational energy transitions and chemical reactions in a flow. On the contrary, in the state-to-state approach the gas temperature characterizes only translational-rotational energy which decreases in an expanding flow much faster than the vibrational energy due to differences in relaxation times.

In Figs. 3(a,b), variation of number densities of molecules and atoms found in the state-to-state and one-temperature approaches in dependence on the distance from the critical cross section is presented. A sharper decrease the temperature in the state-to-state approximation (Fig. 2a) leads to more rapid relaxation, and number densities are frozen earlier than in the case of one-temperature model. The number densities are frozen immediately after throat ($x/r^* \leq 1$) with the exception of the number densities of nitrogen atoms due to the high global rates of exchange reactions in which N atoms are involved. Note the non-monotonic behaviour of N_2 and O_2 number densities obtained in the frame of one-temperature model: slight increase in the number of particles due to reaction dissociation and subsequent increase as a result of atoms recombination.

TABLE 1. The gas temperature and number densities of air species at $x/r^* = 50$ for different kinetic schemes.

	T, K	$\Delta T, \% ^*$	n_{N_2}/n	n_{O_2}/n	n_{NO}/n	n_N/n	n_O/n
All reactions	641,6	—	0.752	0.159	0.027	$4.15 \cdot 10^{-11}$	0.062
Without exchange reactions	648,1	1	0.764	0.17	$3.75 \cdot 10^{-5}$	0.00013	0.065
Without recombination	573,3	10,6	0.739	0.138	0.0213	$8.5 \cdot 10^{-12}$	0.102
Without VV	468,2	27	0.745	0.15	0.0318	$6.15 \cdot 10^{-10}$	0.0728
Without VT	652,1	1,6	0.742	0.148	0.045	$1.017 \cdot 10^{-9}$	0.065

* The deviation of temperature from that obtained for the case of all reactions.

In order to estimate the role of different reactions and processes in air nozzle flows calculations were done for five kinetic schemes: 1) using all reactions (2)–(7), 2) neglecting exchange reactions (6), (7) with NO molecules at the zero-th vibrational state, 3) neglecting recombination, 4) neglecting VV vibrational energy exchanges and 5) neglecting VT energy transitions.

The values of flow parameters in the cross section $x/r^* = 50$ for all cases are given in Table 1. It should be noted that the gas temperatures obtained within 2nd and 5th cases differ insignificantly from temperature calculated for the complete reaction scheme. Neglecting recombination, whose role increases with decreasing the gas temperature, leads to an underestimation of T values up to 10,6 %. Under the considered conditions neglecting of VV energy transitions

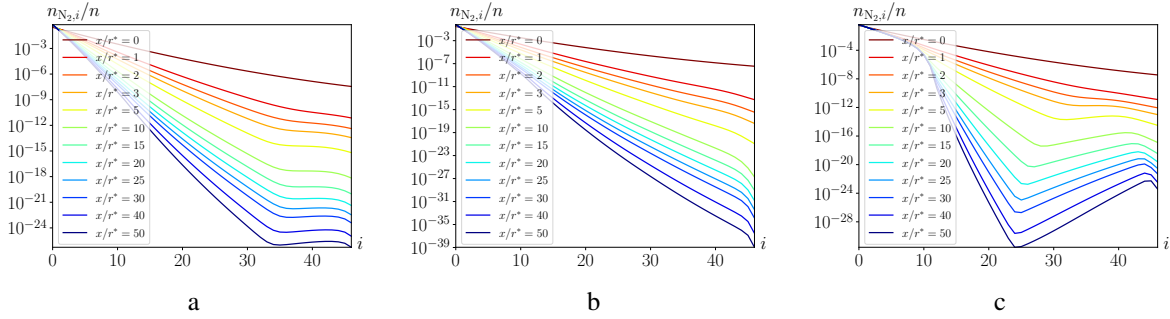


FIGURE 4. The vibrational distributions $n_{N_2,i}/n$ in various cross-sections x/r^* for different kinetic schemes: all reactions (a), without recombination (b), without VV energy exchanges (c).

results in the most dramatic temperature decrease and the greatest difference of temperature values in comparison with the other cases.

Analyzing the Table 1, one can come to the conclusion that the greatest impact of the exchange reactions is on the numerical densities of NO molecules and N atoms. Maximum difference in values reaches two and eight orders of magnitude, respectively. The values of these macroscopic parameters also strongly depend on the exchanges of vibrational and translational energy. Values of number density of the N_2 molecules depend weakly on the choice of the kinetic scheme. For all cases the relative percentage difference does not exceed 1,8 %. The absence of recombination strongly affects all numerical densities. The difference in values reaches 13,5 % for n_{O_2}/n , 19,9 % for n_{NO}/n , 79 % for n_N/n and 64 % for n_O/n . The number densities of molecules are underestimated, and the number densities of atoms are overestimated with respect to the values obtained under the complete reaction scheme.

On the basis of analytical calculations [12] it has been proved that plateau region formation on intermediate vibrational levels happens owing to dominant resonant VV processes with the presence of a vibrational energy dissipation channel at the intermediate and high levels. This fact is clearly illustrated in Figs. 4(a,b,c). One can see on the example of the nitrogen vibrational distributions that under the considered conditions the dissipation is caused not only by VT transitions, but mainly by recombination. In the case of its absence (Fig. 4b), the shape of the vibrational distribution does not have a plateau region while the absence of VV transitions leads to the significant overpopulation of intermediate levels. A similar shape of the nitrogen vibrational distribution has been obtained in [8].

CONCLUSIONS

Quasi-one-dimensional non-equilibrium flows of reacting air mixture $N_2/O_2/NO/N/O$ in a nozzle are studied in the frame of the state-to-state and one-temperature flow description. Vibrational excitation of N_2 and O_2 molecules is taken into account as well as various vibrational energy transitions, N_2 and O_2 dissociation, recombination of atoms and Zeldovich exchange reactions of NO formation. The equations for N_2 and O_2 vibrational level populations, number densities of species, the gas temperature and flow velocity are solved numerically for the flow in a conic nozzle. Variation of vibrational distributions of nitrogen and oxygen molecules, number densities of species and the gas temperature and velocity along a nozzle axis is studied. Comparison of the results obtained in the state-to-state and one-temperature approximation showed that the use of the simplified thermal equilibrium kinetic model leads to overestimated values for the gas temperature and flow velocity and underestimated vibrational level populations. In the case of the state-to-state approach, formation of non-equilibrium non-Boltzmann distributions of N_2 and O_2 molecules with a plateau part at intermediate vibrational levels is shown. The influence of exchange reactions, recombination, VV and VT energy exchanges on the gas flow parameters is also studied in the paper. A strong effect of recombination and VV transitions on the gas temperature and N_2 and O_2 vibrational distributions was established.

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REFERENCES

- [1] B. D. Shizgal and F. Lordet, *J. Chem. Phys.* **104**, 3579–3597 (1996).
- [2] E. V. Kustova, E. A. Nagnibeda, T. Y. Alexandrova, and et al., *Chem. Phys.* **276**, 139–154 (2002).
- [3] C. Park and S. H. Lee, *J. Thermophys. Heat Trans.* **9**, 9–16 (1995).
- [4] G. Colonna, M. Tuttafesta, M. Capitelli, and D. Giordano, “NO formation in one dimensional nozzle air flow with state-to-state non-equilibrium vibrational kinetics,” in *7th AIAA/ASME Joint Thermophysics and Heat Transfer Conference* (American Institute of Aeronautics and Astronautics, 1998), pp. 1–10.
- [5] C. Park, *J. Thermophys. Heat Trans.* **20**, 689–698 (2006).
- [6] S. S. Bazilevich, K. A. Sinitsyn, and E. A. Nagnibeda, “Non-equilibrium flows of reacting air components in nozzles,” in *AIP Conference Proceedings*, Vol. 1084 (AIP, 2009), pp. 843–848.
- [7] A. Guy, A. Bourdon, and M. Y. Perrin, *Chem. Phys.* **420**, 15–24 (2013).
- [8] M. Capitelli, G. Colonna, E. Kustova, and E. Nagnibeda, “State-to-state kinetics and transport properties in supersonic air nozzle flows,” in *Fourth Symposium on Aerothermodynamics for Space Vehicles*, Vol. 487, edited by R. A. Harris (ESA, Capua, Italy, 2002) p. 137.
- [9] E. V. Stupochenko, S. A. Losev, and A. I. Osipov, *Relaxation in Shock Waves* (Springer, Berlin, Heidelberg, 1967).
- [10] O. Kunova and E. Nagnibeda, “On the influence of state-resolved rates of zeldovich reactions on shock heated air flow parameters,” in *Journal of Physics: Conference Series*, Vol. 815 (IOP Publishing, 2017) p. 012009.
- [11] R. N. Schwartz, Z. I. Slawsky, and K. F. Herzfeld, *J. Chem. Phys.* **20**, 1591–1599 (1952).
- [12] B. F. Gordiets, A. I. Osipov, and L. A. Shelepin, *Kinetic processes in gases and molecular lasers* (Nauka, Moscow, 1980).
- [13] G. G. Chernyi, S. A. Losev, S. O. Macheret, and B. V. Potapkin, *Physical and Chemical Processes in Gas Dynamics: Cross Sections and Rate Constants, Volume I. Progress in Astronautics and Aeronautics* (American Institute of Aeronautics and Astronautics, 2002).
- [14] P. Marrone and C. Treanor, *Physics of Fluids* **6**, 1215–1221 (1963).
- [15] E. Nagnibeda and E. Kustova, *Nonequilibrium Reacting Gas Flows. Kinetic Theory of Transport and Relaxation Processes* (Springer Verlag, Berlin, Heidelberg, 2009).
- [16] L. F. Shampine, *Numerical Solution of Ordinary Differential Equations* (Chapman and Hall, New York, 1994).
- [17] D. Ramjaun, “Test case 2: Definition of shock tunnel test cases for gas radiation prediction in a planetary atmosphere,” in *Proceedings of the International Workshop on Radiation of High Temperature Gases in Atmospheric Entry. Part II*, edited by K. Fletcher (ESA Publications Division, The Netherlands, 2004).