

Multi-temperature models for shock heated flows of CO₂/CO/O mixture.

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Abstract

In the paper non-equilibrium flows of the CO₂/CO/O mixture in the relaxation zone behind shock waves are numerically studied taking into account vibrational energy transitions and dissociation of CO₂ molecules. The three-temperature kinetic theory approximation is applied for derivation of flow equations and CO₂ dissociation rate coefficients. The governing equations for the translational temperature T , two vibrational temperatures of coupled (symmetric-bending) and asymmetric CO₂ modes T_{12} , T_3 , flow velocity and number densities of species are solved numerically for a inviscid flow behind a plane shock wave for different free stream conditions. The obtained results are compared with those found in the frame of the simplified two-temperature and one-temperature CO₂ kinetic models. The impact of CO₂ vibrational distributions and free stream conditions on the evolution of flow parameters and CO₂ dissociation rate behind a shock front is shown.

1. Introduction

Investigation of non-equilibrium vibrational and chemical kinetics in CO₂ flows behind shock waves occurring in hypersonic flows is important for prediction of flow parameters on the trajectory of space vehicles entering into the Mars atmosphere. Different models for vibrational-chemical coupling in high-temperature CO₂ flows have been proposed in a number of papers¹⁻⁶. In the frame of the most accurate state-to-state flow description^{3,7} the equations for macroscopic gas dynamic parameters should be solved jointly with a lot of equations for populations of various vibrational states of molecular species. In the present time this approach is successfully developed and applied for numerical modeling of air flows behind shock waves⁸ and in nozzles⁹. However, serious difficulties rise while the state-to-state description is used for prediction of CO₂ flow parameters. In this case a set of governing equations includes considerably more equations for populations of vibrational states than for diatomic gas mixtures because level populations of three vibrational CO₂ modes (symmetric, bending and asymmetric) should be taken into account. This approach is considered in details and applied in the paper⁷ for CO₂ flows in the boundary layer.

More simple and suitable for applications CO₂ models are based on multi-temperature vibrational distributions. Using this approach, instead of many equations for vibrational level populations, one should consider equations for much less number of macroscopic parameters. Thus, only several equations for vibrational temperatures should be solved jointly with equations for gas dynamic parameters and mixture composition. For high-temperature non-equilibrium reacting CO₂ mixture flows multi-temperature models for relaxation and transport properties are derived from the kinetic theory in^{2,10} and used for numerical simulations of flow parameters in a shock layer near the space vehicle MSRO¹⁰.

In the present paper the three-temperature CO₂ kinetic model derived in² is applied for numerical study of the CO₂/CO/O mixture flow in the relaxation zone behind a plane shock wave. Recently this model was used in¹¹ for modeling of vibration-dissociation coupling in the spatially homogeneous CO₂/CO/O mixture. The model is based on the relations between the rates of CO₂ vibrational energy transitions within and between different vibrational modes of CO₂ molecules^{12,13}. Rapid intra-mode VV_{*m*} vibrational energy exchanges within all three (symmetric, bending and asymmetric) modes ($m=1,2,3$) as well as near-resonant VV₁₂ energy transitions between the symmetric and bending modes make it possible to introduce two vibrational temperatures: T_{12} for the combined symmetric-bending mode and T_3 for the asymmetric mode. Finally, the set of governing equations for the one-dimensional flow of the considered mixture in the relaxation zone behind a plane shock wave includes equations for number densities of species $n_{CO_2}(x)$,

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$n_{CO}(x)$, $n_O(x)$, the gas temperature $T(x)$ and velocity $v(x)$ as well as for vibrational temperatures $T_{12}(x)$, $T_3(x)$ (x is the distance from the shock front).

The mixture state ahead the shock front is considered to be equilibrium. A rapid gas compression within the thin shock front results in a temperature jump which calls fast equilibration of translational and rotational degrees of freedom. Along with these processes, rapid VV_{12} , VV_3 exchanges proceed within the shock front whereas the mean vibrational energies of combined and asymmetric modes do not change. Slow processes including VT_m vibrational energy transitions and CO₂ dissociation are supposed frozen within the shock front and are considered in the relaxation zone behind the shock front along with changing of macroscopic mixture parameters. In the end of the relaxation zone the thermal equilibrium one-temperature distributions of species are established.

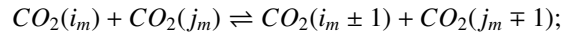
In order to solve governing equations in the relaxation zone, the initial values of mixture parameters just behind a shock should be found. In the paper, the values of flow parameters in the very beginning of the relaxation zone are connected with those in a free stream by the conservation equations for momentum, total energy and two conservation equations of the mean vibrational energies of the combined symmetric-bending and asymmetric mode.

Variation of the temperatures T , T_{12} , T_3 , flow velocity and mixture composition along the relaxation zone is studied in the paper for different Mach numbers, the gas temperature and pressure ahead a shock front. The obtained results are compared with those found in the frame of the two-temperature and one-temperature CO₂ kinetic models introduced for the cases $T_{12} = T_3 = T_v$ and $T_v = T$. The first case corresponds to the vibrational relaxation of all three CO₂ modes with the same vibrational temperature $T_v(x)$ whereas the second case represents the thermal equilibrium flow of the considered mixture with the gas temperature $T(x)$. The impact of CO₂ vibrational distributions and free stream conditions on the variation of flow parameters and CO₂ dissociation rate behind a shock front is studied in the paper.

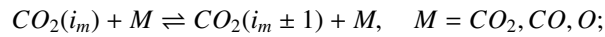
1.1 Vibration distributions and governing equations

Linear three-atomic CO₂ molecules have three modes of vibrations $m=1,2,3$ (symmetric, bending and asymmetric) with frequencies of vibrations ν_m . CO₂ vibrational-chemical kinetics in the considered mixture includes the following basic processes:

- VV_m vibrational energy exchanges within the each m mode:



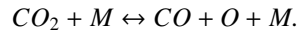
- VT_m vibrational-translational transitions :



- VV_{12} exchanges between the symmetric and bending modes:



- CO₂ dissociation:



The existing data on the rates of considered processes show that the following relation for characteristic times is valid for a wide temperature range² :

$$\tau_{VV_m} \sim \tau_{VV_{1-2}} \ll \tau_{VT_2} \sim \tau_{VV_{2-3}} \sim \tau_{VV_{1-2-3}} < \tau_{VT_3} < \tau_{diss} \sim \theta, \quad m = 1, 2, 3, \quad (1)$$

here θ is the mean time of variation of macroscopic mixture parameters.

Rapid VV_{12} energy exchanges between bending and symmetric modes and VV_3 asymmetric mode energy exchanges make it possible to introduce the vibrational temperatures T_{12} for the coupled symmetric-bending mode and T_3 for the asymmetric mode. In this case CO₂ vibrational level populations take the form² (see also^{4,14}) :

$$n_{i_1 i_2 i_3}(T_{12}, T_3) = \frac{n_{CO_2} s_{i_1 i_2 i_3}}{Z_{vibr}^{CO_2}(T_{12}, T_3)} \exp \left[-\frac{i_1 \varepsilon_{100} + i_2 \varepsilon_{010}}{kT_{12}} - \frac{i_3 \varepsilon_{001}}{kT_3} \right], \quad (2)$$

$$Z_{vibr}^{CO_2}(T_{12}, T_3) = \sum_{i_1, i_2, i_3} s_{i_1 i_2 i_3} \exp \left[-\frac{i_1 \varepsilon_{100} + i_2 \varepsilon_{010}}{kT_{12}} - \frac{i_3 \varepsilon_{001}}{kT_3} \right]$$

is the partition function, $s_{i_1 i_2 i_3} = i_2 + 1$ is the statistical CO₂ weight, k is the Boltzmann constant.

CO molecules are assumed to be in the thermal equilibrium with the Boltzmann vibrational distribution:

$$n_i^{CO}(T) = \frac{n_{CO}}{Z_{vibr}^{CO}(T)} \exp\left(-\frac{\varepsilon_i^{CO}}{kT}\right).$$

In this paper we use the harmonic oscillator model for vibrational energies:

$$\varepsilon_{i_1 i_2 i_3} = \sum_{k=1}^3 h\nu_k i_k = i_1 \varepsilon_{100} + i_2 \varepsilon_{010} + i_3 \varepsilon_{001}, \quad \varepsilon_i^{CO} = ih\nu_{CO}.$$

Vibrational energies of CO₂ and CO molecules are counted from the zero level energy, h is the Planck constant.

If anharmonic effects are taken into account, level populations depend not only on vibrational temperatures but also on the gas temperature T (see⁴).

Under the condition (1) the closed set of the equations for species number densities, gas temperature, velocity and vibrational temperatures T_{12} , T_3 is derived from the kinetic theory in the paper².

In the present paper we applied these equations for study of the one-dimensional non-viscid flow of considered mixture in the relaxation zone behind a plane shock wave. In this case we obtain the governing equations for number densities of species $n_{CO_2}(x)$, $n_{CO}(x)$, $n_O(x)$, the gas temperature $T(x)$, flow velocity $v(x)$ and two vibrational temperatures $T_{12}(x)$, $T_3(x)$ of symmetric-bending and asymmetric CO₂ modes depending on the distance from the shock front x :

$$\frac{d(n_{CO_2}v)}{dx} = R_{CO_2}^{dis-rec}, \quad (3)$$

$$\frac{d(n_{CO}v)}{dx} = \frac{d(n_Ov)}{dx} = -R_{CO_2}^{dis-rec}, \quad (4)$$

$$\frac{d(\rho_{CO_2}vE_{12})}{dx} = R_{12} - m_{CO_2}E_{12}R_{CO_2}^{dis-rec}, \quad (5)$$

$$\frac{d(\rho_{CO_2}vE_3)}{dx} = R_3 - m_{CO_2}E_3R_{CO_2}^{dis-rec}, \quad (6)$$

$$\rho v = \rho_0 v_0, \quad (7)$$

$$\rho v^2 + p = \rho_0 v_0^2 + p_0, \quad (8)$$

$$h + \frac{v^2}{2} = h_0 + \frac{v_0^2}{2}, \quad (9)$$

where the terms $R_{CO_2}^{dis-rec}$, R_{12} , R_3 describe CO₂ dissociation, CO and O recombination and vibration energy transitions.

The vibrational energies E_{12} , E_3 of the combined and asymmetric CO₂ modes are specified by the expressions:

$$\rho_{CO_2}E_{12}(T_{12}) = \frac{n_{CO_2}}{Z_{12}(T_{12})} \sum_{i_1, i_2} (i_1 \varepsilon_{100} + i_2 \varepsilon_{010})(i_2 + 1) \exp\left(-\frac{i_1 \varepsilon_{100} + i_2 \varepsilon_{010}}{kT_{12}}\right),$$

$$\rho_{CO_2}E_3(T_3) = \frac{n_{CO_2}}{Z_3(T_3)} \sum_{i_3} i_3 \varepsilon_{001} \exp\left(-\frac{i_3 \varepsilon_{001}}{kT_3}\right),$$

$$Z_{12}(T_{12}) = \sum_{i_1, i_2} (i_2 + 1) \exp\left(-\frac{i_1 \varepsilon_{100} + i_2 \varepsilon_{010}}{kT_{12}}\right), \quad Z_3(T_3) = \sum_{i_3} \exp\left(-\frac{i_3 \varepsilon_{001}}{kT_3}\right).$$

In the Eqs.(7)-(9) ρ is the mixture density, $p = nkT$ is the pressure, $h = E + p/\rho$ is the enthalpy per unit mass, E is the total energy:

$$\rho E = \frac{3}{2}nkT + (n_{CO_2} + n_{CO})kT + \rho_{CO_2}E_{vibr}^{CO_2}(T_{12}, T_3) + \rho_{CO}E_{vibr}^{CO}(T) + n_{CO_2}\varepsilon_{CO_2} + n_{CO}\varepsilon_{CO} + n_O\varepsilon_O,$$

ε_{CO_2} , ε_{CO} , ε_O are the formation energies, $E_{vibr}^{CO_2}(T_{12}, T_3)$, $E_{vibr}^{CO}(T)$ are the CO₂ and CO vibrational energies:

$$\rho_{CO_2}E_{vibr}^{CO_2}(T_{12}, T_3) = \sum_{i_1, i_2, i_3} \varepsilon_{i_1 i_2 i_3} n_{i_1 i_2 i_3}(T_{12}, T_3),$$

$$\rho_{CO}E_{vibr}^{CO}(T) = \sum_i \frac{n_{CO}}{Z_{vibr}^{CO}(T)} \varepsilon_i^{CO} \exp\left(-\frac{\varepsilon_i^{CO}}{kT}\right).$$

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In the three-temperature approximation flow parameters just behind a shock front are connected with those in a free stream by the conditions of conservation of mixture composition, momentum, total energy and energies of combined and asymmetric modes.

If all VV vibrational energy exchanges within and between three CO₂ modes proceed faster than VT_m transitions and dissociation the total vibrational temperature $T_v = T_{12} = T_3$ for CO₂ molecules may be introduced and vibrational distributions (2) take the form:

$$n_{i_1 i_2 i_3}(T_v) = \frac{n_{CO_2}(i_2 + 1)}{Z_{vibr}^{CO_2}(T_v)} \exp\left(-\frac{i_1 \varepsilon_{100} + i_2 \varepsilon_{010} + i_3 \varepsilon_{001}}{kT_v}\right). \quad (10)$$

In this case the system of governing equations contains, instead of two equations (5), (6), only one equation:

$$\frac{d(\rho_{CO_2} v E_{CO_2}^{vibr}(T_v))}{dx} = R_{CO_2} - m_{CO_2} E_{CO_2}^{vibr}(T_v) R_{CO_2}^{dis-rec},$$

$$\rho_{CO_2} E_{CO_2}^{vibr}(T_v) = \frac{n_{CO_2}}{Z_{vibr}^{CO_2}(T_v)} \sum_{i_1, i_2, i_3} \varepsilon_{i_1 i_2 i_3} (i_2 + 1) \exp\left(-\frac{\varepsilon_{i_1 i_2 i_3}}{kT_v}\right).$$

In the two-temperature approach mixture parameters ahead and just behind a shock front are connected by conservation equations for mixture composition, momentum, total energy and for CO₂ vibrational energy.

If the vibrational relaxation of mixture components occurs considerably faster than dissociation, vibrational level populations are described by the Boltzmann thermal equilibrium distributions (10) with $T_v = T$. In this case non-equilibrium chemical reactions are simulated on the basis of maintaining thermal equilibrium vibrational distributions. The set of equations for macroscopic parameters n_{CO_2} , n_{CO} , n_O , v , T contains dissociation equations with rate coefficients depending only on the gas temperature. In this case parameters just behind a shock are found with the use of classical conservation equations for mixture composition, momentum and total energy.

1.2 Production terms

Production terms in Eqs.(3) describe CO₂ dissociation and recombination CO and O:

$$R_{CO_2}^{dis-rec} = \sum_M n_M (k_{rec,CO_2}^M(T) n_{CO} n_O - k_{diss,CO_2}^M(T, T_{12}, T_3) n_{CO_2}),$$

here k_{diss,CO_2}^M , k_{rec,CO_2}^M are the coefficients of CO₂ dissociation and CO and O recombination rate. $M=CO_2, CO, O$ is a collision partner.

The dissociation rate coefficient may be written in the form of the generalized Treanor-Marrone model for the three-temperature approximation² :

$$k_{diss,CO_2}^M(T, T_{12}, T_3) = k_{diss,CO_2}^{eq,M}(T) Z(T, T_{12}, T_3).$$

The equilibrium dissociation rate coefficient $k_{diss,CO_2}^{eq,M}(T)$ is defined by the Arrhenius law for which the parameters were taken from¹⁵, $Z(T, T_{12}, T_3)$ is the non-equilibrium factor:

$$Z(T, T_{12}, T_3) = \frac{Z_{vibr}^{CO_2}(T)}{Z_{vibr}^{CO_2}(-U) Z_{vibr}^{CO_2}(T_{12}, T_3)} \sum_{i_1, i_2, i_3} (i_2 + 1) \exp\left(\frac{i_1 \varepsilon_{100} + i_2 \varepsilon_{010}}{k} \left(\frac{1}{T} - \frac{1}{T_{12}}\right) + \frac{i_3 \varepsilon_{001}}{k} \left(\frac{1}{T} - \frac{1}{T_3}\right) + \frac{\varepsilon_{i_1 i_2 i_3}}{kU}\right),$$

U is a model parameter, in calculations we had $U = D/6k$.

In the two-temperature approach the non-equilibrium factor is as follows:

$$Z(T, T_v) = \frac{Z_{vibr}^{CO_2}(T)}{Z_{vibr}^{CO_2}(-U) Z_{vibr}^{CO_2}(T_v)} \sum_{i_1, i_2, i_3} (i_2 + 1) \exp\left(\frac{\varepsilon_{i_1 i_2 i_3}}{k} \left(\frac{1}{T} - \frac{1}{T_v} + \frac{1}{U}\right)\right).$$

In Fig. 1 the temperature dependence of the dissociation rate coefficients $k_{diss,CO_2}^{eq,CO_2}(T)$, $k_{diss,CO_2}^{CO_2}(T, T_v)$, $k_{diss,CO_2}^{CO_2}(T, T_{12}, T_3)$ calculated in three approximations is shown for fixed vibrational temperatures T_{12} , T_3 and T_v . It is seen that the non-equilibrium two-temperature and three-temperature dissociation rate coefficients exceed the equilibrium ones if $T_v > T$ or for the values T_{12} , T_3 when $Z(T, T_{12}, T_3) > 1$.

Recombination rate coefficients are determined on the basis of the detailed balance principle² :

$$k_{rec,CO_2}^M(T) = k_{diss,CO_2}^{eq,M}(T) \left(\frac{m_{CO_2}}{m_{COMO}} \right)^{3/2} (2\pi kT)^{-3/2} h^3 \frac{Z_{vibr}^{CO_2}(T) Z_{rot}^{CO_2}(T)}{Z_{vibr}^{CO}(T) Z_{rot}^{CO}(T)} \exp \left(-\frac{\varepsilon_{CO_2} - \varepsilon_{CO} - \varepsilon_O}{kT} \right),$$

here $Z_{rot}^{CO_2}(T)$, $Z_{rot}^{CO}(T)$ are the rotational partition functions.

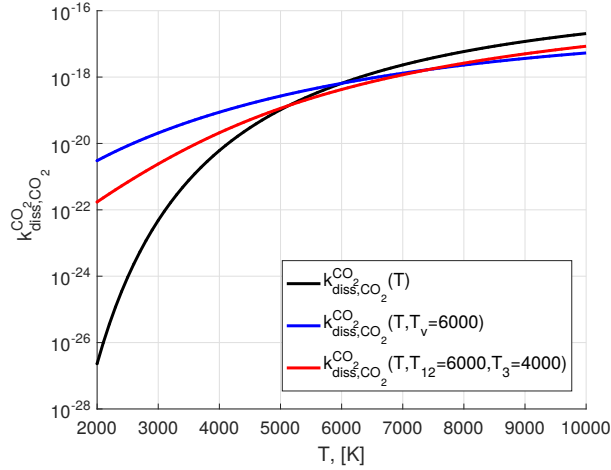


Figure 1: Dissociation rate coefficients in dependence on the gas temperature T with fixed vibrational temperatures: $T_v = 6000K$, $T_{12} = 6000K$, $T_3 = 4000K$.

The right hand parts of Eqs.(5), (6) R_{12} and R_3 describe changing of vibrational energies E_{12} and E_3 due to slow vibrational energy transitions VT_2 , VV_{2-3} , VV_{1-2-3} , dissociation and recombination. These terms are considered in the next form² :

$$R_{12} = R_{12}^{VT_2} + R_{12}^{VV_{2-3}} + R_{12}^{VV_{1-2-3}} + R_{12}^{dis-rec},$$

$$R_3 = R_3^{VT_2} + R_3^{VV_{2-3}} + R_3^{VV_{1-2-3}} + R_3^{dis-rec},$$

where the terms responsible for dissociation may be written as:

$$R_{12}^{dis-rec} = \sum_{i_1, i_2, i_3} (i_1 \varepsilon_{100} + i_2 \varepsilon_{010}) R_{i_1, i_2, i_3}^{dis-rec}, \quad R_3^{dis-rec} = \sum_{i_1, i_2, i_3} i_3 \varepsilon_{001} R_{i_1, i_2, i_3}^{dis-rec}.$$

$$R_{i_1, i_2, i_3}^{dis-rec} = \sum_M n_M (k_{rec, i_1 i_2 i_3}^M n_{CONO} - k_{i_1 i_2 i_3, diss}^M n_{i_1 i_2 i_3}),$$

$k_{i_1 i_2 i_3, diss}^M$, $k_{rec, i_1 i_2 i_3}^M$ are the state specific rate coefficients of dissociation and recombination from/to the corresponding vibrational level. The state depending dissociation rate coefficients were calculated with the use of the Treanor-Marrone model generalized in the state-to-state approximation for CO₂ molecules⁵.

Following the paper⁵ we use approximate expressions of the terms responsible for VV, VT exchanges via relaxation times τ_γ :

$$R_{12}^{VT_2} + R_{12}^{VV_{2-3}} + R_{12}^{VV_{1-2-3}} = \rho_{CO_2} \sum_\gamma \frac{E_{12}^{eq}(T) - E_{12}(T_{12})}{\tau_\gamma},$$

$$R_3^{VT_2} + R_3^{VV_{2-3}} + R_3^{VV_{1-2-3}} = \rho_{CO_2} \sum_\gamma \frac{E_3^{eq}(T) - E_3(T_3)}{\tau_\gamma},$$

where $\gamma = VT_2, VV_{2-3}, VV_{1-2-3}$.

The relaxation times τ_γ were calculated using analytical approximations proposed in the papers^{16,17} on the basis of experimental data. It should be noted that VT_1 and VT_3 transitions are much less probable comparable to VT_2 processes and are not taken into account in calculations (see^{2,10}).

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1.3 Results

The system of equations for the flow of the considered mixture behind the shock front is numerically solved in the framework of the three-temperature, two-temperature and one-temperature approaches. The solution is obtained for the following conditions before a shock front typical for the entry regime of a space body in the Mars atmosphere: $T_0 = T_{12}^{(0)} = T_3^{(0)} = T_v^{(0)} = 271$ K, $\rho_0 = 3.141 \cdot 10^{-5}$ kg/m³, the Mach numbers $M = 10, 15$ are considered. The free stream is assumed to consist only of CO₂ molecules. To solve the system of Eqs.(3)-(9) we used the Gear method with a variable step of integration and order of the method. This method is based on implicit multi-step difference schemes and is most effective in solving of rigid systems of equations.

Variations of the gas temperature, mixture composition and vibrational temperatures, flow velocity and CO₂ dissociation rate coefficients along the relaxation zone found with the use of different vibrational distributions and various Mach numbers in the free stream are presented in Figs. 2-7. First, we will consider the impact of vibrational distributions on flow parameters and dissociation rate coefficients behind the shock front with $M=15$ (Figs. 2-4).

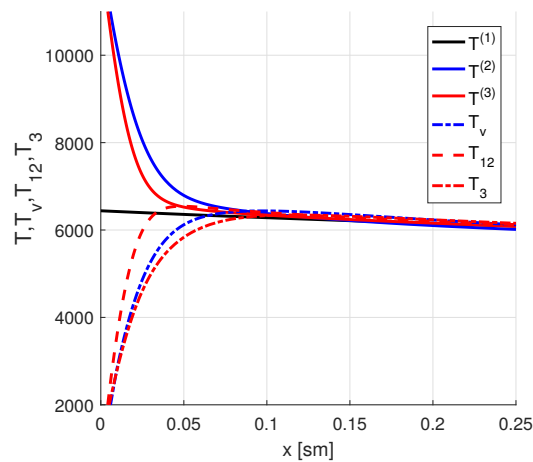


Figure 2: The gas temperature T and the vibrational temperatures T_{12} , T_3 , T_v in dependence on x ; 1 – one-temperature, 2 – two-temperature, 3 – three-temperature approach.

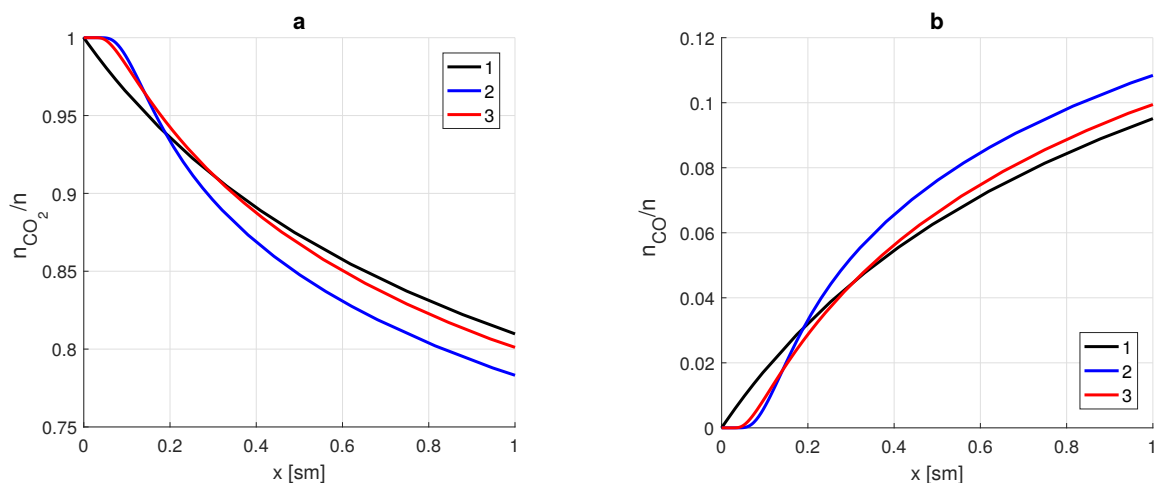


Figure 3: The relative number density of CO₂ (a) and CO (b) in dependence on x ; 1 – one-temperature, 2 – two-temperature, 3 – three-temperature approach.

The values of the gas temperature immediately behind the shock front in the two-temperature and three-temperature approximations are much higher than in the one-temperature approximation (see Fig. 2), since it is assumed that the vibrational levels of CO₂ molecules are excited with vibrational temperature $T_{12} = T_3 = T_v = T_0$ in the front. A sharp drop of the gas temperature and increase of T_v and T_{12} , T_3 in the two-temperature and three-temperature approximations

is due to the vibrational relaxation caused by the rapid inter-mode exchanges and translational-vibrational energy transitions. The difference between the temperature values in the one-temperature and three-temperature approximations near the shock front reaches 40% and 12% between T values in the two-temperature and three-temperature approximations. Excitation of the combined mode occurs faster than of the third mode and causes a rapid increase in the vibrational temperature T_{12} in comparison with the temperature T_3 . Further along the relaxation zone the dissociation proceeds actively with decrease of T , T_{12} , T_3 , T_v until the flow reaches the thermal equilibrium regime.

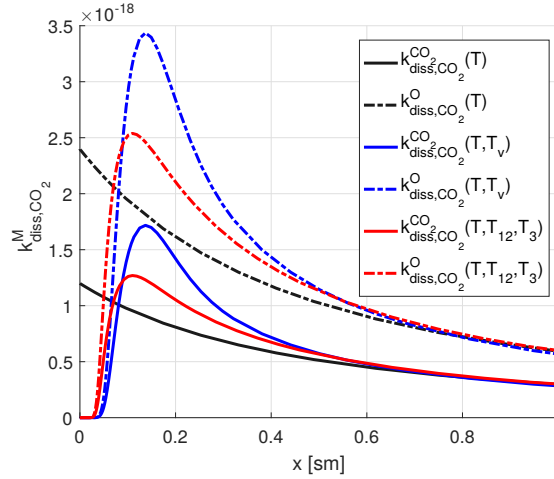


Figure 4: Dissociation rate coefficients in dependence on x .

Comparing the relative numerical densities of CO₂ molecules and dissociation products CO and O (see Fig. 3 (a, b)), we can observe the dissociation delay in the two-temperature and three-temperature approximations, which is explained by the fact that the translational energy close to the shock front passes into the vibrational energy due to the fast TV transitions whereas dissociation starts later.

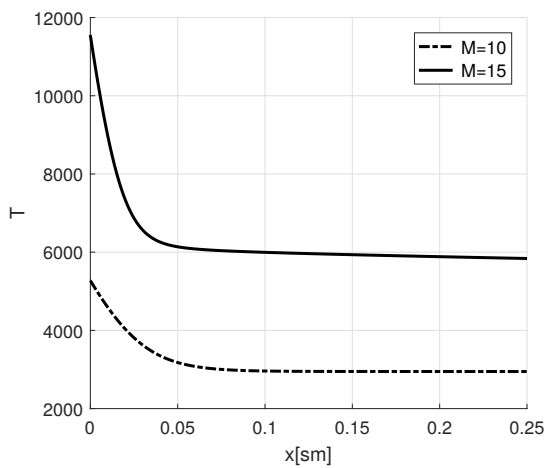


Figure 5: The gas temperature T in dependence on x .

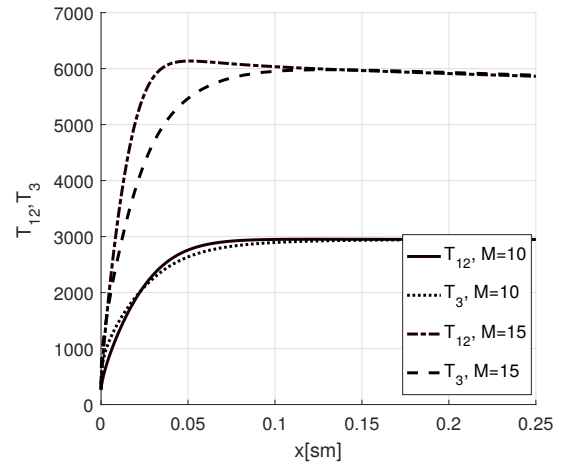


Figure 6: The vibrational temperature T_{12} , T_3 in dependence on x .

The dissociation rate coefficients corresponding to the variation of the parameters behind the shock front are shown in Fig. 4 as functions of x . It should be noted that the dissociation of CO₂ is more active in the collision with atoms O, since the coefficient k_{diss,CO_2}^O is greater than $k_{diss,CO_2}^{CO_2}$. Again we can see a delay of dissociation in the three-temperature and two-temperature approximations close to the shock front. In the one-temperature approximation dissociation rate coefficients exceed $k_{diss,CO_2}^M(T, T_v)$ and $k_{diss,CO_2}^M(T, T_{12}, T_3)$ for small values of x . The non-monotonic behaviour of two-temperature and three-temperature dissociation rate coefficients is explained by the increase of vibrational temperatures close to the shock front and then their slow decrease approaching to the equilibrium. The greatest deviation from the equilibrium value is observed in Fig. 4 for the two-temperature coefficient $k_{diss,CO_2}^{CO_2}(T, T_v)$ and is

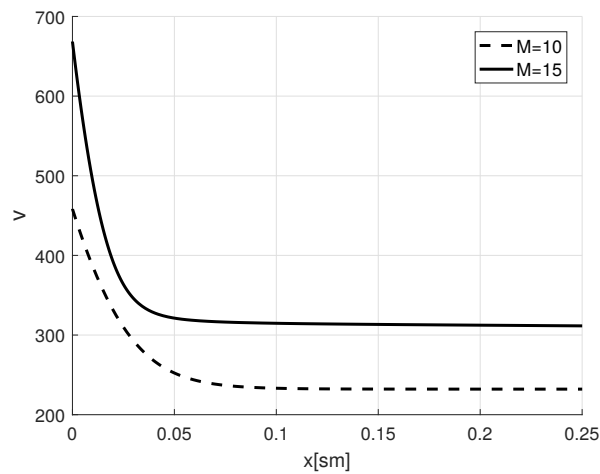
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Figure 7: The velocity of the flow in dependence on x .

consistent with large deviations of the number densities of CO₂ and CO molecules from the equilibrium values at Fig. 3 (a, b).

Now, in Figs. 5-7 we compare flow parameters behind the shock front found in the three-temperature approximation for different Mach numbers in the free stream.

An increase in the Mach number leads to a significant rise in the gas temperature within the shock front and then to high T values immediately behind the front and along the relaxation zone (Fig. 5). The influence of Mach numbers on the vibrational temperatures in the relaxation zone is more noticeable for T_{12} than for T_3 and becomes lower with x rising (Fig. 6). It can be noted that for higher Mach numbers, the relaxation of the mixture proceeds somewhat faster because of the greater initial translational energy immediately behind the shock front (Fig. 5, 6). The velocity variation along the relaxation zone is shown in Fig. 7. A significant difference can be noticed for velocity values obtained for $M=10$ and $M=15$.

2. Conclusions

The relaxation zone structure behind a shock wave occurring in the flow of the mixture CO₂/CO/O is studied numerically in the three-temperature kinetic theory approximation. Governing equations for the mixture composition, gas temperature, velocity and vibration temperatures of combined symmetric-bending and asymmetric modes are solved numerically for the one-dimensional inviscid flow of the considered mixture behind the plane shock wave. The results are compared with those found in the frame of simplified two-temperature and one-temperature flow descriptions. The influence of vibrational distributions and conditions ahead a shock front on variation of macroscopic flow parameters along the relaxation zone is shown.

The results obtained on the basis of the two-temperature and three-temperature approximations show a significant effect of non-equilibrium vibrational excitation on the flow parameters near a shock front and on the dissociation rates. However, as the distance from the shock front x increases, the non-equilibrium effects become smaller. Non-monotonic behaviour of the three-temperature and two-temperature CO₂ dissociation rate coefficients along the relaxation zone is found. The highest values of CO₂ dissociation rate coefficients are obtained for the collisions of CO₂ molecules with O atoms. The comparison of macroscopic parameters for various Mach numbers showed an increase of the gas temperature and flow velocity immediately behind a shock front for higher M .

3. Acknowledgments

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