Cylindrical Flame Acceleration and Deflagration-to-Detonation Transition in Confinement Space

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1 Introduction

Experimental and theoretical studies of outward flame propagation in cylindrical bomb geometry [1-3] have shown that the flame propagation speed is modified due to cylindrical boundary confinement and results in a significant distortion of the flame surface. Flame structure is also changed by intrinsic instabilities [4]. Kelley *et al.* [5] studied propagation of a premixed flame in the confined vessel filled with combustible fluid by using large activation energy asymptotic. Xin *et al.* [3] investigated self-accelerated cylindrical flame by numerical simulation. While flame acceleration in confinements has drawn intense research interests in recent years [6], most studies focused mainly on flame propagations in tubes and channels. Wang *et al*. [1] found experimentally that the transition to a detonation usually occurred near wall as a flame propagates in internal engine combustor with high temperature and pressure. Wu & Kuo [7] have observed DDT of a flame ring circularly expanding in a gap filled with stoichiometric ethylene/oxygen mixtures initially at atmospheric pressure and temperature. Overall, cylindrical flame acceleration and DDT have been studied, while the mechanism of DDT still is not clear.
In the paper, a high-resolution parallel code is employed to simulate the propagation of cylindrical flame in bounding space with ethylene-oxygen mixture. Goal is to investigate flame acceleration and identify the mechanism of DDT inside of the cylindrical bounding space.

2 Numerical model and specifications

A circle computational domain with diameter of 79.6cm is filled with the ethylene-oxygen mixture. The specific heat ratio is γ=1.4. The reaction model is the Arrhenius law, $\omega = -KY exp(-E_a/R_uT)$, where E_a the activation energy, R_u the gas constant, M the molecular weight, K the constant pre-exponential factor and Y is mass fraction. The mixture parameters are obtained by the GasEQ for stoichiometric ethylene-oxygen combustion [8]. A weak ignition source is set at the center (x=39.8, y=39.8), in which the temperature is 2400K. Bounding boundary is non-slip and adiabatic wall. The simulation is carried out for these two cases: (a) p_0=0.5atm and T_0=300K; (b) p_0=2atm and T_0=600K.

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The compressible and reactive flow Navier-Stokes equations including convection, diffusion and reaction source are used to describe the flame propagation. The flame thickness is defined as $f_l = \nu/\mathrm{Pr}S_l$, where S_l is laminar flame speed, ν is the molecular kinetic viscosity and Pr = 0.75 is Prandtl number. The laminar flame speed S_l is 4.5m/s and the flame thickness is 0.05mm. To numerically solve the governing equations, we apply the fifth-order characteristics-based WENO conservative finite difference scheme [8] to discretize the advection term and the sixth-order center difference is used for the diffusion term, with third-order TVD Runge-Kutta for time discretization. We carried out simulations with the minimum grid sizes of 0.005mm that is obtained by refining adaptively mesh so that grid-resolution level of 10 point/flame thickness can be obtained. It is done in high performance cluster by using 512 cores.

3 Verification of grid convergence

Firstly grid convergence is verified by using grid-resolution level with adaptive refine mesh for Case 2. The gird resolution of Δx=0.05mm is used as base grid (*bg*), and the minimum grid size is 0.01mm (1/5*rbg*) and 0.005mm (1/10*rbg*) by refining. The evolution of flame fronts with different levels of grid resolutions is shown in Figure 1.

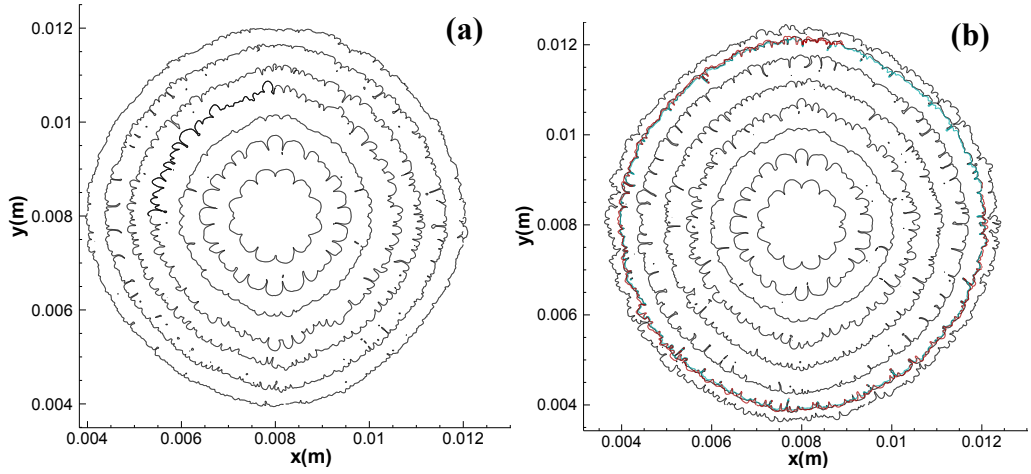

Figure 1 Relative grid convergence: (a) 0.05mm; (b) 0.01 (red line), 0.005mm (green line).

For Δx =0.01mm the flame surface is relatively smooth as the flame propagates to x ~1.2cm (Fig. 1(a)), while small-scale structure appears at the front for 1/5*rbg* and 1/10*rbg* in Fig. 1(b), demonstrating that the mesh resolution of Δx =0.01mm is not enough for capturing the finer structure. For 1/5*rbg* and 1/10*rbg*, the flame fronts are almost overlapping at the same time (see red and blue lines in Fig. 1(b)), showing a good grid convergence is obtained. Although the 1/10*rbg* can capture the finer structure, the larger computational resource leads to very low computing efficiency. Hence, 1/5*rbg* is selected by compromising the resolution and computing resource to simulate the flame propagation.

4 Numerical results and discussions

In this section, we mainly discuss propagation of cylindrical flame at different initial pressures. Figure 2 shows three typical flame structures. Initially, an expanding flame is created by weak source energy at the center and develops into cellular flame due to intrinsic instability (Fig. 2(b)), which increases the surface of the flame and further accelerates the flame propagation. As the flame accelerates, compression wave

appears in front of flame and preheats the un-reacted gas, which leads to the formation of preheated zone shown in Fig. 2(c). Eventually, the turbulent flame is formed and subsequently develops into deflagration due to interaction of the reflection wave from the wall. Figure 3 shows the formation of pressure wave as cellular flame propagates. At t=0.94ms, the flame has taken cellular structure and unreacted gas is chipped between two flame-let heads. Collision of the flame-let head induces upstream weakly and locally curved pressure wave in the vicinity of the flame front, which intersects into net structure; see Fig. 3(a). The cellular flame also modifies the upstream flow and renders it non-uniform. Interplay pressure waves preheat the unreacted gas at the intersection in front of the flame front and create hot spots here; see Fig. 3(b). The flame goes into the preheated unreacted gas with non-uniform flow and becomes turbulent flame, which leads to faster acceleration. The compression wave strengthened by the accelerated flame enhances the positive feedback mechanism that makes it overlap into shock wave. The shock wave reflects from the wall and interacts with the flame, and eventually leads to strong deflagration flame. Nevertheless, due to the lower initial pressure the deflagration flame is not able to transit to detonation.

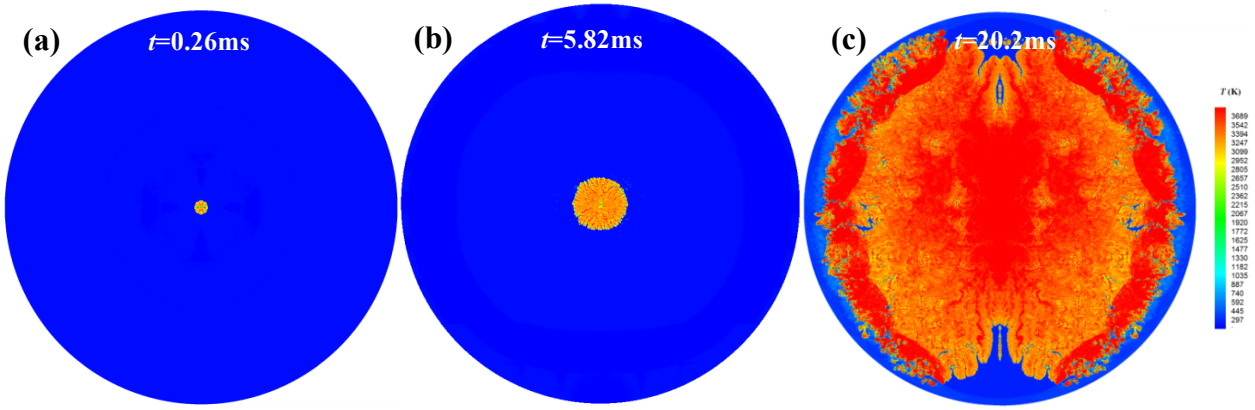

Figure 2 cellular flame and strong deflagration wave

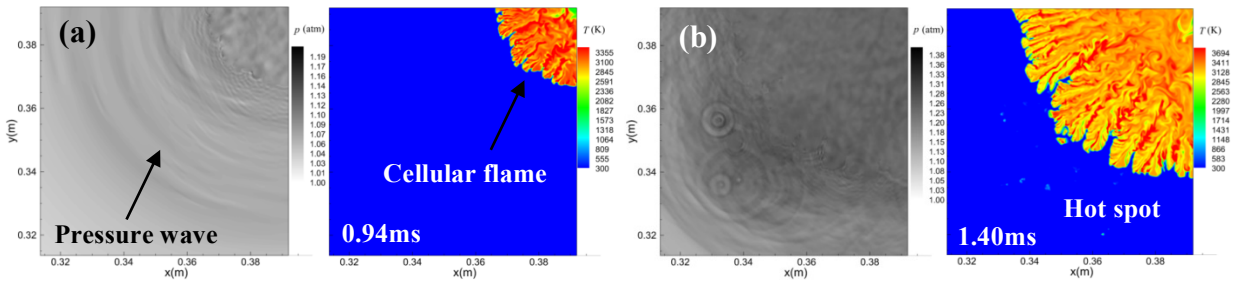

Figure 3 Formation of cylindrically cellular flame: p_0=0.5atm

However, initial pressure increases to 2atm the flame initially takes on cellular front and eventually the detonation can be triggered due to local explosion near wall; see Figure 4. At t=2.25ms, the cylindrical flame has cellular front structure, and accelerates constantly. At t=16.8, DDT occurs and the formed detonation wave reflected from the wall propagates to the center and rapid burns out the other unreacted gas; see Fig. 4(b, c). Note that, appearance of the detonation is not symmetry. This is due to extremely high susceptibility of DDT to small perturbations that are caused by the numerical error. The interaction of the detonation wave with the cellular flame also is seen in Fig. 4(d). Figure 5 shows the onset of the detonation. As the cellular flame accelerates, resulting shock wave interacts with upstream gas, leading to

the early burning near wall; see Fig. 5(a). Early-burning flame further increases the pressure in the unreacted gas between it and wall, and here temperature shocked enhances further, leads to an environment with high pressure and temperature; see Fig. 5(b). Here autoignition time of gas is extremely short. A small perturbation or gradient will trigger local explosion and then leads to the transition to detonation. Furthermore, in initial stage the averaged velocity of globally cylindrical flame can be calculated by the means of the averaged flame front in ref. [2], shown in Figure 6. It is observed that flame initially accelerates exponentially and then linearly [2]. In the simulation by Xin et al., the boundary is open and therefore the confinement effect of the wall has no influence on the flame structure. Hence, the present simulation agrees with the results of Xin because perturbations reflected from wall still do not affect the flame front in the initial stage.

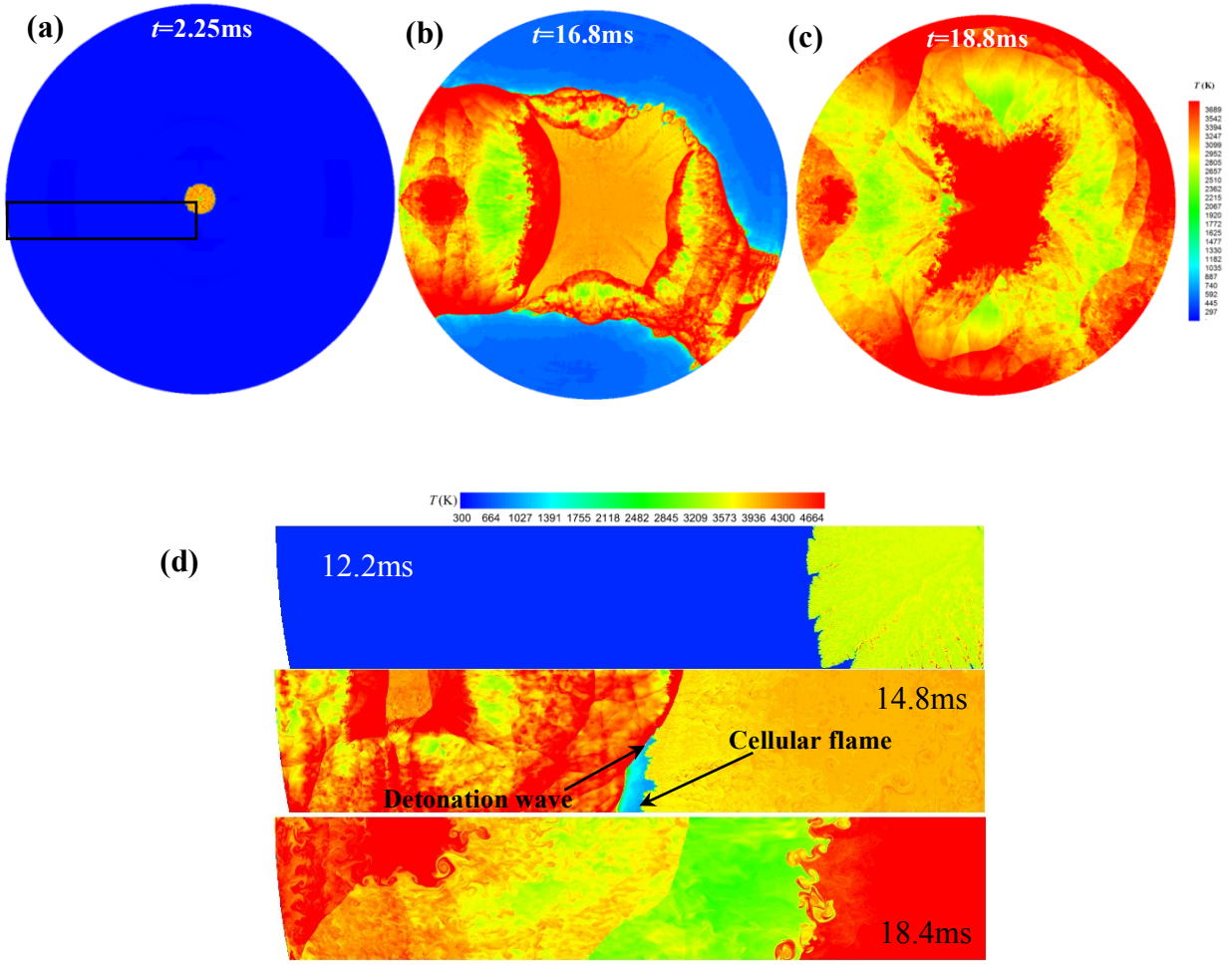

Figure 4 Cellular flame and detonation wave (p_0=2atm): zone boxed by black line in (a) is amplified in (d).

The increase in initial pressure lowers the acceleration rate of the flame. Furthermore, the change of average pressure along the wall as function of time is shown in Figure 7. It is seen that for p_0=0.5atm DDT do not occurs and the maximum pressure (~10atm) at wall is lower, while for p_0= 2atm DDT occurs and the maximum pressure at wall reaches ~70atm. In high temperature and pressure condition, the phenomenon also is observed experimentally by Wang *et al*. [7].

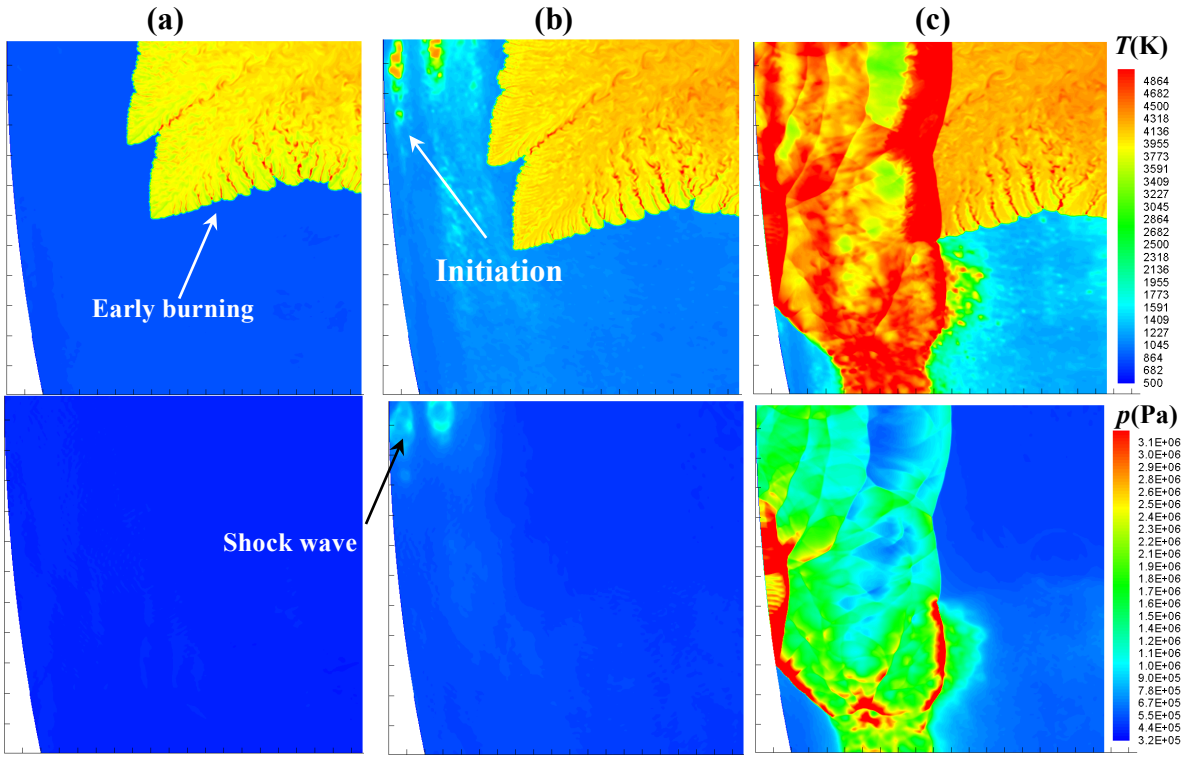

Figure 5 Formation mechanism of the detonation (p_0=2atm)

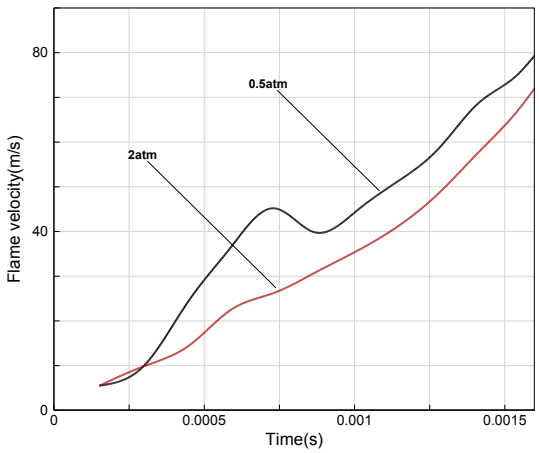

Figure 6 Change of flame speed as function of time

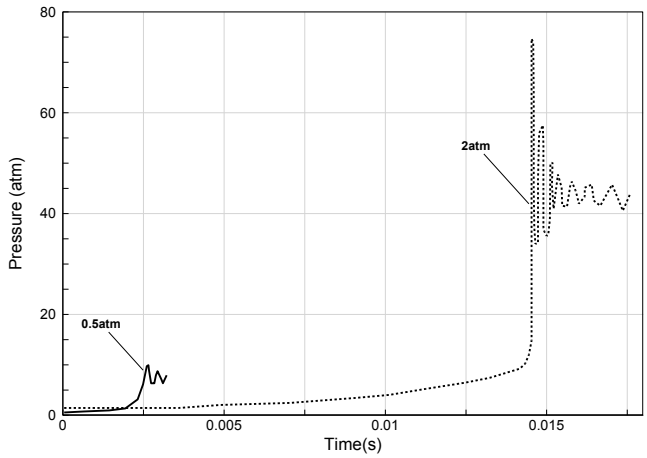

Figure 7 Change of pressure on the wall as function of time

5. Conclusions

In the paper outward propagation of cylindrical flame in confinement geometry is investigated by high-resolution simulations. It is first found that globally cylindrical flame acceleration contains: exponential

self-acceleration and linear acceleration. For the lower initial pressure, linear acceleration is as result of gas compressibility, coupling positive-feedback mechanism. While turbulent flame is formed, the transition to detonation does not occur. As the initial pressure and temperature increases, DDT appears near wall due to the interaction of shock wave with the preheated unreacted gas.

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