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A Microscopic Study of One-Dimensional H_2-O_2 Detonation Using DSMC Method

Chao Yang[1, a)], Heji Huang[2, 3, b)] and Quanhua Sun[2, 3, c)]

[1]Laboratory for Aerospace Science and Technology, Institute of Mechanics, Chinese Academy of Sciences, Beijing, China
[2]State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, CAS, Beijing 100190, China
[3]School of Engineering Science, University of Chinese Academy of Sciences, Beijing 100049, China

a)yangchao@imech.ac.cn
b)huang@imech.ac.cn
c)qsun@imech.ac.cn

Abstract. The global and local behaviors of detonation waves are affected by the thermo-chemical coupling process which requires the understanding at molecular level due to its microscopic complexity. In present study, one-dimensional H_2-O_2 detonation is numerically investigated through DSMC method. The detailed balance between forward and reverse reactions is achieved through a modified reaction model, which improves the simulation accuracy of combustion system. Results show that the overall structure of detonation is in accordance with the CFD result, but the microscopic fluctuation of auto-ignition affects detonation in both initiation and propagation stages. Analysis of the detailed structure in the induction zone shows that the auto-ignition process is strongly coupled with the vibrational relaxation process. The lower vibrational temperature decreases the chemical reaction rates, resulting in an increase of ignition delay time and induction zone length.

INTRODUCTION

Combustion consists of complex thermal and chemical non-equilibrium processes, which are often coupled in different degree for many problems. For shock-induced combustion phenomena such as detonation, the coupled thermo-chemical processes are especially important due to the fact that vibrational relaxation and auto-ignition of premixed gas occurs simultaneously behind the leading shock. Taking H_2-O_2 combustion as an example, although the influence of vibrational temperature on chemical reaction rate is relatively weak for the 3-step chain reactions comparing with typical dissociation reactions [1], the close time scale [2] of vibrational relaxation and auto-ignition can still cause a strong thermo-chemical coupling effect in detonation.

Recent computational fluid dynamics (CFD) studies [3, 4] have shown that for H_2-O_2 detonation the effect of thermo-chemical non-equilibrium coupling reduces chain reaction rates in the induction zone, therefore increases the ignition delay time and the induction zone length, finally leads to a larger detonation cell size. In CFD method, the thermo-chemical coupling is often modeled by relaxation equation (such as Landau-Teller equation) and two-temperature reaction rates. However, due to the microscopic nature of thermo-chemical process and the complexity in combustion mechanism, detailed analysis at molecular level is required.

Molecular simulation methods such as the Direct Simulation Monte Carlo (DSMC) method have been widely applied to study thermo-chemical flows in high-temperature air, and the application fields have been expanded to combustion problems such as auto-ignition [5, 6], diffusive and premixed flames [7, 8] as well as detonation [9-12] in the past decade. Early DSMC studies [9, 10] of detonation used irreversible model reaction with simplified hard sphere particle, and recent DSMC studies by Bondar et al. [11, 12] simulated H_2-O_2 detonation using a detailed reaction mechanism and structured molecules with rotational and vibrational energy. Their 1-D result agreed well with the Chapman–Jouguet (C-J) velocity and the Zeldovich–von Neumann–Doering (ZND) model, meanwhile the

detailed balance property of microscopic reaction model was found to be important for the microscopic simulation of H$_2$-O$_2$ combustion.

In this paper, H$_2$-O$_2$ detonation is further studied through DSMC method. Microscopic reaction model is evaluated for chain reactions and a modified reaction model is proposed to satisfy the principle of detailed balance. One-dimensional H$_2$-O$_2$ detonation is then simulated through DSMC method; both overall process and detailed structure are analyzed through the numerical result.

DSMC METHOD AND REACTION MODEL

DSMC Method

The DSMC method is a powerful numerical tool for simulating rarefied gas flows, and its application can also be expanded to non-equilibrium thermo-chemical flows by modeling inelastic collisions and reactive collisions.

For inelastic collisions, both the relaxation collision number and the energy redistribution method should be determined. The relaxation collision number can be converted from the macroscopic relaxation rate with a DSMC modification [13]. The Larsen-Borgnakke (L-B) model [14] is often used for energy redistribution, which ensures the equipartition of different energy modes at thermal equilibrium state.

For reactive collisions, the reaction cross section can be modeled by different reaction models. Building and applying state-specific models for all element reactions is difficult for a real combustion system, and a more practical way is to use phenomenological reaction models which are generally based on the collision theory of chemical reactions. For a specific reaction model, both the vibrational favor character and the equilibrium property (such as detailed balance) are important for the DSMC simulation of combustion system.

In this paper, the Variable Hard Sphere (VHS) [15] model is used to model elastic collisions. The internal energy of molecules assumes a continuous form of rotational energy and a discrete form of vibrational energy (simple harmonic oscillator (SHO) model with a cutoff at the dissociation limit). The rotational degrees of freedom ξ_{rot} and vibrational characteristic temperature θ_v of diatomic and polyatomic molecules in H$_2$-O$_2$ combustion are given in Table 1. Based on this, the temperature-dependent relaxation collision number and the L-B model are used for inelastic collisions. For reactive collisions, the Total Collision Energy (TCE) model [15] is used for forward reactions and a modified form (given in the next section) is used for reverse reactions in order to achieve the detailed balance.

Table 1. The rotational freedom ξ_{rot} and vibrational characteristic temperature θ_v for each species in H$_2$-O$_2$ combustion

| Specis	ξ_{rot}	θ_v (K)
H$_2$	2	6159
O$_2$	2	2256
OH	2	5360
H$_2$O	3	5261, 2294, 5432 (3 modes)

Reaction Model

The TCE model is a widely applied reaction model in DSMC method, which assumes the reaction probability P_{reac} is a function of the total collision energy E_c. The expression can be written as follows,

$$P_{reac} = C_1 \frac{(E_c - E_a)^{C_2}}{E_c^{C_3}} \tag{1}$$

where E_a is the activation energy, C_1, C_2, C_3 are constants determined by molecular properties and Arrhenius form reaction rate.

The TCE model is not a typical vibrationally-favored model, because each part of the total collision energy contributes to the reaction probability in the same way. However, the vibrational energy of reactant still has a weak influence on the TCE reaction probability, which is found to be suitable for H$_2$-O$_2$ chain reactions with low activation energy. Here TCE model is evaluated for one of the 3-step chain reactions, H+O$_2$→OH+O. Figure 1(a)

shows the distribution of vibrational energy levels of reacted O_2 molecules at a thermal equilibrium state of 2000K. Obviously, the distribution is biased to higher vibrational energy level comparing with the Boltzmann distribution. Figure 1(b) shows that the non-equilibrium reaction rate ($T_{tr} \neq T_v$) predicted by TCE model agrees well with the Park two-temperature model modified by quasi-classical trajectory (QCT) calculation [1], indicating that TCE model is a proper choice for H_2-O_2 chain reactions with weak vibrational favor.
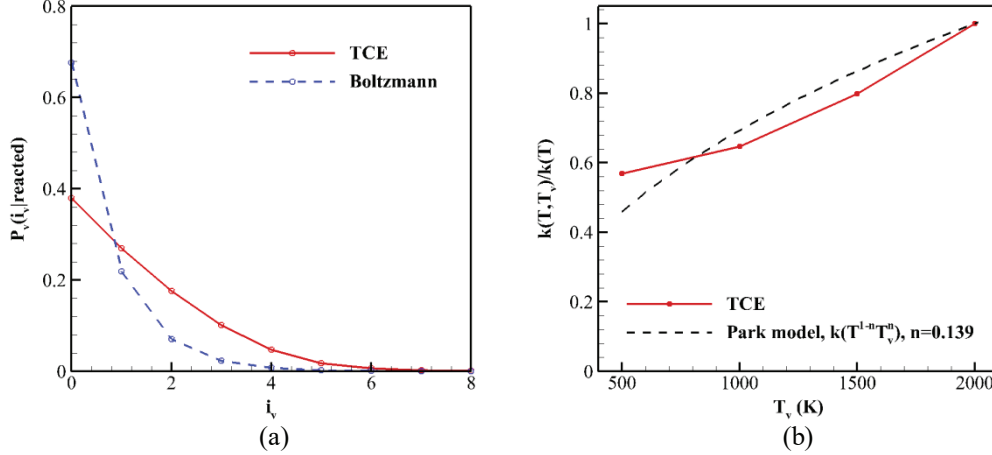
FIGURE 1. Evaluation of TCE model for chain reaction "H+O_2→OH+O". (a) Distribution of vibrational energy levels of reacted O_2 molecules in a thermal equilibrium bath of 2000 K for TCE model. (b) Normalized non-equilibrium reaction rate predicted by TCE model comparing with a modified Park model [1], $T_{vib}<T$=2000 K.

    The equilibrium property of TCE model is another critical problem for combustion modeling. Apparent breakdown of thermal equilibrium at chemical equilibrium state has been observed in several DSMC simulations of H_2-O_2 combustion [11, 8] using TCE model for all elemental reactions and L-B model for energy redistribution of reactive collisions. It has been pointed out that thermal equilibrium cannot be achieved at chemical equilibrium state unless detailed balance between forward and reverse reaction is accurately satisfied [16]. In order to satisfy detailed balance, different modifications were proposed for combustion simulation. Using anharmonic oscillator (AHO) model of vibrational energy and a corresponding VFD reaction model [17], Bonder et al. [12] found that detailed balance between dissociation and recombination of polyatomic molecules cannot be achieved unless dissociation of polyatomic molecules of which the total vibrational energy is larger than the dissociation energy is prohibited. Using SHO model of vibrational energy and TCE reaction model, Sebastião et al. [8] proposed a two-step energy redistribution model for reactive collisions, which significantly reduces the difference between translational and vibrational temperatures at chemical equilibrium state. Although the above two modifications work well in practice, achieving an exact detailed balance requires a more precise method focusing on microscopic collision process of forward and reverse reactions. Therefore, a theoretical analysis and a modified reaction model are shown below.

    In order to satisfy detailed balance, the thermal effect of forward and reverse reaction has to be canceled by each other at chemical equilibrium state. Taking exchange reaction

$$AB + C \rightleftharpoons AC + B \tag{2}$$

as an example, two specific requirements have to be satisfied,

$$v_f n_{AB} n_C P_{reac,f}\left(E_{c,f}\right) f\left(E_{c,f}\right) = v_r n_{AC} n_B P_{reac,r}\left(E_{c,r}\right) f\left(E_{c,r}\right), \tag{3}$$

$$P_{redist}\left(E_{i,AC} \mid E_{c,f}\right) = P_{reacted}\left(E_{i,AC} \mid E_{c,r}\right). \tag{4}$$

In equation (3), the subscript f and r refer to the forward and reverse reactions respectively, v is the molecular collision rate, n_i is the species number density at chemical equilibrium state, E_c is the total collision energy which contains relative translational energy and molecular internal energy and $f(E_c)$ is its distribution function at equilibrium state. An implicit restriction for $E_{c,f}$ and $E_{c,r}$ is

$$E_{c,f} - E_{c,r} = E_{a,f} - E_{a,r} = E_{heat} \tag{5}$$

where E_a is the activation energy, E_{heat} is the reaction heat. Equation (4) is the energy redistribution model, in which P_{redist} is determined by the internal energy distribution of AC produced by forward reaction and $P_{reacted}$ is determined

by the internal energy distribution of AC consumed by reverse reaction. The energy redistribution model for AB produced by reverse reaction can be written down in the same way.

The energy redistribution method for reactive collision has been discussed a lot in previous studies; however, as a precondition equation (3) received little attention. It is easy to prove that if TCE model is used to determine the forward and reverse reaction probabilities, equation (3) and therefore detailed balance are usually not satisfied. So in order to satisfy detailed balance, we propose a modified model for reverse reaction as a counterpart to the TCE model for forward reaction.

The number densities of species in equation (3) can be eliminated by introducing the chemical equilibrium constant K_{eq}, which can be calculated using a statistical expression as follows [15]

$$K_{eq} = \frac{k_f}{k_r} = \frac{n_{AC}n_B}{n_{AB}n_C} = \frac{Q_{AC}Q_B}{Q_{AB}Q_C} \exp\left(-\frac{E_{heat}}{kT}\right) \tag{6}$$

where E_{heat} is the difference between the forward and reverse activation energies, Q is the partition function of each species. Each partition function can be further written as the product of translational, rotational, vibrational and electronic partition functions. In the temperature range of 1000 K to 4000 K for typical H_2-O_2 combustion problems, the electronic partition function can be treated as a constant. In order to get a better accordance with the experimental value of K_{eq}, a correction factor may be used for each species.

After some simplification of equation (3), the terms related to the macroscopic temperature T are all eliminated. Therefore, the reaction probabilities of forward and reverse reactions satisfy the following equation,

$$\frac{P_{reac,f}\left(E_{c,f}\right)}{P_{reac,r}\left(E_{c,r}\right)} = \frac{C_r \sum\limits_{E_{v,r}<E_{c,r}} \left[\left(\frac{E_{c,r}-E_{v,r}}{kT_{ref}}\right)^{1.5-\omega_r+\frac{\xi_{rot,r}}{2}}\right]}{C_f \sum\limits_{E_{v,f}<E_{c,f}} \left[\left(\frac{E_{c,f}-E_{v,f}}{kT_{ref}}\right)^{1.5-\omega_f+\frac{\xi_{rot,f}}{2}}\right]} \tag{7}$$

where C is a constant, ω is the temperature exponential coefficient of viscosity, ξ_{rot} is the total number of rotational degrees of freedom, E_v is the total vibrational energy, E_c is the total collision energy and the subscript f and r refer to the forward and reverse collision pairs. The summation symbol refers to all possible discrete vibrational energy E_v that is smaller than E_c. The constant C for forward and reverse collision pair is (subscript f and r are omitted)

$$C = \frac{\varepsilon_{coll}^{-1}\sigma_{T,ref}m_{reduce}^{-0.5}\left(m_1 m_2\right)^{1.5}}{\Gamma\left(2.5-\omega+\frac{\xi_{rot}}{2}\right)\prod\limits_i \left[g_{e,i}^{-1}\varepsilon_{rot,i}\left(\theta_{rot,i}/T_{ref}\right)^{\frac{\xi_{rot,i}}{2}}\right]} \tag{8}$$

where m_1 and m_2 are the molecular mass of the two species in forward or reverse collision pair, m_{reduce} is the reduced mass, ε_{coll} is the symmetric factor of collision pair, $\sigma_{T,ref}$ is the reference cross section. For each reactant i, $g_{e,i}$ is the electronic partition function which is used as a constant, $\theta_{rot,i}$ is the characteristic rotational temperature, $\xi_{rot,i}$ is the rotational degree of freedom, $\varepsilon_{rot,i}$ is the molecule symmetric symbol.

Unlike exchange reaction, recombination reaction involves three molecules. As a result, the relation between recombination and dissociation reaction probabilities is a little different from equation (7). Taking reaction

$$A + B + M \rightleftharpoons AB + M \tag{9}$$

as an example, the total collision energy for recombination reaction consists of the collision energy between A and B as well as the collision energy between AB and M, thus a corresponding adjustment should be made to the original TCE expression [15]. In order to have a formal consistency with the original TCE expression, the relative translational energy between AB and M is considered as an extra term to the total collision energy while a corresponding freedom of 3 is added to the internal energy freedom. By doing so, the adjusted expression still reproduces the Arrhenius reaction rate. Based on this adjustment, the reaction probabilities of forward (recombination) and reverse (dissociation) reactions satisfy the following equation,

$$\frac{P_{reac,f}\left(E_{c,f}\right)}{P_{reac,r}\left(E_{c,r}\right)}=\frac{C_r\displaystyle\sum_{E_{v,r}<E_{c,r}}\left[\left(\frac{E_{c,r}-E_{v,r}}{kT_{ref}}\right)^{1.5\text{-}\omega_r+\frac{\xi_{rot,r}}{2}}\right]}{C_f\displaystyle\sum_{E_{v,f}<E_{c,f}}\left[\left(\frac{E_{c,f}-E_{v,f}}{kT_{ref}}\right)^{3\text{-}\omega_f+\frac{\xi_{rot,f}}{2}}\right]}. \tag{10}$$

where C_f and C_r become

$$C_f=\frac{\varepsilon_{coll}^{-1}\sigma_{T,ref}m_{reduce}^{-0.5}\left(m_A m_B\right)^{1.5}\left(\frac{2\pi}{h^2}\right)^{1.5}\left(kT_{ref}\right)^{1.5}}{\Gamma\left(2.5\text{-}\omega+\dfrac{\xi_{rot}}{2}+1.5\right)\prod_i\left[g_{e,i}^{-1}\varepsilon_{rot,i}\left(\theta_{rot,i}/T_{ref}\right)^{\frac{\xi_{rot,i}}{2}}\right]} \tag{11}$$

$$C_r=\frac{\varepsilon_{coll}^{-1}\sigma_{T,ref}m_{reduce}^{-0.5}m_{AB}^{1.5}}{\Gamma\left(2.5\text{-}\omega+\dfrac{\xi_{rot}}{2}\right)\prod_i\left[g_{e,i}^{-1}\varepsilon_{rot,i}\left(\theta_{rot,i}/T_{ref}\right)^{\frac{\xi_{rot,i}}{2}}\right]}. \tag{12}$$

In practice, the reaction probability of forward reaction is calculated through TCE model directly, while the reaction probability of reverse reaction is calculated through equation (7) or (10) and the corresponding reaction probability of forward reaction though TCE model. Although mapping all the possible vibrational states satisfying $E_{v,f}<E_{c,f}$ when calculating equation (7) and (10) takes more CPU cost, it has only a small influence on the overall efficiency because reactive collisions are a small part of all collisions in typical combustion problems below 4000K.

For H_2-O_2 combustion, the necessary parameters to calculate constants C_f and C_r, i.e. the term in middle bracket in the denominator for each species i, is listed in Table 2. Although the rotational degree of freedom is 0 for monatomic molecules, the characteristic rotational temperature θ_{rot} is still set to the reference temperature (T_{ref}=273K) for calculation convenience. Besides, a correlation factor α_i for each species is multiplied to that term in order to get a better accordance with the experimental value of K_{eq} in typical temperature range for combustion.

Table 2. Necessary parameters in the modified reaction model for H_2-O_2 combustion.

| Specis i	$g_{e,i}$	$\varepsilon_{rot,i}$	$\theta_{rot,i}$ (K)	α_i
H_2	1	2	85.4	0.9158
H	2	1	T_{ref}	1
O_2	3	2	2.07	0.8183
O	9	1	T_{ref}	1
OH	4	1	26.6	0.9119
H_2O	1	1	21.6	1.135

Verification of Reaction Model

Verification for the above reaction models is made through a DSMC simulation of H_2-O_2 auto-ignition. All collision models (elastic, inelastic and reactive) used in DSMC simulation can be found in "DSMC method" section. A detailed reaction mechanism [18] of 6 species and 14 element reactions is used, in which forward reactions are simulated by the TCE model and reverse reactions re simulated by the modified model.

A stoichiometric H_2-O_2 mixture of T=2000 K and n=10^{25} m^{-3} is initially filled in a constant-volume box with spectacular wall condition, and the initial particle number is 10^6. Figure 2(a) shows that the ignition process cannot achieve thermal equilibrium at chemical equilibrium state using TCE model for both forward and reverse reactions. Figure 2(b) shows that the deviation between vibrational and translational temperatures at chemical equilibrium state

vanishes by using TCE model for forward reactions and modified model for reverse reactions. The vibrational relaxation collision number in Fig.2(a) and Fig.2(b) correspond to a macroscopic vibrational relaxation rates determined by the Millikan-White equation [19, 20]. However, as shown by G.Bird [16], if detailed balance is satisfied, adiabatic reacting systems should relax towards thermal equilibrium regardless the value of Z_V. Therefore, another simulation which is similar to Fig.2(b) but completely turns off vibrational relaxation (i.e. infinity values for Z_v) is shown in Fig.2(c). The excellent agreement between vibrational and translational temperatures at chemical equilibrium state in Fig.2(c) proves that detailed balance is completely satisfied.
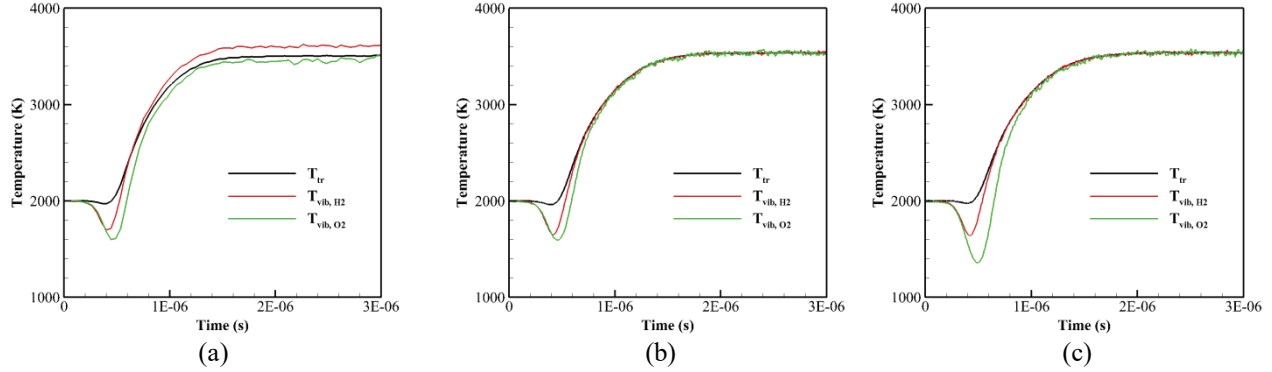
FIGURE 2. The time history of translational and vibrational temperatures in auto-ignition process.

(a) TCE model for forward reactions, modified model for reverse reactions and physical values of Z_v.

(b) TCE model for forward and reverse reactions and physical values of Z_v.

(c) TCE model for forward reactions, modified model for reverse reactions and infinity values of Z_v.

NUMERICAL SIMULATION AND RESULT ANALYSIS

Simulation Setup

The initial condition of 1-D H_2-O_2 detonation is shown in Fig.3. The driver section gas is on the left side and the upstream gas is on the right side. For upstream gas, T_1=300 K and p_1=1 atm; for driver gas, T_2=3000 K and p_2=100 atm. The initial mole concentration for both sides is H_2:O_2=67%:33%. The domain length in x direction is 0.01 m and the driver section is set to be 0.0002 m to ensure enough energy for a direct initiation. The minimum and maximum boundaries in x direction are both specular reflecting walls. The cell size is 1μm in x-direction. Each cell is further divided into 3 sub-cells, and the nearest collision partner method is used to select collision pairs in sub-cells. At the beginning of simulation, the number of simulated particles is about 1.22 million in driver section and 5.99 million in upstream section. Domain decomposition with MPI parallel is used to accelerate the simulation and running one case takes about 10 days by using 96 CPUs. The DSMC models used in detonation case are identical to those in the auto-ignition case.


FIGURE 3. The sketch of 1-D H_2-O_2 detonation problem

A CFD simulation is also conducted for the same case as a comparison. The reactive Euler equations are solved using a dispersion-controlled dissipative (DCD) scheme [21]. The reaction mechanism is the same one used in DSMC simulation. The thermodynamic data of each species use the statistical expression determined by translational, rotational and vibrational energies which are also identical to the DSMC simulation.

Analysis of the Overall Process: Initiation and Propagation

The initiation process of detonation is shown in Fig.4. After the breakdown of the initial discontinuity, a shock wave forms first and is quickly enhanced by a pressure pulse produced by the auto-ignition of the driver gas. While the shock wave propagates, an induction zone forms behind it. Auto-ignition events successively occur in the induction zone and new pressure pulses produced by heat release enhance the leading shock to higher strength. In Fig.4, there are three obvious increases of shock wave pressure due to auto-ignition events, and an overdriven detonation finally forms at about $X=0.0012$ m after the last increase of pressure.
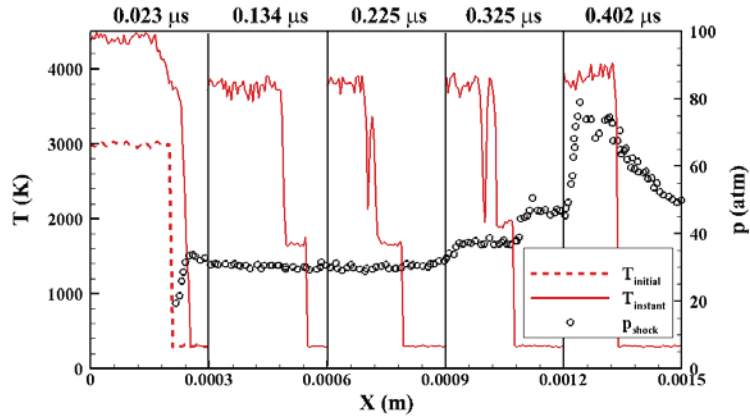
FIGURE 4. The temperature profiles of different instantaneous moments in the initiation process and the evolution of shock wave pressure.

The auto-ignition and pressure increase in DSMC result are found to be affected by the microscopic fluctuation of chemical reactions. Figure 5 compares the time history of shock wave pressure of two independent DSMC cases and also with the CFD result calculated under a grid size of 1 μm. In the second DSMC case, detonation initiation occurs directly after the second pressure increase at about $X=0.001$ m. The effect of microscopic fluctuation is supposed to play a more important role if the initiation energy decreases to a certain critical value, and this issue needs a detailed study in future work focusing on detonation initiation.
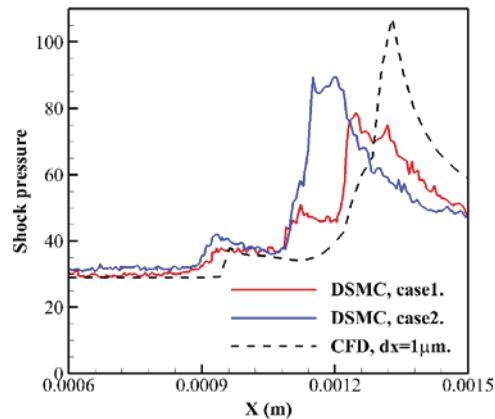
FIGURE 5. The time histories of shock wave pressure in the initiation process for two statistically independent DSMC cases.

After the initiation, the overdriven detonation wave gradually decays to the C-J detonation. The detonation velocity is 2921 m/s, which is linear fitted by the positions of detonation wave front between (0.002 m, 0.01 m). The overdriven degree is about 1.03, which is defined as the ratio of detonation velocity to C-J detonation velocity. It is known that 1-D H_2-O_2 detonation is highly unstable unless the mixture is diluted by a large amount of non-

combustible gas. Due to the intrinsic instability, the propagation of detonation front develops into a periodic oscillation mode, shown in Fig.6(a). Periodic oscillation with relatively small amplitude appears first, and the amplitude gradually increases as the degree of overdrive decreases in the propagation. The temperature profiles of three typical moments in one oscillation period are compared in Fig.6(b) under the shock-wave coordinate. The moments t_A and t_C represent the situation of maximum shock wave pressure, and their temperature profiles are qualitatively in accordance with the CFD result calculated under a grid size of 10 μm. The moment t_B represents the situation of minimum shock wave pressure, in which auto-ignition has been greatly delayed due to the fluctuation of ignition delay time. Previous studies [21] have shown that, at microscopic scale, the fluctuation of ignition delay time is strongly affected by the stochastic and discrete natures of reactive collisions. In present DSMC simulation, the limited particle number in the induction zone causes a similar fluctuation of ignition delay time. Such a microscopic fluctuation becomes a physical disturbance to the unstable system, which is supposed to be one of the many reasons that cause the periodic oscillation in 1-D H_2-O_2 detonation.
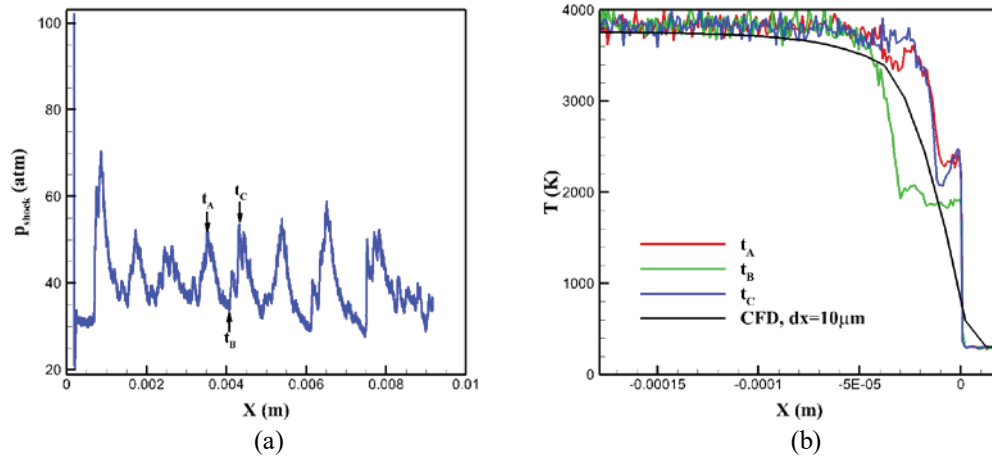

FIGURE 6. Detonation instability in the propagation process. (a) The oscillation of shock wave pressure. (b) The temperature profiles of three typical moments.

Analysis of the Thermo-Chemical Coupling Effect

Due to the fluctuation of auto-ignition process, it is difficult to quantitatively analyze the thermo-chemical coupling effect in the induction zone. Therefore, a statistical averaged profile of instantaneous results of the entire oscillation period is used. Figure 7 shows the averaged profiles of temperature, pressure and species concentrations in the shock-wave coordinate.

Figure 7(a) shows that the vibrational temperatures of H_2, O_2, OH and H_2O all deviate from translational temperature greatly in the induction zone, indicating that auto-ignition after the leading shock is coupled with a strong thermal non-equilibrium process which is dominated by the relaxation of H_2 and O_2. In the relaxation process, translational temperature has a slight decrease because its energy is transferred to the vibrational mode of H_2 and O_2. Besides, due to the fact that O_2 molecules with higher vibrational energy are more easily consumed by chain reactions, the vibrational temperature of O_2 molecules stays steady for a while in its relaxation process, indicating a two-way interaction between thermal relaxation and chemical reaction. In Fig.7(b), the variation of H_2 and O_2 concentration in the shock wave layer is caused by the mass diffusion effect of light (H_2) and heavy (O_2) molecules, which has been discussed in many theoretical and numerical studies.

To quantitatively study the thermo-chemical coupling effect in the induction, the above result is compared with a thermal-equilibrium case in which vibrational relaxation number is set to be 1. Similar statistical average strategy is used in the thermal-equilibrium case in order to get a smooth averaged profile. Figure 8 shows that the length of the induction zone is obviously larger in the thermal non-equilibrium case; and the half reaction thickness, which is defined as the distance between shock wave front and the position where H_2 concentration drops to half of its upstream value, is 29.9% larger than that in the thermal equilibrium case. This means the relaxation process reduces chain reaction rates and increases the ignition delay time in present H_2-O_2 detonation case.
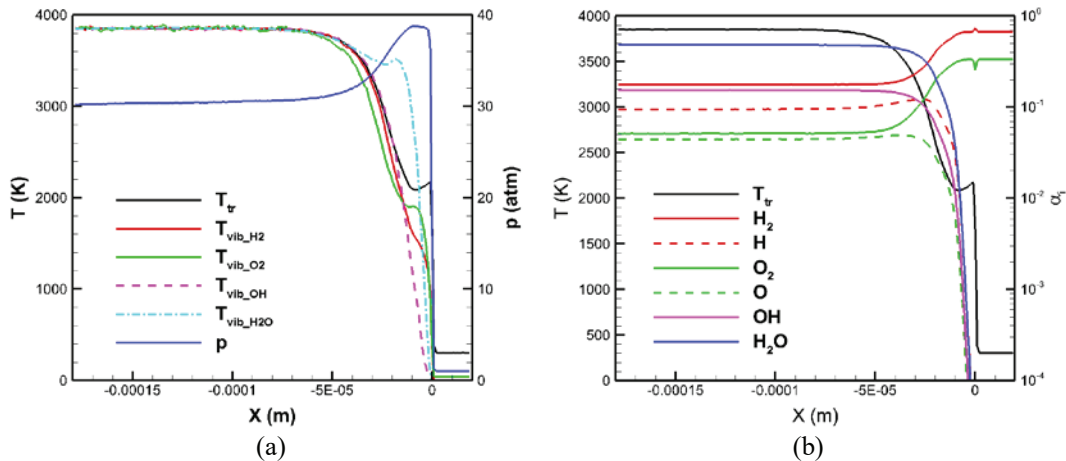
FIGURE 7. The detailed structure of detonation. (a) Pressure and temperature. (b) Species concentrations.
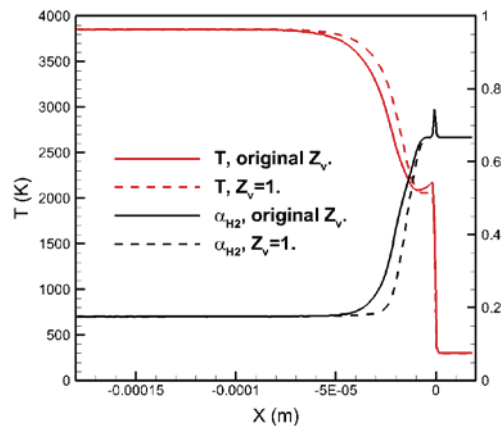

FIGURE 8. Effect of vibrational relaxation on the induction zone length.

CONCLUSION

One-dimensional H_2-O_2 detonation is numerically studied by DSMC method. Microscopic detailed balance of combustion system is achieved through TCE model and a modified reaction model for reverse reaction. DSMC result shows that the initiation and propagation processes of H_2-O_2 detonation are affected by the microscopic fluctuation of auto-ignition, which is important in microscopic scale. The detailed structure of the induction zone is analyzed by the statistical averaged profile, and the comparison with thermal-equilibrium result shows that vibrational relaxation reduces the chain reaction rates and therefore increases the auto-ignition process and induction zone length. Future study will analyze the thermo-chemical coupling effect in different upstream conditions, especially the dilution degree and equivalence ratio.

ACKNOWLEDGMENTS

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