Effect of Vertical Concentration Gradient on Detonation Behavior with Detailed Reaction Mechanism

Wenhu Han[1, *], Wenjun Kong[1, 2], Ning Du[1, 2], Zaigang Liu[1, 2]
[1] Key Laboratory of Light-Duty Gas-Turbine, Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing 100190, China

[2]University of Chinese Academy of Sciences, Beijing 100049, China

1 Introduction

Fuel-air mixtures that accumulate in large spaces, such as those that may be encountered in industrial settings, are likely to be highly non-uniform. Investigating behaviors of the detonations propagating in the non-uniform explosive mixture is important both for detonation physics and in analysis of practical applications. Ishii et al. [1] have shown that concentration gradient is able to enhance detonation instability. Thomas et al. [2] discussed the influence of concentration gradient on the propagating behaviors of detonations, and observed the quenching and reinitiating behaviors. Kessler et al. [3] studied numerically transverse instabilities and the quenching probability for the detonation with a one-step reaction model. Ettner et al. [4] used detailed reaction mechanism to study numerically the global structure of the detonation with concentration gradients. Overall, the detonation propagating in non-uniform mixture is closely related to reactivity gradient, depending strongly on the detailed chemical reaction mechanism. Goal of this study are to show numerically the structure and propagating mode of the detonation in the mixture with a transverse concentration gradient, based on detailed reaction mechanism for H_2-O_2 system.

2 Computational details

Reactive flow Euler equations containing multi-species and detailed reactions are used to describe detonation propagation. The spatial discretization is by using the 5th-order WENO scheme [5]. To solve stiff problems, the explicit-implicit Additive Runge-Kutta schemes [6] are used to time discretization. The species are H_2, O_2, OH, O, H, H_2O_2, HO_2 and H_2O, and the involving reaction mechanism is seen in [7]. The channel is filled with H_2-O_2 mixture. Planar source energy is set at the left as the ignition zone, while in the rest the gas is stationary, and its initial pressure and temperature is respectively 6.67KPa and 298K [8]. The left side is inlet and the right side is outflow. The grid convergence is verified by simulating the detonation with three grid-resolution levels of the minimum mesh size Δx_{min}=0.02mm, 0.01mm and

Correspondence to: hanwenhu@iet.cn

0.005mm. It is seen from Fig. 1(b, c) that the cell size is ~ 9mm, which agrees with results obtained by Hu et al. [8] and in the detonation database by Kaneshige & Shepherd et al. [9]. It is seen further that the solution with Δx_{min} =0.01can converge well into that with Δx_{min} = 0.005mm, showing that the present grid resolution of Δx_{min} =0.01mm is valid to describe the global characteristics. Consequently, the grid resolution of Δx_{min} =0.01mm is selected for the following simulations.

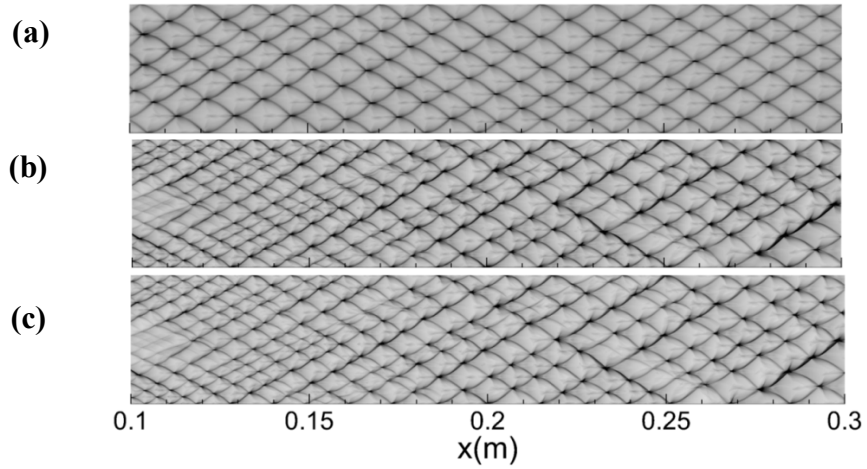

Figure 1 Verification of grid-resolution convergence: (a)0.02mm, (b)0.01mm, (c)0.005mm

In the following simulations, the channel width and length is respectively 288mm and 960mm. A concentration gradient is given by a linear distribution from the bottom (mass fraction f_{H2}=0, f_{O2}=1) to the top (f_{H2}=1, f_{O2}=0), leading to the mixture with a transition from the fuel-poor to the fuel-rich layers to study systematically the influence of the concentration gradient on the detonation instability.

3 Results and discussions

Figure 2 shows the histories of shock pressure in the detonation propagation. It is interestingly seen that a highly unstable detonation is led by the concentration gradient, taking periodically on galloping characteristics and resembling the mode observed by Gamezo et al. [10]. The tracks of the maximum pressure look like "wing" shape, in which finer structure also is observed. The shock pressures along the lines of y=1, 2, 4, 6, 8 and 10cm are shown in Figure 3. It is seen that in the fuel-lean layer the shock pressures behave obviously periodic oscillation around the average value of 1.75atm; see Fig. 3(a). In the vicinity of the stoichiometry (y ~4cm) the track has relatively wider span and bifurcates, while in the fuel-rich layer it becomes wider but is weakened largely. For the line of y=10cm, the pressure peak decreases to ~0.5atm and is lower than $10p_0$, showing that here detonation has quenched and decayed to an inert shock wave; see Fig. 3(b).

Here we are to discuss the formation of the galloping detonation in one cycle. Observed from Figure 4, the front includes a triple shock (TS) consisting of incident shock (IS), reflection shock (RS) and transverse wave (TW) extending to downstream, shown in Fig. 4(a). The contact discontinuity is caused by the TS, at which small-scale vortices led by the R-M instability also appear. These vortices can promote mixing of the product and the fresh fuel, enhancing burning rate of the downstream unreacted mixture in the fuel-rich layer. From Fig. 4(a), the IS almost decouples with the reaction layer except that in the fuel-lean layer near the bottom. Meanwhile, the flow behind the IS is supersonic and cut off the downstream influence, leading to intensification of the reaction rate and further the shock. Consequently, local explosion near the bottom

occurs and leads to strongly overdriven detonation at y ~3cm, shown in Fig. 4(b). This is also reasonable because here mixture is closer to stoichiometry. The advancing wave is leading detonation with Mach Shock (MS), while that propagating upward develops into transverse detonation (TD) shown in Fig. 4(c). The TD includes finer structure in the front, see Fig. 4(c). As the TD moves further to the fuel-rich layer, it decays into inert transverse wave (TW) decoupling with the reaction layer. Simultaneously, the MS expands fast and leads to subsonic flow behind the front. The downstream influence makes the strong overdriven detonation decay. As a result, the reaction layer starts to recede from the MS in the fuel-rich layer and then that in the fuel-lean, shown in Fig. 4(d). Eventually, the MS decays into incident shock (Fig. 4(a)) followed by supersonic flow behind it and the process repeats itself, hence constituting the observed galloping feature. As the TD decays to inert shock and the MS becomes IS, new triple shock forms and moves upward, leading to new contact discontinuity and R-M instability, shown in Fig. 4(d). Eventually, when the detonation front reaches ~96cm the front structure with the leading and transverse detonations still goes on and the unreacted band is formed in fuel-rich layer, shown in Fig. 4(e).

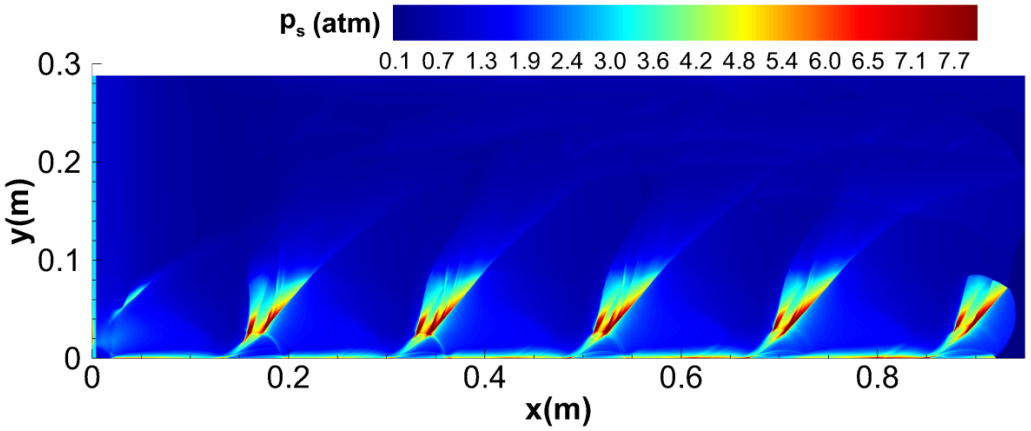

Figure 2 Maximum pressure histories.

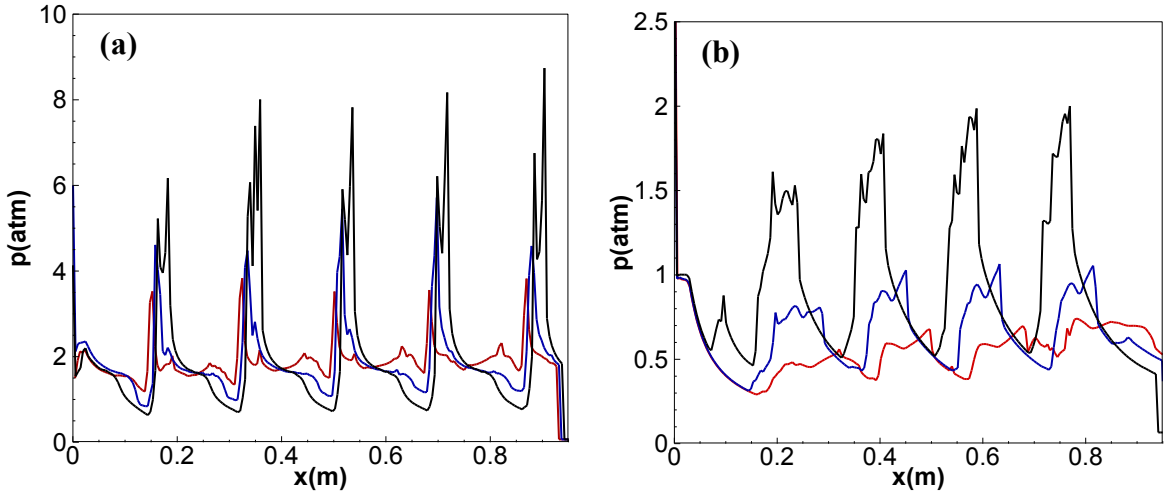

Figure 3 Maximum pressure along lines of different transverse positions: (a) y=1cm (red line), 2cm (blue line) and 4cm (black line); (b) y=6cm (black line), 8cm (blue line) and 10cm (red line)

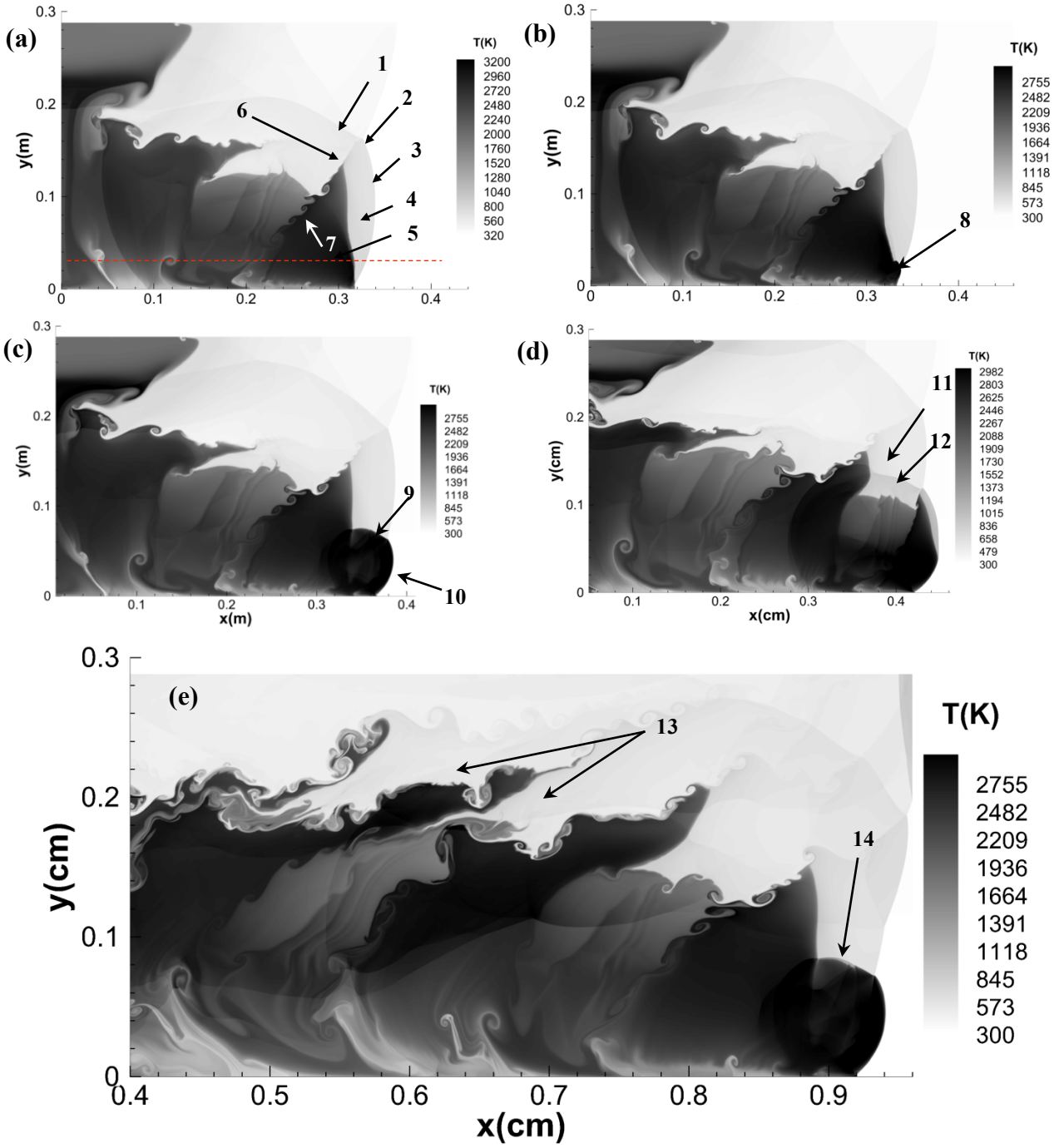

Figure 4 Detonation structure for highly unstable detonation: (a) 149.5μs, (b) 157.5μs, (c) 169.0μs, (d) 196.6μs, (e) 416.2μs; 1, transverse wave; 2, triple shock; 3, incident wave; 4, induction zone; 5, reaction layer; 6, contact discontinuity; 7, R-M instability; 8, reinitiation; 9, transverse detonation; 10, Mach shock (leading detonation); 11, unreacted gas; 12, transverse wave; 13, unreacted gas band; 14, fine structure; red line is stoichiometric position.

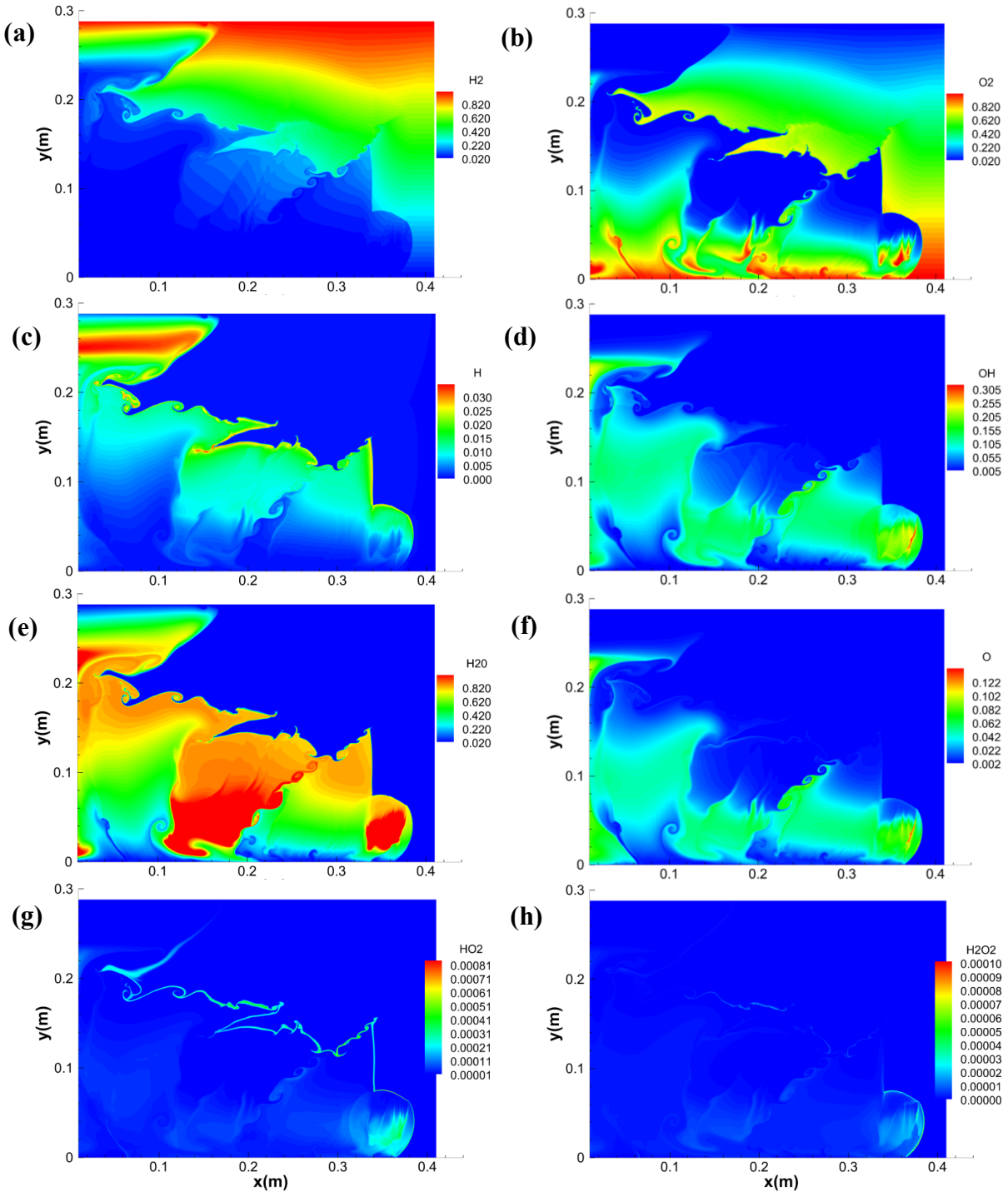

Figure 5 Mass fraction contours of species in highly unstable detonation

We take Fig. 4(c) as the typical feature to reveal species distribution in detonation structure since the local explosion has formed and the transverse detonation is fully developed. Globally, the mass fraction of each species is relatively large in the detonation zone, showing that all of them are important for accurate

prediction of the initiation. Radical H and HO_2 are mainly at reaction surfaces including the MS and TD fronts as well as the downstream reaction front; see Fig. 5(c, g). H_2O_2 is mainly in the TD and MS fronts, shown in Fig. 5(h). This is also reasonable because reactions involving H_2O_2 are more important in the condition of high pressure [9]. OH and H_2O are produced in the high temperature zone since the reactions involving them usually are high temperature reactions; see Fig. 5(d, e).

4 Conclusions

The behavior of the detonation in the mixture with the concentration gradient is simulated by using a high-resolution code. Numerical results show that the concentration gradient enhances the cellular instability, leading to the galloping behave. The detonation feature may be understood as a coupling of a galloping detonation in the fuel-lean layer near the bottom with the transverse detonation that is responsible for the transverse propagation to the fuel-rich layer. This coupling is not simple overlap of them since the propagation of transverse detonation waves is accompanied by pulsations produced by unstable overdriven parts of the leading detonation front.

Acknowledgements

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