Propagation of Hydrogen-Oxygen Cellular Detonation with Ozone Sensitivity in Open Space

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1 Introduction

Gaseous detonation is intrinsically unstable [1] and shows cellular instability in multi-dimensions [2]. The evolution of detonation is dependent on the induction and reaction time associated with initial mixture properties [3,4]. Previous researches have shown that detonability limits in channels or tubes can be determined through a characteristic parameter, called the detonation cell size associating with the induction length of a combustible gas [5,6]. It has been known that as a detonation propagates from a narrow tube to an open space, its sustenance always meets the semiempirical criterion of $\lambda = D/13$ for the most of fuels [7-9]. Lots of works have studied the propagation and cellular structures of gaseous detonations in the bounding space, and the reflection and reamplification of transverse waves play ley role in the sustaining propagation. It is well known that a detonation can propagate at the CJ speed in the cylinder of explosives without bounding conditions. However, whether a gaseous detonation can sustain at the CJ state still is not known clearly so far as the bounding condition is withdrawn or weakened. It may require very high reactivity for combustible gases, corresponding to extremely thin induction length. Hence, it is interest to identify whether a gaseous detonation sustains at a CJ speed in an open space and the relationship of the sustenance to the induction length (reactivity).

Note that adding trace amounts of ozone in mixtures significantly reduces induction length of a detonation without affecting heat capacity and heat release [10]. This work studies the sustenance of a detonation in a channel with weak confinement by numerical simulations and establish the relationship of induction length to the propagation by adding ozone into the system.

2 Numerical Specifications

The reactant layer is stoichiometric H_2/O_2 mixture with 0.05%, 1% and 5%O_3 additions and its width is respectively 12cm and 16cm width, which is bounded by N_2 inert layer with the height of h = 3cm, in which an oblique shock and reflection disturbance from the top and bottom boundaries are not able to influence on the propagation of cellular detonation. The initial pressure is p_0 = 0.04 atm and the initial temperature is T_0 = 300 K. A formed detonation with cellular structures is set at the left as initial condition and then propagates toward the right. The left is inlet flow, while the other boundaries are free flow. The model is shown in Figure 1.

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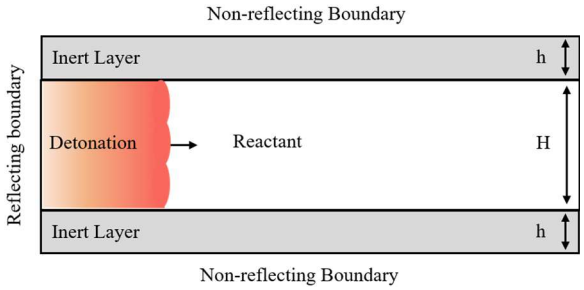


Figure1: Computational model.

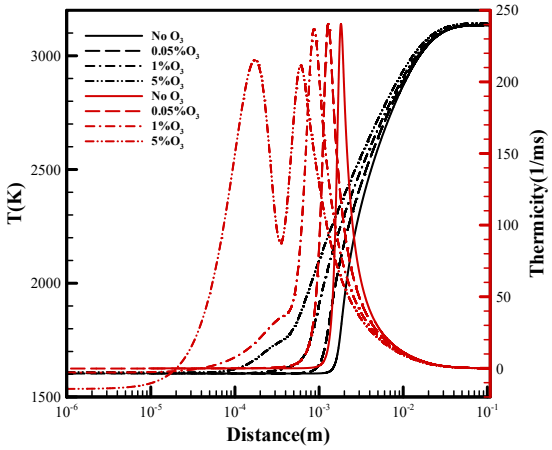


Figure 2: Steady ZND of detonations.

Figure 2 show steady ZND solution with different O_3 addition. It is seen that slightly varying O_3 addition can substantially affect the induction length, while the thermicity peak is minimally affected. Note that, as 5%O_3 there are two peaks in thermicity profile, which is led by low-temperature chemistry of O_3. We study the effect of O_3 addition on the propagation of cellular detonation in a weak confinement and reveal the role of transversal waves on the propagation of cellular detonation. For 5% O_3 addition, the induction length is 0.173mm. In the following simulations, we take the gird size of 0.001mm to describe the induction zone of the corresponding ZND. Hence, the grid resolution is 173points/L_{in}, where L_{in} is the induction length. The gird resolution is enough for the simulations of weakly unstable and stable detonations.

3 Results and discussion

4.1 Propagating characteristics of cellular detonations in unconfined space

By changing the channel width and O_3 addition, the formed cellular detonation propagates in the open space. The sustenance of the cellular detonation is shown in Table 1. It is seen that for the cases without O_3 addition, the detonation fails to sustain in both 6 cm and 16 cm reactant layers. As 0.05%O_3 addition, the detonation quenches for both 6 cm and 12 cm reactant layers, while it can sustain in the 16cm layer. As 5%O_3 is added to the mixture, the detonation can propagate in both 12 cm and 16 cm reactant layers. The propagation of cellular detonation in the open space is related to the ratio of reactant layer height to induction length and the reactivity of mixture, determined by O_3 addition.

Table 1: Summary of the results and parameters of a detonation propagating.

Case	O_3	H	Sustenance	Induction length(L)
1	No	6cm	F	1.821mm
2		16cm	F	
3	0.05%	6cm	F	1.286mm
4		12cm	F	
5		16cm	S	
6	5%	6cm	F	0.173mm
7		12cm	S	
8		16cm	S	

Figure 3 shows the average velocity of cellular detonations for different cases. It is seen that the velocity depends on the height of reactant layer and O_3 addition. In the 6cm reactant layer, the velocity without

O_3 addition decreases fast, with strong oscillations, and eventually the minimum is lower than 0.5CJ value, showing the detonation quenches. Although O_3 additions just make the decay delay slightly, the fact that the detonation quenching cannot be changed and the velocities for different O_3% eventually decay to be lower than 0.5 CJ value. In the 12cm layer, the velocity with 0.05%O_3 takes strong oscillations and the minimum is ~ 0.7CJ value at x = 0.38m; while for 5%O_3 the oscillation weakens significantly and the averaged velocity tends to be steady, with ~ 0.8CJ value. However, in the 16cm reactant layer, the velocity decays more slowly and its oscillation is weaker than those in the 12cm and 6cm reactant layers; at x = 0.33cm - 0.43cm in which the velocity tends to be stable, the deficit of the average velocity is ~ 0.9CJ value for 5%O_3 addition, and 0.85CJ for 0.05%O_3 addition.

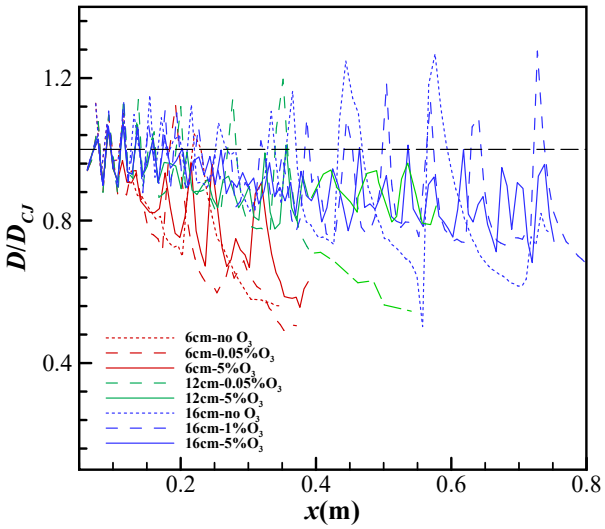
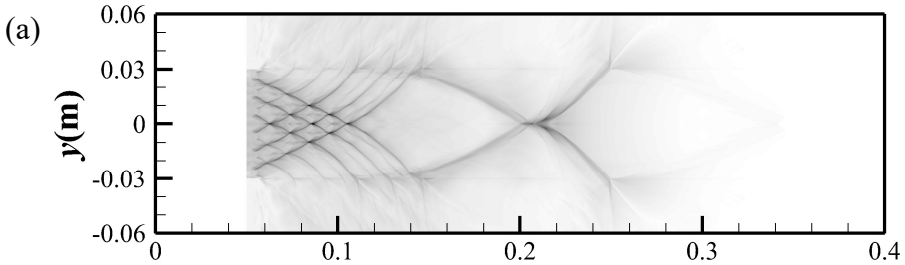


Figure 3: Detonation velocity evolution process under different cases.

Figure 4 shows the numerical smoke foil produced by recoding the maximum pressure histories in the whole domain. In the 6cm reactant layer, about six detonation cells is accommodated to make the detonation sustain in the confined space. However, the six cells are not insufficient to sustain the detonation in weak confined space; for no O_3 addition, because of low reactivity, transversal wave arrivals the inert layer and weakens significantly due to the lack of strong reflection role. As a result, two triple points only are left in the reactant layer and reflected from the inert surface; and the reflected triple points collide each other at x ~ 0.2m, move separately toward the inert layer and weakens further; eventually, it quenches at x ~ 0.3m due to the lack of reestablishing mechanism of transversal waves and the regeneration mechanism of new transversal waves. As 5%O_3 is added, a cellular detonation can be reestablished, while it cannot propagate stably and quenches at x > 0.35m.



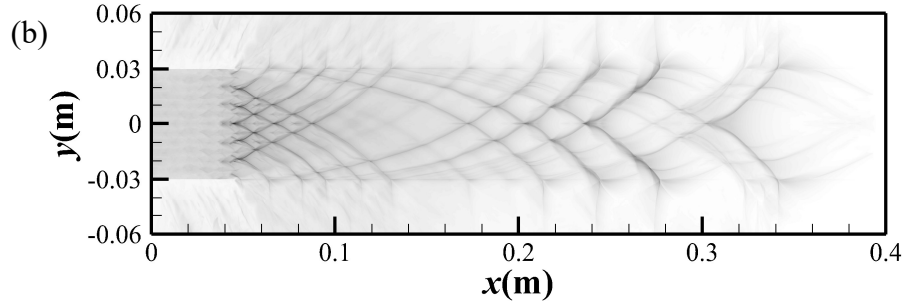


Figure 4: Maximum pressure histories of detonations in the 6cm layer: (a) no O_3, (b) 5%O_3.

As the height of reactant layer increases to 16cm and is able to accommodate 16 cells, the sustenance of detonation is significantly enhanced. Nevertheless, for the case with O_3 addition, although it can be reestablished at $x \sim 0.35$m, while eight triple points just are left at the front; eventually, the cellular detonation quenches after taking long distance. As 5%O_3 addition, high reactivity renders the formed cellular detonation easier to survive by regenerating new triple points at the front. At $x \sim 0.38$m, there are 22 triple points at the front, being more than the number of initial those. The mechanism of sustenance of cellular detonation in the weak confinements is discussed below.

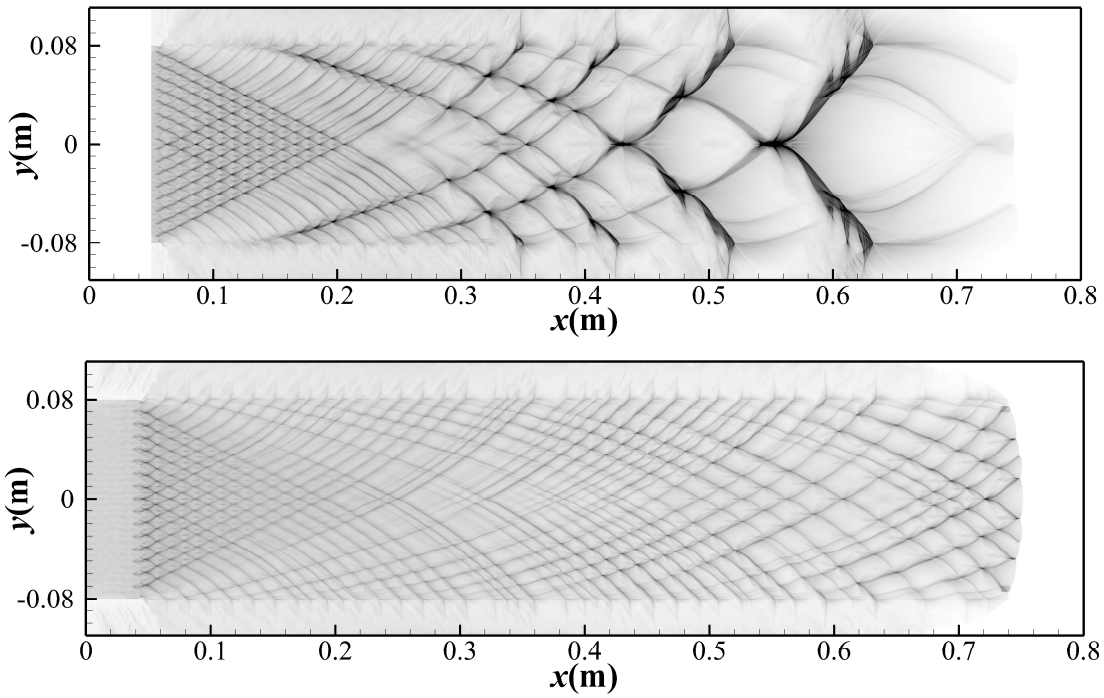


Figure 5: Numerical smoke-foil images of a detonation propagating in the 16cm reactant layer: (a) no O_3, (b) 5%O_3.

Figure 6 shows typical chemical structures of detonations propagating in the 6cm reactant layer for the case without O_3 addition. It is seen that as the shock arrives $x \sim 0.1$m, oblique shock has yet been formed in the inert layer; six triple points are left at the front and those near the inert layer run away the reactant layer. Transverse waves propagate to the inert layer and play role in subsequent propagation. As a result, two triple points are present in the front at $x \sim 0.2$m and the oblique shock in the inert layer is formed fully. The partial energy in the reactant layer is brought into the inert layer so that the leading shock decouples with the reactant layer. The leading shock further is weakened and the detonation quenches eventually. The reflected shock waves generated by the Mach shock wave adhere to the interface and no new triple points are generated. The formed shock wave propagates to the center of reactant layer

and maintains the propagation of detonation. After the central section collision, the dominant shock wave is decoupled from the reactant layer, and the detonation cannot sustain.

For 5%O_3 addition, the propagating ability of detonations in the unconfined space is enhanced by high reactivity. As the detonation reaches 0.3m, its front contains of six triple points and the leading shock still couples with the reaction layer, shown in Fig. 6(b). It is obviously seen that at $x < 0.3$m, H_2 reactant does not slip into the inert. The expansion downstream may not influence on the sustenance of detonation in the open space because average sonic surface can cut off any disturbance downstream, which will be explained later. However, in this narrow reactant layer, the sustenance of detonations depends strongly on the reinforcement of transversal wave. As transversal wave slightly weakens near the inert layer, it cannot sustain. Hence, it is seen that at $x \sim 0.4$m, the leading shock recedes the main reaction layer and the detonation quenches.

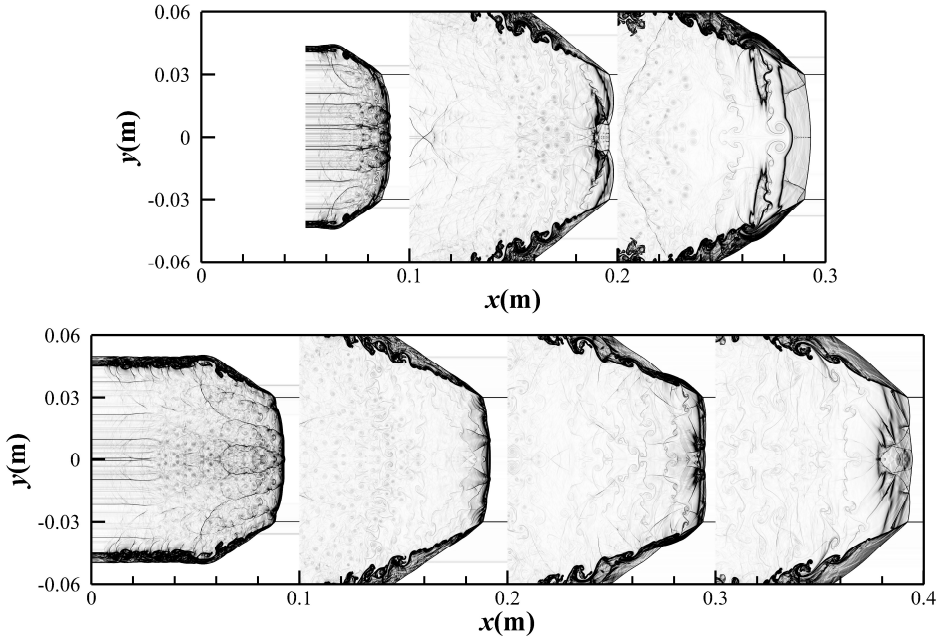
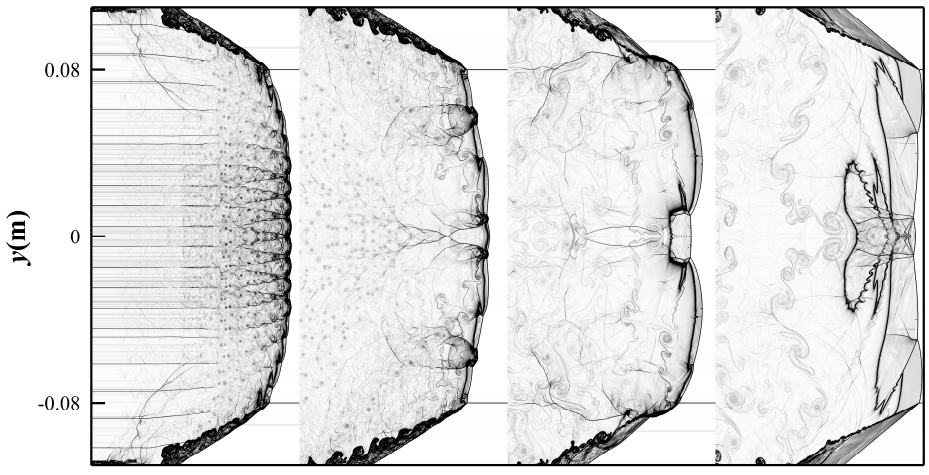


Figure 6: Numerical schlieren in the 6cm reactant layer: (a) no O_3 addition, (b) 5% O_3.



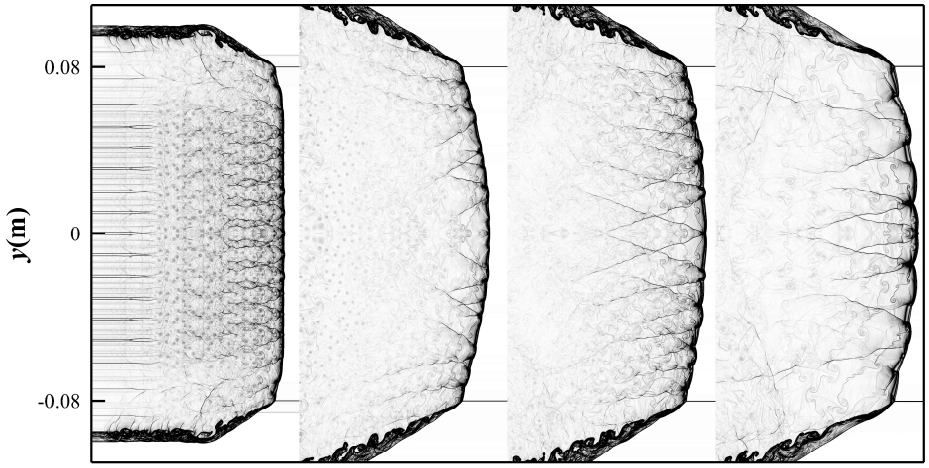


Figure 7: Numerical schlieren in the 16cm reactant layer: (a) no O_3 addition, (b) 5% O_3.

When the reactant layer is widened 16cm, more triple points permit a longer distance of propagation in the open space. For the case without O_3, when the detonation arrives 0.4m there are six triple points left at the front. Nevertheless, global shock waves become weak and induction zone elongates due to low reactivity. Weakening transversal waves has little influence on sustenance of detonation in the open space because H_2 in the reactant does not slip into while the product downstream expands into the inert layer. The propagation is more related to reactivity associating with O_3 addition. For no O_3 addition, eventually the detonation quenches at $x > 0.4$m due to no regeneration and reinforcement of transversal wave.

However, for 5% O_3, high reactivity makes the reestablishment of newly cellular detonation easier and the regeneration of transverse waves allows sustaining of detonation. As the front is ~ 0.2m, the number of triple points is 22 in the front, while the number increases to be 26 in the front of ~ 0.4m. The regeneration of triple points is able to set off the role of unconfined boundary. The detonation can sustain in the unconfined space.

In summary, sufficient triple points and high reactivity in the reactant layer are required to guarantee the sustenance of cellular detonation in the open space, in which transversal wave cannot be reinforced by the boundary confinement. Ozone reactions are able to shorten the induction length, enhance the reactivity so that new transverse wave is generated, which improves significantly the self-sustaining ability of detonation in the unconstrained space. The present results show that in the 2-D problem, the ratio of the channel width to the induction length needs to be larger than 693.5 if a cellular detonation sustain in the open space. It is well known that the detonation cell size for hydrogen-oxygen mixture is about 20 times as the induction length. Hence, it can be calculated that for 5%O_3, the cell size is about 3.5mm, and the reactant layer is about 5 times as the same as the cell size, which agrees magnitudinally with the criterion of $d_c = 13\ \lambda$, where λ is the detonation cell size.

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