Effects of Disturbance on Direct Detonation Initiation in $H_2/O_2/Ar$ Mixture

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1 Introduction

Direct detonation initiation is an important fundamental combustion problem, which is related to the development of high-performance detonation engines and the control of accidental explosion. The instability development was considered as the key mechanism of detonation initiation [1]. Therefore, many studies investigated the influence of disturbances on direct detonation initiation.

For one-dimensional direct detonation initiation, Chue et al. [2] examined the influence of periodic perturbation in density on detonation development. They found that the frequency of applied perturbation plays an important role in direct detonation initiation. Mazaheri [3] and Ng and Lee [4] found that local density disturbances can promote the onset of detonation due to the amplification of local disturbance/instability. Qi and Chen [5] assessed the effects of local temperature perturbation on 1D direct detonation initiation. They found that at small amplitude of temperature perturbation, i.e., a cold/hot spot, can promote/inhibit direct detonation initiation. Such unexpected observation was shown to be caused by the opposite effects of temperature perturbation: local low temperature reduces the chemical reaction rate while it also increases the local volumetric energy density when the pressure remains unchanged [5].

To include multi-dimensional effects, Radulescu et al. [6] examined the influence of cellular instability on the direct initiation of 2D weakly unstable detonations. Their results indicate that multi-dimensional perturbations and cellular instabilities inhibit the initiation of inviscid detonations. Ng et al. [1] noticed that a large wave length of perturbation was used by Radulescu et al. [6] and thereby they examined the effects of perturbation wavelength and channel size on direct initiation of 2D weakly unstable detonations. They found that high frequency, small amplitude perturbations can generate fine scale instabilities which can accelerate the heat-release rate and thereby promote the onset of detonation. Li et al. [7] examined the effects

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of spatial heterogeneity on near-limit propagation of a pressure-dependent detonation. They found that the detonation wave speed depends on the wave length of heterogeneity.

In most of above studies mentioned above, one-step reaction model was used. However, as demonstrated by Mazaheri [3] and emphasized by Lee and Higgins [8], successful detonation initiation can always be achieved due to the absence of the cross-over temperature in one-step chemistry model. Therefore, one-step chemistry model cannot predict a distinct value for the critical initiation energy below which no detonation occurs and it has limitation in the study of direct detonation initiation. In the present study, a detailed chemical mechanism for hydrogen oxidation is considered in the simulation and it consists of 13 species and 25 elementary reactions [9]. Two-dimensional numerical simulations are conducted to investigate the influence of disturbance on direct detonation initiation in $H_2/O_2/Ar$ mixture.

2 Numerical model and methods

The numerical setup for the initiation of a 2D detonation in $H_2/O_2/Ar$ mixture with mixing zone non-uniformity is sketched in Fig. 1. The parallel mesh refinement framework AMROC [10] is adopted to simulate the multi-component compressible Navier-Stokes equations. This efficient and adaptive solver has been extensively validated for supersonic combustion and detonation problems [11,12]. The length of the computational domain is x=30 cm; and the height is y=1 cm. Adiabatic, reflective wall boundary conditions are used for all four boundaries. The spatial mesh size before refinement is 0.5 mm × 0.5 mm; and the finest possible mesh size is 31.2 μm × 31.2 μm. The initial mesh distribution is shown in Fig. 2. The gradients of temperature, density and pressure are used to control the dynamic refinement and coarseness. Initially, a static stoichiometric H_2/O_2 mixture with 85% argon dilution (i.e., H_2:O_2:Ar=2:1:17) is uniformly distributed in the whole computation domain. To initiate detonation in the 2D channel, a thin region of high temperature (T_L=1000 K) and high pressure (P_L=50 atm) is placed near the left wall. The mixture on the right side is at the temperature of T_R=298 K and pressure of P_R=0.2 atm. A disturbance is introduced on the surface of high energy slab at x=1 cm and a sinusoidal perturbation with the amplitude of A and wavelength of λ is imposed in the y-direction.

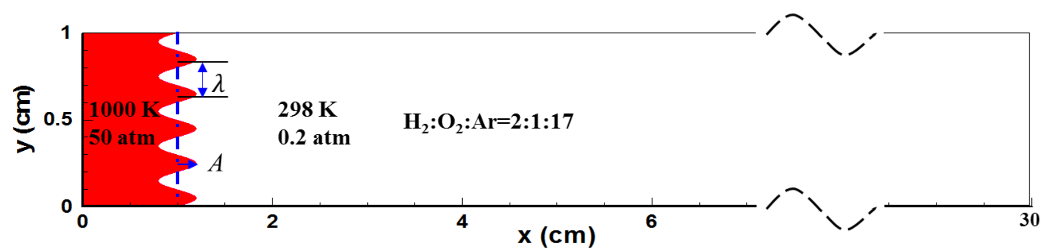

Figure 1. Schematic of mixing zone non-uniformity for direct detonation initiation.

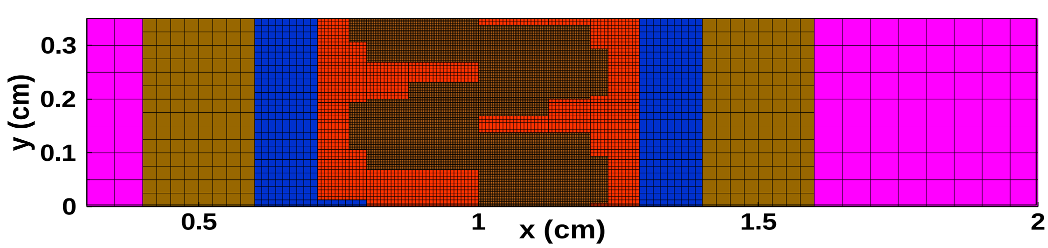

Figure 2. Distribution of initial mesh with five level mesh refinement for A=2 mm and λ=2 mm.

3 Results and discussion

We first consider direct detonation initiation without disturbance (i.e., $\lambda=\infty$). The results are shown in Fig. 3. At the beginning, a leading shock wave propagates from the left to the right. The mixture behind the shock front is compressed; and its temperature and pressure become 1312 K and 3.0 atm respectively. At t=34 μs, the shock front reaches *x*=4.97 cm and autoignition happens around x=4.18 cm which is behind the shock wave. The local autoignition results in an abrupt increase of the temperature and pressure. The burned gas expands toward the left and right sides and pressure wave is generated. The mixture behind the leading shock is further compressed by the pressure wave, which triggers further autoignition. Eventually, the coherent coupling between pressure wave and sequential autoignition yields detonation development according to the SWACER mechanism [13]. At t=56 μs, the reaction front catches up and couples with the leading shock. Afterwards, a stable detonation propagates to the right.

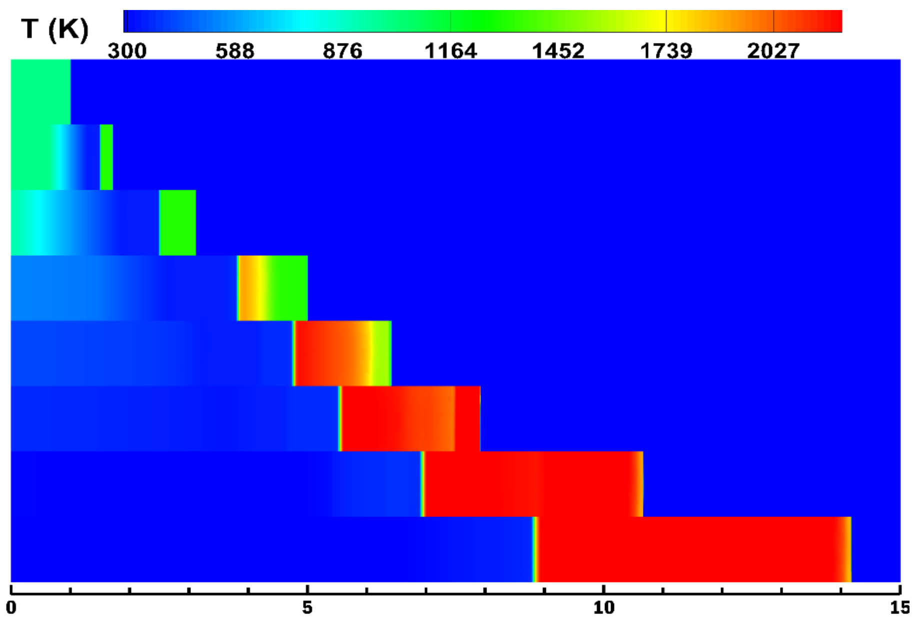

Figure 3. The evolution of temperature contour for the case without disturbance (i.e., $\lambda=\infty$). The time sequence from upper to lower is: 0 μs, 6 μs, 18 μs, 34 μs, 46 μs, 56 μs, 74 μs, 98 μs.

We then consider the case with disturbance on the surface of high energy slab. The amplitude and wavelength of the sinusoidal profile are *A*=2 mm and λ=10 mm, respectively. The results are shown in Fig. 4. The shock wave is formed at the beginning and propagates to the right side with low pressure. The disturbance results in a complex shock wave interaction, which yields hot spots with very high local temperature above 2600 K. Autoignition can occur immediately at these hot spots. With the development of an autoignition zone, the pressure wave propagates upwards and reflects on the upper wall, which results in autoignition in a broad near-wall region at t=10 μs. The reaction front couples with the shock wave, which is further enhanced during t=10~54 μs. Eventually, a planar detonation is formed at t=67 μs.

To further explain the interaction of shock wave, enlarged temperature contours are shown in Fig. 5. Local autoignition caused by initial shock wave interaction generates pressure wave propagating outwardly. When the pressure wave reaches and reflects on the upper wall, the mixture temperature further increases and regional autoignition occurs. The pressure wave is enhanced and it propagates towards the lower wall, which induces further regional autoignition.

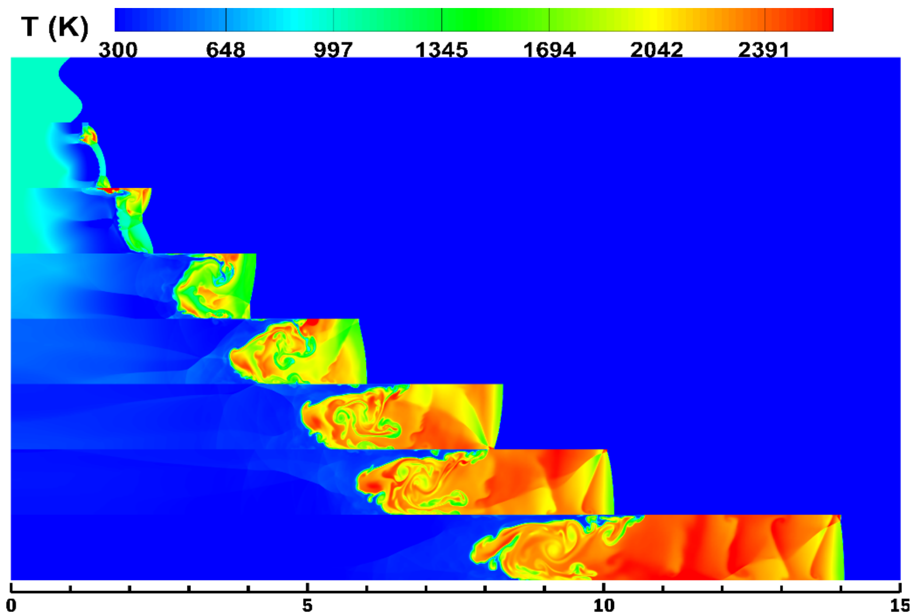

Figure 4. The evolution of temperature contours for the case with disturbance of A=2 mm and λ=10 mm. The time sequence from upper to lower is: 0 μs, 4 μs, 10 μs, 24 μs, 38 μs, 54 μs, 67 μs, 94 μs.

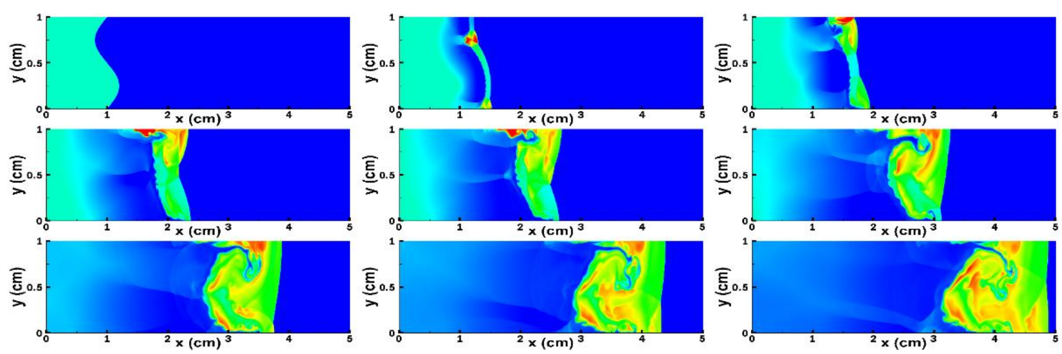

Figure 5. Enlarged temperature contours for those shown in Fig. 4. The time sequence from left to right and upper to lower is: 0 μs, 3 μs, 6 μm, 9.8 μs, 12.2 μs, 17 μs, 22 μs, 26 μs, 30 μs.

We also examine the effects of disturbance wave length on direct detonation initiation. Different wave lengths of λ=∞, 10 mm, 5 mm and 2 mm are considered and the results are compared in Fig. 6. It is found that smaller perturbation wavelength induces more complex shock wave interaction at the initial stage of shock propagation. Consequently, as shown in Fig. 6, global detonation development in the channel occurs earlier for smaller wave length: the time is reduced from 56 μs for the case without disturbance (i.e., λ=∞) to 15 μs for the case of λ=2 mm. Figure 6 also shows that at the same time of t=84 μs, the detonation wave position changes with the wavelength: farther propagation of the detonation is observed for the smaller wavelength. There are set to the same initial condition for different wavelength cases, however, the detonation wave position changes little. Therefore, the wave length of the disturbance has great impact on direct detonation initiation and the disturbance with small wave length promotes the onset of detonation.

Li et al. [7] concluded that the existence of an optimal size of heterogeneity at which the effect is the greatest corresponding to a wavelength that is approximately 10 to 50 times the half reaction zone length of the ideal CJ detonation. We were sure that behaves of disturbance as if it was homogeneous for a very small wavelength. In our simulations, the half reaction zone length is about 0.1 mm, so we did not consider the very small wavelength (i.e., the wavelength is less than 1 mm) because it does not happen in reality.

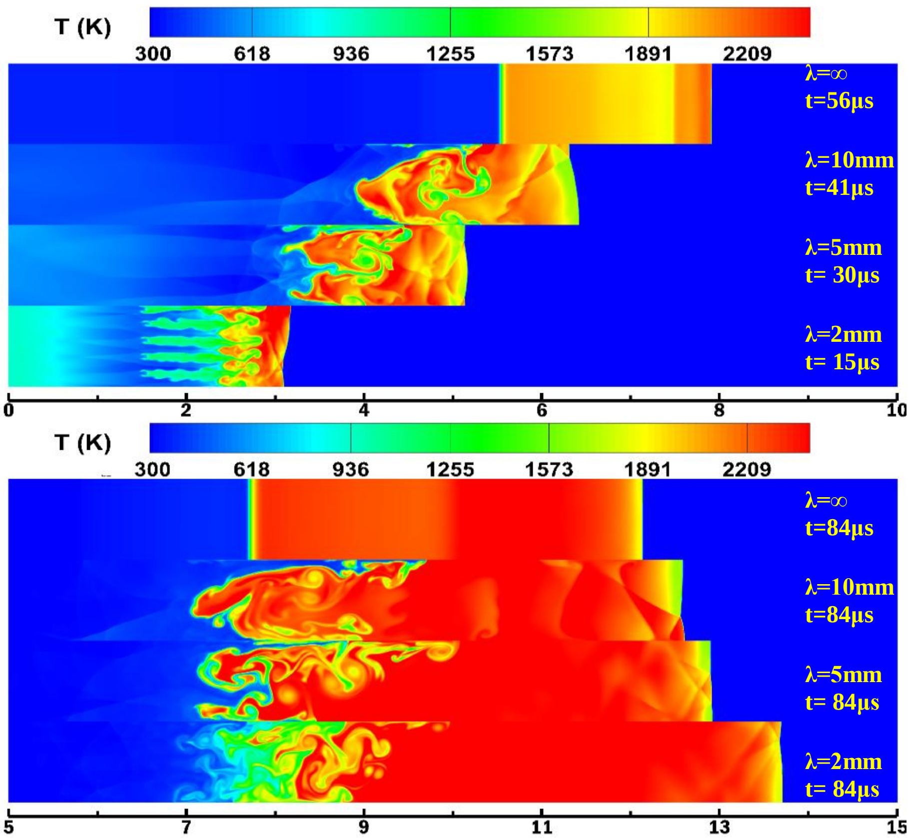

Figure 6. Temperature contours for different wave lengths of $\lambda=\infty$, 10 mm, 5 mm, 2 mm and fixed amplitude of A=2 mm. The upper figure shows the results at the time of global detonation development in the channel; and the lower figure shows the detonation propagation at the same time of t=58 μs.

4 Conclusion

Two-dimensional numerical simulation for direct detonation initiation in $H_2/O_2/Ar$ mixture is conducted. Detailed chemistry is considered and structured adaptive mesh refinement is used to efficiently resolve the detonation development. A disturbance is introduced on the surface of high pressure and high temperature initiation region. The influence of disturbance on direct detonation initiation is examined. It is observed that the disturbance induces complex shock wave interaction, which promotes autoignition and onset of detonation. Disturbances with different wave lengths are considered. It is found that the wave length of the disturbance has great impact on direct detonation initiation. The smaller the perturbation wavelength, the more complex the shock wave interaction and thereby the shorter the detonation development time. Therefore, disturbance with small wave length promotes the onset of detonation.

It is noted that symmetrical reflective boundary conditions are used for the upper and bottom walls, where the normal flow speed is zero while the tangential flow speed is not zero. Simulation for non-slip wall will be conducted and the effects of wall boundary will be examined. Besides, periodical boundary conditions will also be used for the upper and bottom walls and thus the effects of wall confinement will be examined. These results will be presented during the conference.

Acknowledgements

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