Numerical Simulation on Mechanism of Flame Acceleration and Deflagration to Detonation Transition for Ethylene-Oxygen System

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1 Introduction

A leaking or out bursting of the combustible gas may happen in the process of transport. The low speed laminar flame from a weak ignition source will accelerate to be a deflagration wave by the pipe wall and obstacle interactions. Then local explosion may be triggered and transition to detonation can occur under proper condition, which results in heavy casualties and losses. Therefore it is particularly prominent and urgent to prevent the happening of combustible gas explosion disasters and ensure the safety of gas transport. So carrying out the study of deflagration to detonation has an important application value and long-term protect in the explosion disaster prevention.

A whole process of deflagration-to-detonation transition (DDT) involves rather complicated physical mechanism and is across multiple time and space scales, containing the laminar flame acceleration, the formation of compression wave and the resulting detonation stage. In the small scale DDT, the effect of the viscous role and the heat exchange of wall on DDT and detonation propagation are considered in recent researches [1-5]. For microscale (order of 0.1 mm) DDT, recent experiments study on the DDT of ethylene-oxygen in capillary channels [2, 6]. Wu et al. observes the oscillating flame, steady deflagration and galloping detonation in microscale channels and further discusses the deficit of detonation velocity and the effect of the wall heat exchange on flame acceleration and detonation velocity. Also detonation limits are studied in extremely narrow channels [7]. There are different stages from cellular detonation to spinning detonation, and galloping detonation can be observed in critical diameter of channel for reactive flow Euler system [8]. Pulsating detonations propagating in circular and square tubes are numerically investigated with a two-step reaction model [8]. In their simulation, viscous effect is neglected in governing equations and the effect of thus resistance from the wall on the propagation of detonation cannot explain well. Hence, how do the viscous effect play role in the microscale detonation and the deficit of detonation velocity, and can the detonation sustains without the triple point?

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In macroscale (order of 1cm) DDT, generally flame instability and turbulence are important for the transition of detonation in macroscale channel [9, 10]. A series of the DDT experiments in long channels containing hydrogen-oxygen mixtures were carried out by Oppenheim with collaborators [11-14]. Initially laminar flame, to turbulent flame and transition to detonation caused by local explosion in the flame brush and the formation of reaction gradient mechanism is observed in [12, 13, 14]. Liberman et al. [15] numerically studies of DDT in highly reactive hydrogen-oxygen and ethylene-oxygen mixtures by solving two-dimensional reactive Navier-Stokes equations for a hydrogen-oxygen gaseous mixture. Even through the different transition mode of DDT and the formation of the cellular detonation in different diameters of tube [11] experimentally are observed, the effect of viscous force on the mode of DDT and the formation mechanism of detonation cell and the deficit of detonation velocity still is not clear.

The paper will simulate the whole process of DDT and the propagation of detonation in microscale and macrosacle channels by solving the reacting flow governing equations with the viscous and heat and material diffusion and the reaction model are used to describe flow and energy release characteristics for ethylene-oxygen system. The goal of the simulation is to reveal the effect of the viscous in boundary layers on the mode of DDT and the propagation of detonation.

2 Governing equations

The compressible reaction Navier-Stokes equations including advection, diffusion and reaction source are as following

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j + \delta_{ij} p - \zeta_{ij}) = 0 \tag{2}$$

$$\frac{\partial}{\partial t}(\rho e + \frac{1}{2}\rho u_i u_i) + \frac{\partial}{\partial x_j}(\rho u_j h + \frac{1}{2}\rho u_i u_i u_j + \sigma_j - u_i \zeta_{ij}) = 0 \tag{3}$$

$$\frac{\partial}{\partial t}(\rho Y) + \frac{\partial}{\partial x}(\rho u_i Y - \frac{\mu}{\mathrm{Sc}}\frac{\partial Y}{\partial x_i}) = -A\rho Y \exp(-Ea / R_p T) \tag{4}$$

$$p = \rho R_p T / M \tag{5}$$

here is the mass fraction of combustible gas, $e = QY + C_V T = QY + R_p T / (\gamma\text{-}1)$ is internal energy, $h = QY + C_p T = QY + RpT\gamma / (\gamma\text{-}1)$ is enthalpy, Q is the heat of reaction, C_V and C_p are specific heat at constant volume and the specific heat at constant pressure, respectively. R_p is perfect gas constant, M is the molar mass, γ is the adiabatic exponent of the combustion gas. The stress tensor ζ_{ij} and the energy diffusion vector σ_j are

$$\zeta_{ij} = \mu(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}) \tag{6}$$

$$\sigma_j = \mu(\frac{C_p}{\mathrm{Pr}}\frac{\partial T}{\partial x_j} + \frac{Q}{\mathrm{Sc}}\frac{\partial Y}{\partial x_j}) \tag{7}$$

here $\mu \equiv \rho v$ is dynamic viscosity coefficient, v is molecular kinetic viscosity, Pr = 0.75 and Sc = 0.75 are Prandtl and Schmidt number. δ_{ij} is Kronecker symbol, if $i = j$ ， δ_{ij}=1, if not δij = 0. Furthermore, ρ is the density, p the pressure, T the temperature, Y the reactant mass fraction, Q the heat of reaction, E_a is activation energy, γ = 1.4 the specific heat ratio and A the pre-exponential factor. A high-resolution parallel code based on 5-th order weighted essentially non-oscillatory WENO scheme is used to simulate DDT for ethylene-oxygen system.

3 Results and discussions

Take channel with the width of W=0.22mm and 12mm, and fill it with premixed mixture. A planar flame by weak ignition is set at the left. In the unreacted mixture, initial velocity, temperature and pressure are 0.0m/s, 300K and 1atm respectively. The left of the duct is closed and the right is free outflow. The upper and bottom all is non-slip wall. In numerical simulation, 50 points per one flame thickness is used to mesh the computing domain. An efficient parallel code can be used on a massive parallel platform, as it is done in this work.

3.1 DDT in microscale channel

In microscale channel, the evolution of the flame front in the whole process of DDT is shown in Figure 1. It can be seen that the DDT process contains coarsely three stages: flame acceleration; transition to detonation; detonation. Initially, flame accelerates due to the expansion of hot product from the left end closed. Generally, combustion wave is subsonic and thus perturbations behind the flame front can propagate into upstream as so to change the initial value in unreacted mixture. Hence, as flame forward propagates, flow in the gas ahead to the flame appears. Because of the effect of boundary layers, the flow is fast at the center line and slow near wall. Flame propagates into the thus flow, the flame stretches and takes on a shape liking finger, as shown in zoom of Figure 1. Figure 1 shows the structure of the flame under the condition of no slip wall, which agrees with the results by Wu [2, 6]. We can see that the flame front stretches and becomes curved and longer due to the boundary layers and the thermal expansion, and the flow near the wall is relatively slower than that in the central. As the flame elongate, a finger characteristic appears and flame surface increases. Propagation speed of the flame increases exponentially, compared as the same results by Schmidt and Oran [16, 17]. The accelerated flame constantly preheats the unreacted mixture ahead to the flame front, which in turn makes the flame further accelerate. Then compression wave in front of flame front can be induced by the fast flame and constantly superposition into leading shock with the increase in flame velocity. Noting that from Figure 1, a strongly preheated region of unreacted gas near wall appears and results in a feather with faster flame at wall and slower flame at channel axis, liking a tuliping shape [3]. At x~0.168m, precursor shock couples with the accelerated flame in boundary layers and overdriven detonation forms. Eventually, overdriven detonation decays, as also seen in Figure 2. Figure 2 shows pressure distribution along propagating direction at axis line. From the evolution of pressure profile, it can be seen that in initial stage of laminar flame propagation, pressure is low and close to be initial value in unreacted mixture. Hence, the flame in this stage can be considered as constant-pressure combustion. At x~0.04-0.06m, compression wave forms and the weak discontinuity of the pressure appears. As the flame and the flow ahead to it accelerate, a strong discontinuity of the pressure can be formed and correspondingly leading shock appears. Hence, the profile of pressure contains the combination of the induction region and reaction zone. With the decrease in the induction zone and the increase in the reaction zone, a gradient mechanism of reaction (see Figure 5) can be formed and then the resulting pressure pulse develops into a sharp pressure peak at x~0.15m. The formation of the gradient mechanism eventually leads to the onset of overdriven detonation at x~0.16m and the pressure reaches approximately 75atm.

Figure 3 shows evolution of the temperature, pressure, density and velocity profile along axis line in the laminar flame acceleration. The formation of compression wave and preheated zone shown in Figure 3(b) are observed in detail and that the density shown in Figure 3(a), pressure, temperature and flow velocity of unreacted gas at front of flame all increases. As the compressed and preheated mixture flows into the flame front, heat release in reaction enhances and renders further the flame acceleration. The width and amplitude of the pressure profile is not enough to create a sharp discontinuity but make the ignition time decrease and also enhances the reaction rate. Because the combustion wave is an expansion wave, the products behind flame front has an inverse flow and the velocity of the inverse flow increases along the negative direction, as shown in Figure 3(a), which also agree with that of 1D model in [15]. However, at t = 12.7×10^{-5}s, the leading edge of the profile steepens, which can be observed from 1D simulation, and local perturbation of flow is observed. The

propagating velocity of detonation also shows longitudinally oscillation shown in Figure 4, which also was observed by Sugiyama and Matsuo [8]. In Sugiyama's simulations, strong longitudinal pulsation controls the propagation of detonation due to the lack of the transverse wave, while our numerical results show that the pulsation of detonation is not very strong. The difference may be because the transverse wave is not necessary to the microscale detonation in our simulation and maybe the interaction of shock with boundary layer is more key role in propagating of detonation in microscale channels. It is interestingly found that after overdriven detonation attenuates CJ state at x~0.195m, detonation can propagates at below CJ velocity (about 2200m/s). The present low-speed propagation might be some low-speed detonation previously observed in the literature for detonation in narrow gaps or porous media [2]. In the experiment, due to heat loss at wall and momentum loss in boundary layer detonation velocity is below the CJ value. However, there is no wall heat loss in the simulations. This microscale detonation can propagate at low speed due to the loss of momentum led by the viscous effect on wall.

3.2 DDT in macroscale (12mm) channel

Initially, a planar flame is set at the left end. Local explosion, triggered by the interaction of the resulting shock wave with boundary layer, can be observed obviously between the turbulent and shock wave at t=7.90×10^{-4}s (see Fig.5). Reflected wave also can be seen and supports the explosion wave to catch up with the precursor shock. As the explosion wave propagating forward couples with the precursor shock wave, strong overdriven detonation forms at t=8.04×10^{-4}s. Eventually, with the transverse wave fully developing and the formation of the triple point, the strong overdriven decays and gradually evolves into cellular detonation by the collision of triple point with each other. Meanwhile, noting that, also evident is the retonation wave that propagates back into the combustion products and induces the fast reaction of unreacted gas in the turbulent flame, consistent with the experimental results by Urtiew & Oppenheim (1966). Transition to detonation in the micro- and macro-scale channels takes fundamentally different progresses, as summarized in Figure 6. For micro-detonation, initially flame velocity increases exponentially. As the flame accelerates, the flame velocity linearly increases due to the compressible effect of the gas, and jumps suddenly to 2800m/s and then decays below CJ state. Compared the micro-scale, macro-scale DDT has slower flame instability and acceleration rate initially, so the flame velocity slowly increases. As the turbulent flame forms, the flame velocity rapidly increases to deflagration value that can be kept in longer period (deflagration velocity, 800m/s by Rankine-Hugoniot relation and release heat), and then suddenly jumps to very high value and then decays almost to CJ velocity.

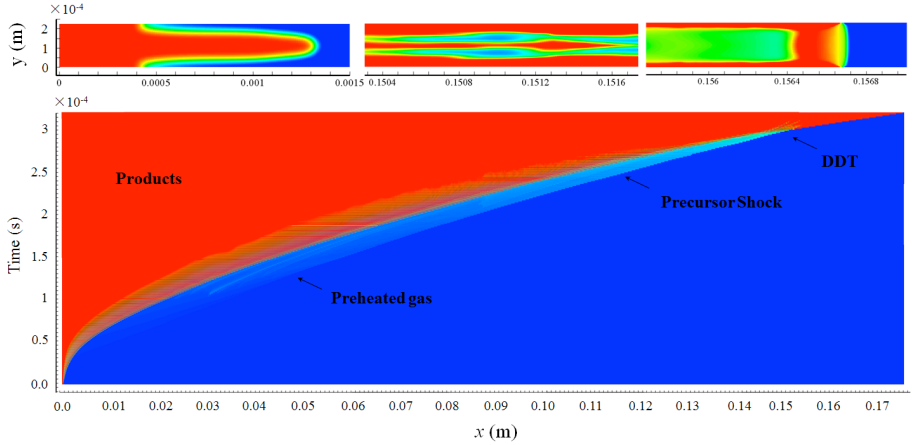


Fig. 1 Laminar flame acceleration and DDT: red region indicates flame and blue region indicates unreacted gas deflagration wave with leading shock and transition to detonation; steady detonation: initially exponent and then linear acceleration of flame.

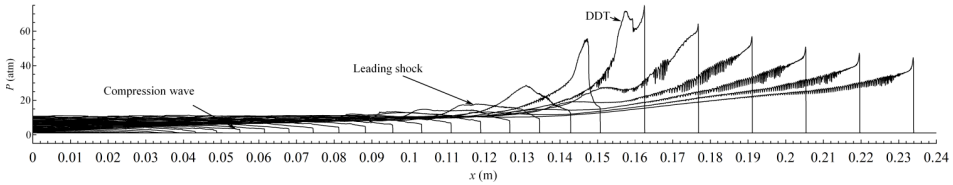
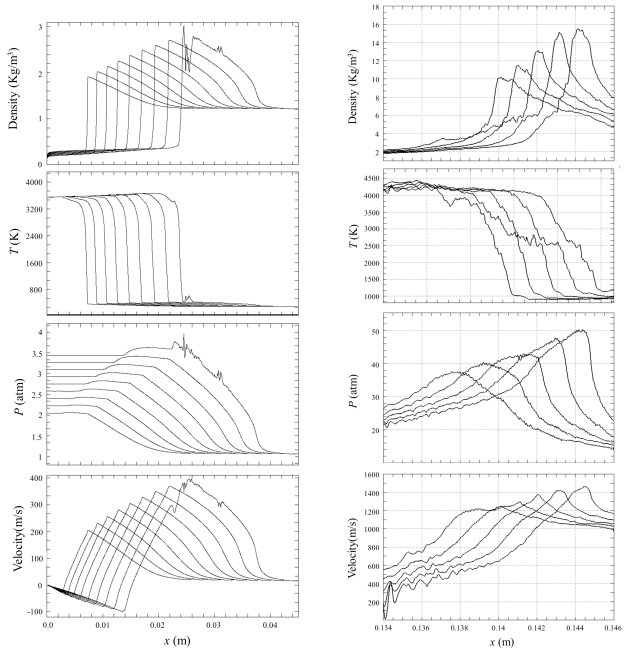


Fig. 2 Evolution of pressure profile in the process of DDT



(a) (b)

Fig.3 Evolution of the temperature profile, pressure, density and velocity at axis line: (a) t=7.40, 8.11, 8.80, 9.49, 10.16, 10.82, 11.47, 12.11, 12.74 $\times 10^{-5}$s; (b) t=2.82, 2.83, 2.84, 2.85, 2.87$\times 10^{-4}$s, responding the curves from the left to right, showing the flame acceleration and formation of preheated zone ahead to the flame front.

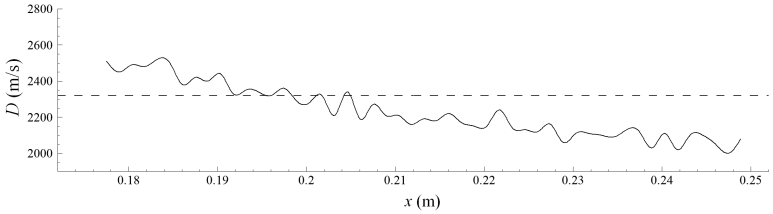


Fig.4 Curves of detonation velocity with propagating distance in the stage of pulsating detonation: *D* denotes detonation velocity (solid line); dash line denotes CJ velocity.

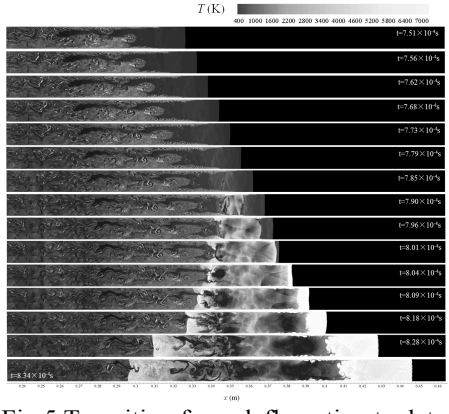


Fig.5 Transition from deflagration to detonation(12mm)

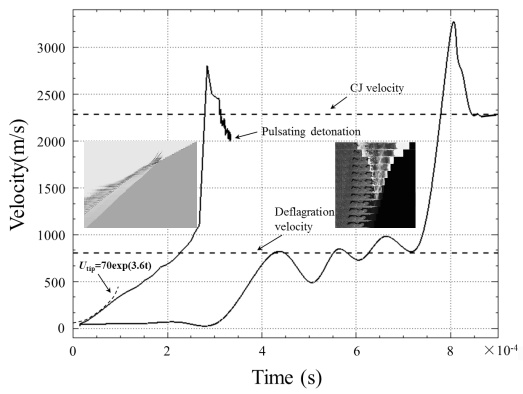


Fig.6 Curves of velocity with time for the two modes

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