

Numerical Studies on the Effects of Ozone Addition on Flame Acceleration and Deflagration-to-Detonation Transition for Hydrogen/Oxygen Mixtures

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1 Introduction

Study on flame acceleration and deflagration-to-detonation transition (DDT) is of considerable importance not only due to industrial safety concerns, but also the potential application to advanced engines [1-2]. Previous literature studies have focused on the understanding the mechanisms of DDT [3-8]. Accelerating DDT has a greater attraction for the propulsion community [9-10]. The thermal and kinetics enhancement are two options for accelerating DDT. The essence of thermal enhancement is to increase the heat release rate of the mixture by increasing fuel concentration and turbulence intensity. Previous studies [10-12] have shown that DDT can be accelerated by increasing fuel concentration. As a result, DDT onset time is the shortest at near stoichiometric conditions due to the maximum heat release rate. Recent studies also have shown that DDT can be accelerated by chemical kinetics by using plasma to produce active radicals [13-14]. Sepulveda et al [14] experimentally showed that the DDT time and onset distance was drastically reduced for C₂H₂/O₂ mixtures in microchannels via addition of plasma generated ozone. Moreover, it was also observed that kinetic enhancement had a much larger effect on DDT time than the thermal enhancement. In order to further understand the chemical kinetic effect of ozone addition on flame acceleration and DDT in a microscale channel, this study aims to investigate the effects mechanism of addition ozone on flame acceleration and DDT for hydrogen/oxygen mixtures by using numerical simulation.

2 Physical model and numerical approach

A numerical simulation of flame acceleration in a two-dimensional channel was conducted. The conservation equations are the compressible NS equations, with advection, diffusion and reaction source terms. The detailed chemistry for hydrogen/oxygen mixtures developed by Ó Conaire et al. [15] is used in the simulations. The ozone chemistry subset developed by Ombrello et al. [16] was incorporated into the above models. CHEMKIN packages [17] are used to calculate chemical reaction rates and temperature-dependent thermal and transport properties. To numerically solve the governing equations, we apply fifth-order local characteristics based on the WENO conservative finite difference scheme to discretize the advection term and the sixth-order central difference to the diffusion term, with third-order TVD Runge-Kutta time discretization. The details of this method can be found in our other papers [18-19].

The width and length of the channel are 0.2 mm and 38.4 cm, respectively. The mesh size is 4 μm [20]. At the initial moment, in order to eliminate the influence of pressure waves on the unreacted mixture during the ignition process, a planar laminar flame is set at the left as the initial ignition source. In the unreacted mixture, the initial velocity, temperature and pressure are 0.0m/s, 300 K and 1atm, respectively. The equivalent ratio of the mixture is unity, and the volume fraction of ozone is 0.67%. Both the upper and lower boundaries are non-slip and adiabatic walls in order to consider the effects of chemical kinetics in isolation.

3 Results and discussion

3.1 Effect of ozone addition on ignition and steady detonation ZND structure

Figure 1 shows ignition delay time as a function of temperature of hydrogen/oxygen mixtures for $\phi = 1$. No ozone addition (black), 0.68% ozone addition (blue) and 1.37% ozone addition (red) are shown. The results show that 0.68% ozone addition reduces the ignition delay time, especially in the low temperature zone (700-900 K), which shortens the ignition delay time by approximately four orders of magnitude compared to no ozone addition. Analysis showed that the effect of ozone addition on ignition delay was primarily due to the production of atomic O by the thermal decomposition reaction $\text{O}_3 (+\text{M}) \rightarrow \text{O}_2 + \text{O} (+\text{M})$ [16]. The atomic O rapidly reacts with the fuel via the branching reaction $\text{O} + \text{H}_2 = \text{H} + \text{OH}$, leading to an exponential increase in radical concentration for ignition. Essentially, the ozone addition shortens the ignition delay time by bypassing the chain initiation reaction $\text{H}_2 + \text{O}_2 = \text{HO}_2 + \text{H}$, which is main initial radical-production source for no ozone addition. Figure 1 implies that the ozone addition enhances the flame propagation speed and the coupling effects between the flame and pressure waves due to the shortening of ignition delay time, leads to accelerating the DDT process through chemical kinetics.

Figure 2 shows the steady ZND structure, Chapman-Jouguet (CJ) velocities and induction length of detonation with different ozone concentration. It is seen that as the ozone mole fraction increased from 0 to 1.67%, the induced length of detonation was shortened, but the temperature, pressure and thermicity in the ZND structure were substantially unchanged, as shown in Fig. 2(a) and (b). Moreover, The CJ velocities D_{CJ} is slightly reduced by 1.34%, and the induction speed of detonation v_i , defined as the ratio of the induction length to the induction time, is only increased by 4.25%, as shown in Fig. 2(c). The results implied that ozone addition does not alter the heat release rate in the detonation reaction zone, merely changing the induced length of the detonation by chemical kinetic.

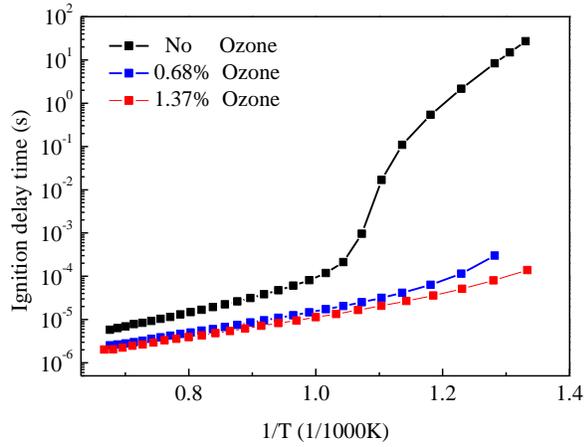


Fig.1 Ignition delay time as a function of temperature of hydrogen/oxygen mixtures for $\phi = 1$. No ozone addition (black), 0.68% ozone addition (blue) and 1.37% ozone addition (red) are shown.

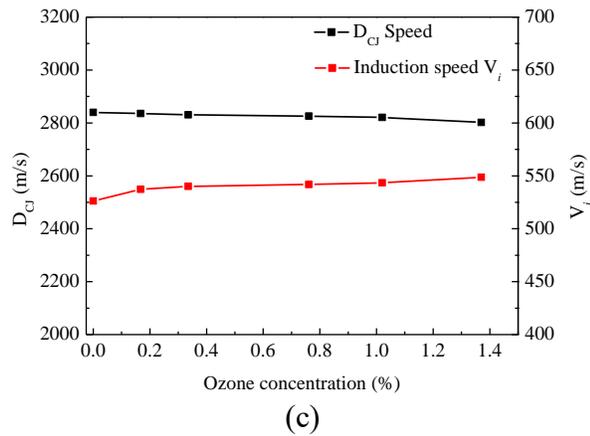
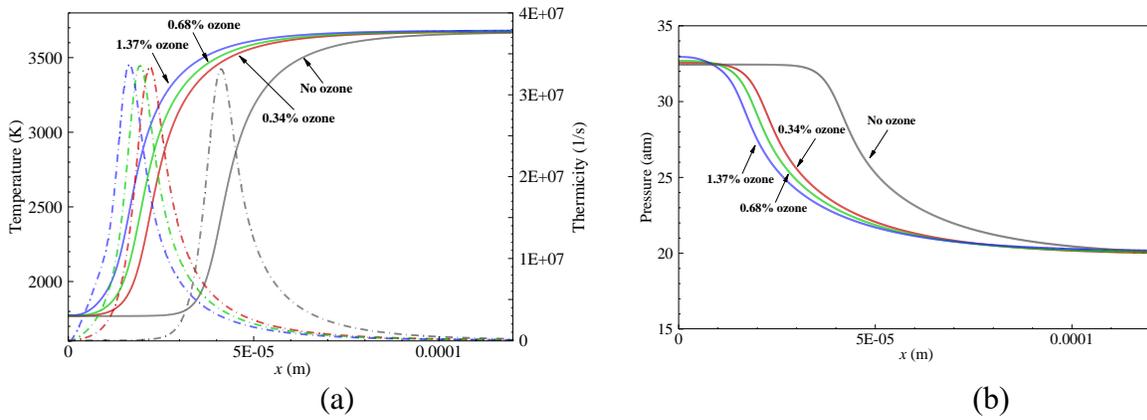


Fig. 2 Steady ZND structure, CJ velocities and induction speed of detonation with different ozone concentration

3.2 Effect of ozone addition on flame acceleration and Deflagration-to-Detonation

Figure 3 shows the flame acceleration and deflagration to detonation transition for hydrogen/oxygen mixtures with 0.68% ozone addition. The contour image represents the temperature.

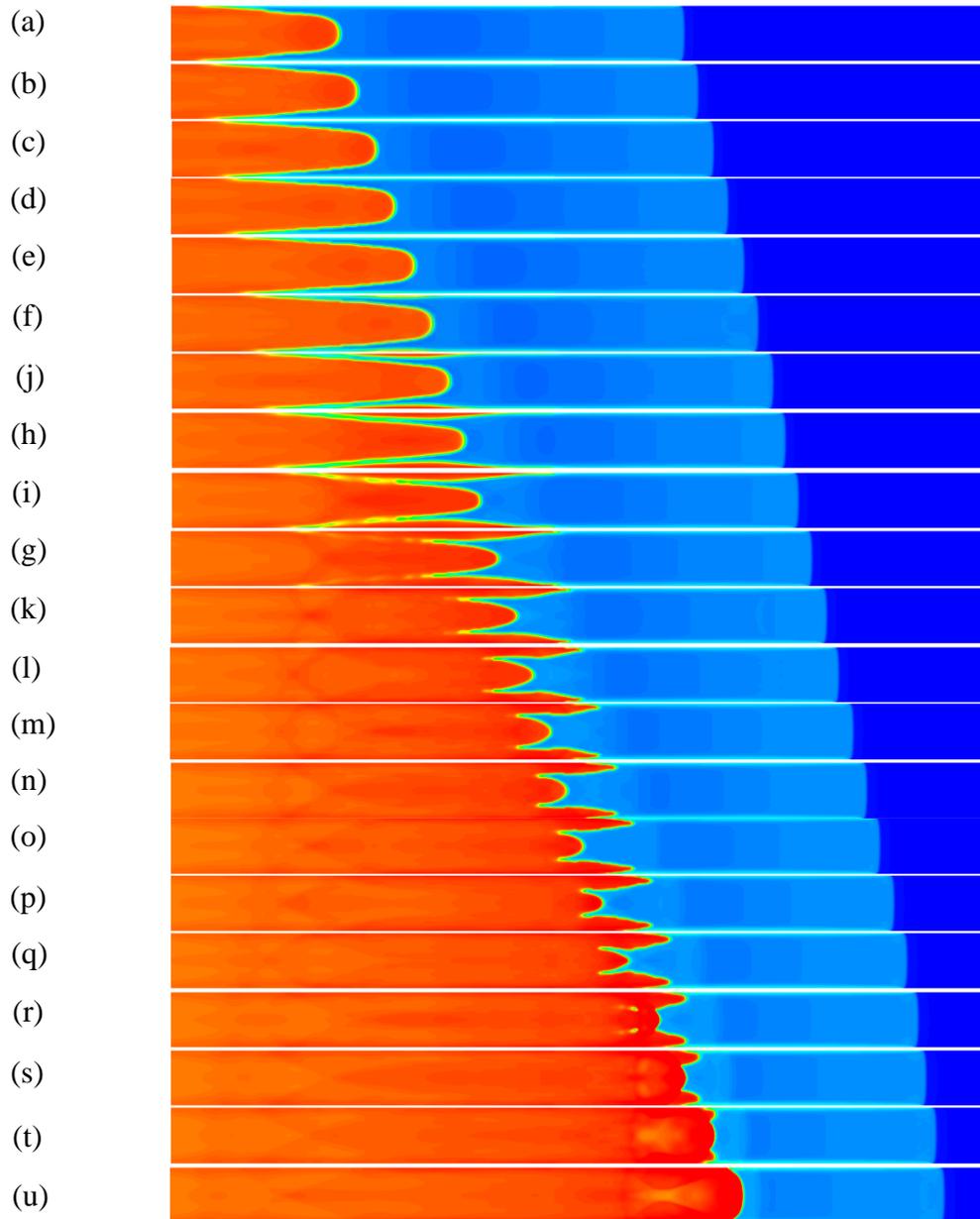


Fig. 3 Flame acceleration and deflagration to detonation transition: (a)-(u) $t=40.78, 40.82, 40.85, 40.89, 40.92, 40.96, 40.99, 41.02, 41.05, 41.09, 41.12, 41.15, 41.18, 41.21, 41.24, 41.27, 41.31, 41.33, 41.35, 41.37$ and $41.39\mu\text{s}$

As $t=40.78\sim 40.92\ \mu\text{s}$, the flame accelerates due to thermal enhancement caused by stretching of the flame surface and kinetic enhancement due to shortening the ignition delay time by adding ozone, as shown in Fig. 3 (a)-(e). As $t=40.96\sim 41.02\ \mu\text{s}$, under the coupling of pressure waves and wall viscous effect, the mixtures near the wall surface auto-ignites due to the shortening of the ignition delay time by ozone addition. Flame acceleration is dominated by kinetic enhancement in this stage, as shown in Fig. 3 (f)-(h). As $t=41.05\sim 41.18\ \mu\text{s}$, the boundary layer flame collides with the mainstream flame and gradually merges into it, as shown in Fig. 3 (j)-(k). As $t=41.21\sim 41.39\ \mu\text{s}$, The upper and lower boundary layer flames begin to move towards the center of the narrow channel and eventually merged together due to a local explosion at the tip of the accelerating flame caused by pressure pulse, and then DDT occurs caused, as shown in Fig. 3 (l)-(u). Figure 4 shows the flame front location and speed as a function of time for hydrogen/oxygen mixtures with 0.68% ozone addition. It is seen that the flame accelerates exponentially and turns into detonation at $t = 41.39\ \mu\text{s}$.

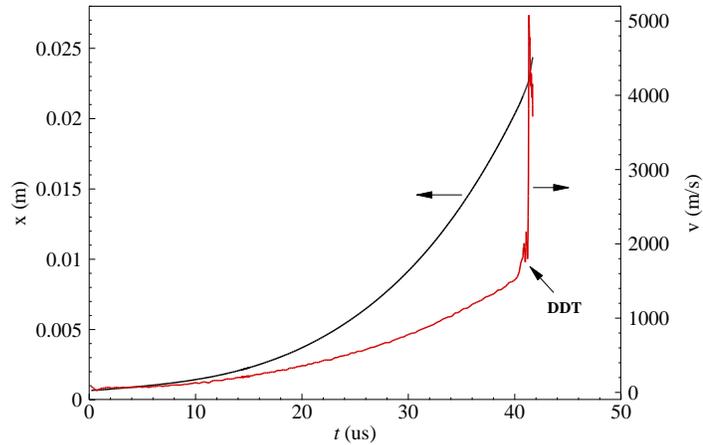


Fig. 4 The flame front location and speed as a function of time for 0.68% ozone addition at $\phi = 1$.

4 Conclusion

This study numerically investigates the effects of ozone addition on flame acceleration and DDT for hydrogen/oxygen mixtures in the microchannel. The study showed that adding a small amount of ozone can greatly reduce the ignition delay time, but does not change the heat release rate in the detonation reaction zone. The flame accelerates in the microchannel due to thermal and kinetic enhancement. In addition, under the coupling of pressure waves and wall viscous effect, the mixtures near the wall surface auto-ignites due to the shortening of the ignition delay time by ozone addition. DDT occurs due to a local explosion at the tip of the accelerating flame caused by pressure pulse.

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