Numerical study on two-dimensional detonation propagation across inert layers

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1 Introduction

Due to its high thermal efficiency, detonation can be used in propulsion systems such as Pulsed or Rotating Detonation Engines (PDE, RDE). In these engines, the fuel and air might not be perfectly mixed and thereby spatial heterogeneity in terms of fuel concentration might occur [1]. The spatial heterogeneity can affect the detonation propagation. Therefore, we need understand the propagation and instability of detonation propagation in non-uniform mixtures.

In the literature, there are many studies on the detonation propagation through a non-uniform mixture. For example, Thomas et al. [2] studied detonation propagation in concentration gradients and found that the reinitiation of detonation is enhanced by smooth concentration gradients at inert/reactive interface. Moreover, Kuznetsov et al. [3] found the driver length, gradient width, and difference in properties of driver and acceptor mixtures play important roles in detonation transmission in nonuniform gaseous mixtures. Li et al. [4] assessed the effect of spatial heterogeneity on near-limit detonation propagation. They found that the presence of a sinusoidal variation in the density of an explosive medium has a significant influence on the propagation of a detonation wave. Boulal et al. [5] found that detonation quenching is controlled by the rates of variation of composition and detonation characteristic lengths. Ishii and Seki [6] demonstrated that the length of the inert gas zone and types of the inert gas can affect the propagation of the transmitted shock wave and flame front. Mi et al. [7, 8] examined the effect of spatial discretization of energy release on detonation propagation. They found that the energy release of one such discrete source drives a blast wave, which initiates the next source after a prescribed delay and ensures successful detonation propagate.

Most of numerical studies mentioned above only used simple one-step chemistry or one-dimensional model. However, the detonation structure is multi-dimensional and it is a coupling between complex reaction kinetics and gas dynamics. Unlike previous studies, in this work both one-dimensional (1D) and two-

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dimensional (2D) numerical simulations are conducted and detailed chemistry and transport are considered. Detonation propagation across inert layers is simulated. The objective is to examine how the appearance of inert layers affects gaseous detonation propagation in $H_2/O_2/N_2$ mixture.

2 Numerical model and specifications

The in-house code A-SURF [9] and the parallel block-structured mesh refinement framework AMROC [10] are respectively used to simulate 1D and 2D detonation propagating across inert layers. The effect of inert layers on gaseous detonation propagation is assessed. The conservation equations for unsteady, compressible, reactive flow are solved in A-SURF using the finite volume method. A-SURF has been successfully used in previous studies on flame propagation, end-gas autoignition and detonation development (e.g.[11]). The detailed chemistry for hydrogen are used in simulation. CHEMKIN packages [12] are incorporated into A-SURF to calculate the thermodynamic and transport properties as well as the reaction rates. AMROC solves the Navier-Stokes equations for unsteady, 2D, multi-component, compressible reactive flows using the second-order accurate MUSCL-Hancock finite volume scheme. AMROC has been extensively validated for supersonic combustion and detonation problems [13, 14]. More details on governing equations and numerical schemes of AMROC can be found in Ref. [10] and thereby are not represented here.

The numerical model is sketched in Fig. 1. The detonation first propagates through a static, homogeneous, stoichiometric H_2/air mixture, which is uniformly distributed in the left computational domain. Then inert layers appear and the mixture becomes heterogeneous. As shown in Fig. 1, the inert and reactive layers appear alternatively in the period of $L=a+w$, where a and w are the thickness of the inert and reactive layers, respectively. In the inert layer, the mixture is pure nitrogen. In order to make the averaged H_2 concentration is the same as that in the homogeneous mixture, the molar ratio in the reactive layer is H_2:O_2:N_2=2:1:x, where $x=6.76\times(W/L)-3$. The mixture is initially static with the initial temperature of T_0=300 K and pressure of P_0=1 atm. In order to accurately and efficiently resolve the propagation of shock wave and detonation, dynamically adaptive mesh refinement technology is adopted in simulation. The finest mesh size is 3.9 μm. The induction length of detoantion under present condition is about 0.19 mm. This indicates that there is more than 40 grids within one induction length. Numerical convergence has been checked and ensured by further decreasing the time step and mesh size in simulation.

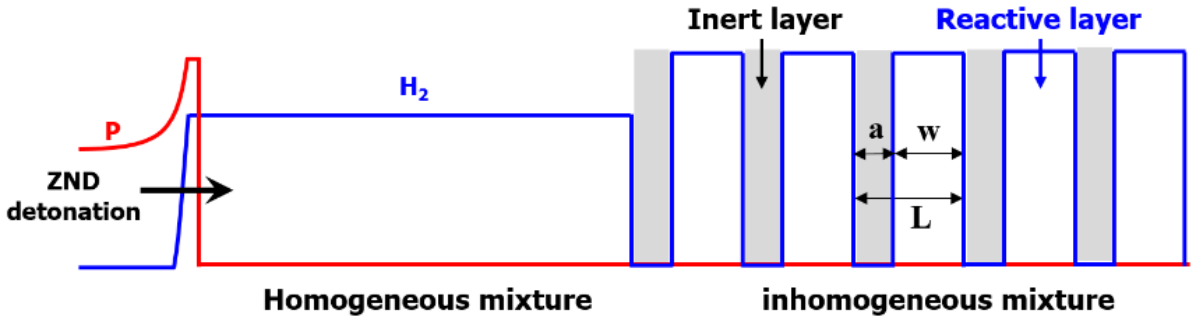

Figure 1. Schematic of the initial conditions and the appearance of inert layers considered in simulation

3 Results and discussion

3.1 One-dimensional detonation propagation

First we consider 1D detonation propagation across inert layers. Figure 2 shows the evolution of the leading shock speed. For a fixed period L, successful detonation propagation is observed for a small value of a=0.1 mm. For a=0.15 and 0.2 mm, the detonation is quenched by the inert layers. The minimum inert layer thickness for successful detonation propagation at a fixed period L is defined as the critical inert layer thickness which is denoted as a_c. At a fixed value for a, successful detonation propagation is observed for a small period of L=1 mm. For L=2 and 3 mm, detonation failure occurs. Although the shock speed decay is nearly the same in the inert layer for these three values of L, the recovery of the shock speed decreases with L due to the decreases of the concentration for H_2 in the reactive layer. Therefore, successful detonation propagation occurs only at relatively small values of a and L.

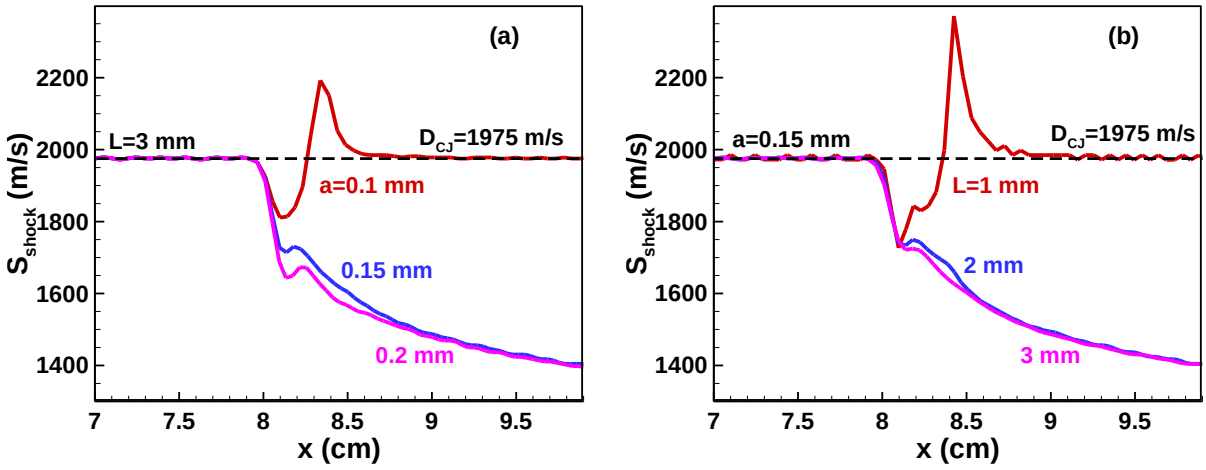

Figure 2. Change of the leading shock speed with its position for (a) fixed value of L and different values of a; (b) fixed value of a and different values of L

3.2 Two-dimensional detonation propagation

Then we consider 2D detonation propagation across inert layers. The evolution of temperature distribution is shown in Fig. 3. The inert layer first appears at x=6 cm and there are fifteen inert layers with the period of L=2 mm. Therefore, homogeneous mixture start to appear again at x=9 cm. First, a steady detonation propagates to the right side until t=28.9 μs (Fig. 3a). At t=31.4 μs, the detonation wave arrives at the inert layer with pure nitrogen. The detonation is quenched and only the leading shock propagates to the right side (Fig. 3b). At t=35.3 μs, the leading shock propagates into the reactive layer. It compresses the $H_2/O_2/N_2$ mixture and eventually triggers local autoignition (Fig. 3c). The heat release from the local autoignition leads to the generation of pressure wave, which further compresses the unburned gas and induces further autoignition. The coherent coupling between autoignition and pressure wave leads to a new detonation development. Therefore, during its propagation across these inert and reactive layers, detonation quenching, autoignition, and detonation development and propagation occur alternatively in turn. After passing through the inhomogeneous mixture, a steady detonation appears and it continuously propagates in the homogeneous mixture as shown in Fig. 3(e).

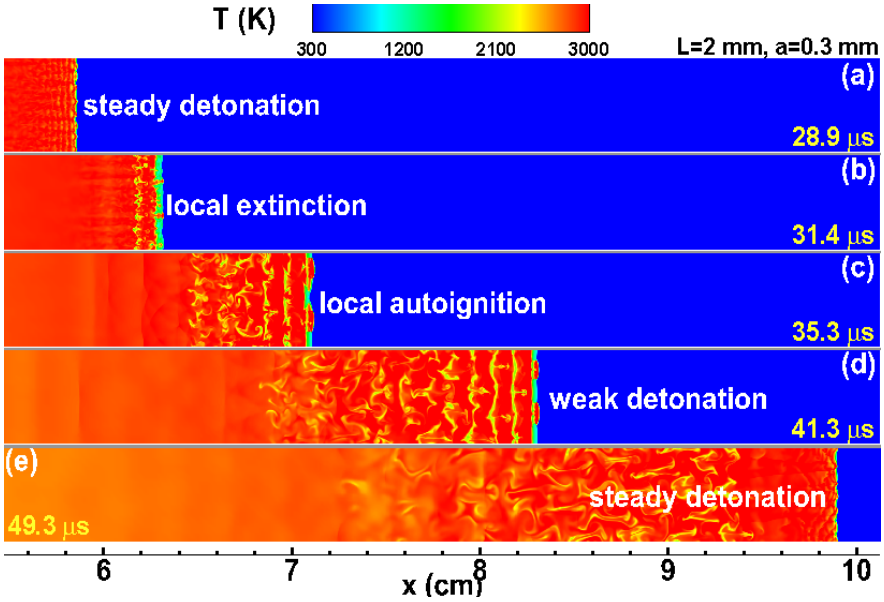

Figure 3. Evolution of temperature contour for L=2 mm and a=0.3 mm

The effect of inert layer thickness and period length on detonation propagation is investigated. Figure 4 compares the cell structures for different inert layer widths of a=0, 0.3 and 0.4 mm and fixed period of L=2 mm. For a=0 mm (i.e. without inert layers), the detonation propagates at C-J speed and regular cellular structure is observed. For all cases, the calculation lengths are enough to fully develop steady detonation. For a=0.3 mm, successful detonation propagation is still observed in the inhomogeneous mixture and the cell size is shown in to be much larger than the homogenous case. For a=0.4 mm, the detonation is quenched. Therefore, similar to the 1D case, in 2D case there is a critical inert layer thickness above which the detonation is quenched in the inhomogeneous mixture.

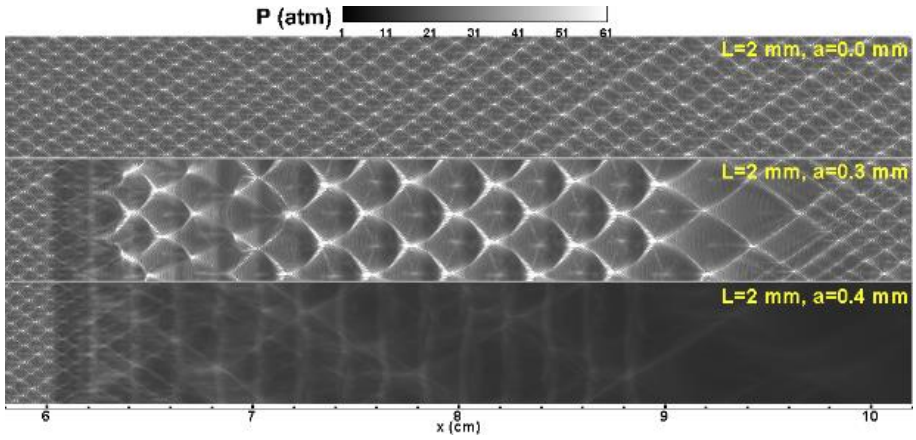

Figure 4. Numerical soot foils for fixed value of L and different values of a

Figure 5 compares the cell structures for different periods of L=1, 2 and 4 mm and fixed inert layer thickness of a=0.3 mm. Successful detonation propagation in the inhomogeneous mixture are always observed. However, there is great change in the cell structure with the increase of the period, L. It is observed that the global cell size increases linearly with L.

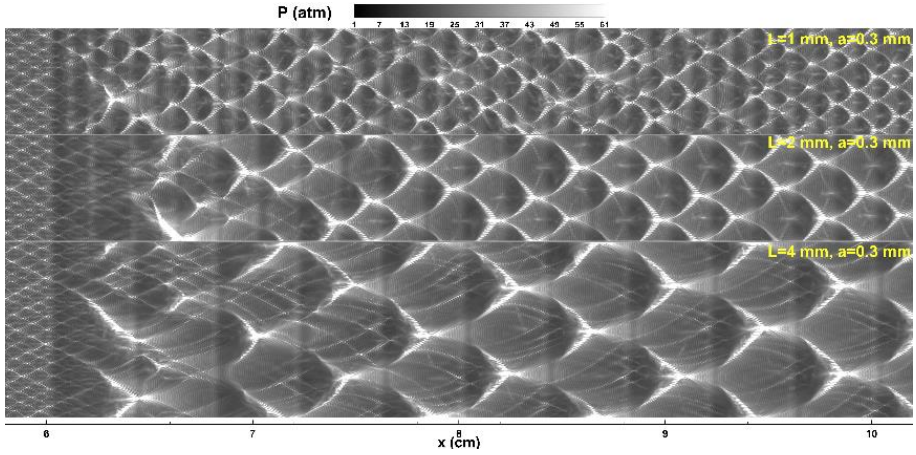

Figure 5. Numerical soot foils for fixed value of a and different values of L

Figure 6 compares the critical inert layer thickness predicated by 1D and 2D simulation. As the period L increases, the normalized a_c first decreases rapidly for L<3mm, and then it approaches to a nearly constant value. As expected, the 2D case has a much larger value of a_c compared to the 1D case since multi-dimensional instability promotes detonation initiation. Moreover, the simulation results indicate that the appearance of inert layers has little influence on the averaged detonation speed once successful detonation propagation is achieved.

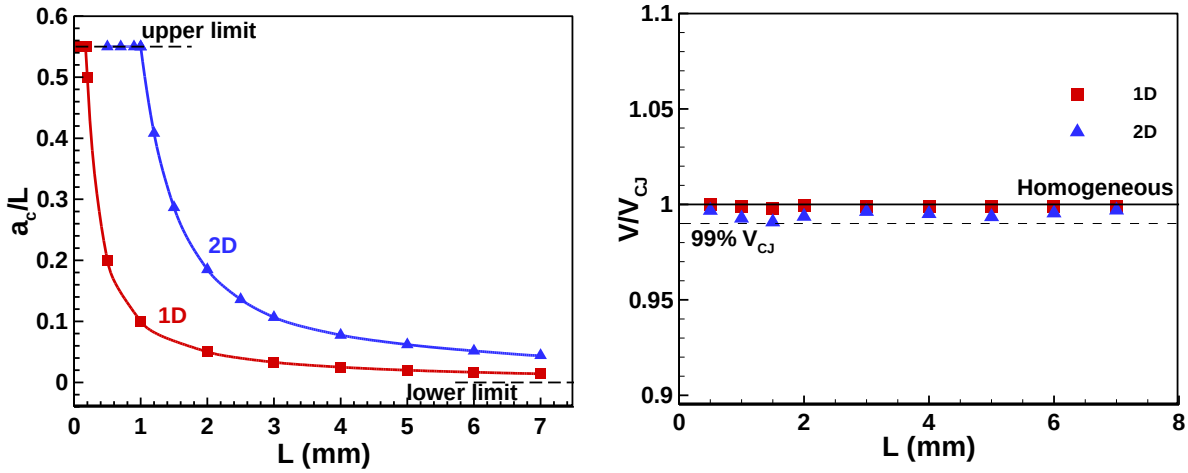

Figure 6. Change of the normalized critical inert layer thickness, a_c/L (left) and the normalized detonation propagation speed, V/V_{CJ} (right) with the period length, L

4 Conclusions

In this study, 1D and 2D simulations considering detailed chemistry are conducted to investigate the effect of inert layers on detonation propagation and detonation structure. For successful detonation propagation across the inert and reactive layers, detonation quenching, autoignition, and detonation development and propagation occur alternatively. The critical inert layer thickness and global cell size are studied for different disturbance period lengths. It is found that successful detonation propagation occurs only at relatively small values of a and L.The critical inert layer thickness for the 2D case is much greater than that for the 1D case

since multi-dimensional instability promotes detonation initiation. Besides, the global cell size increases linearly with disturbance period length. However, the influence of non-uniform mixtures on detonation propagation speed is negligible.

Acknowledgements

This work was supported by National Natural Science Foundation of China (Nos. 91541204 & 91741126).

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