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Numerical study on initiation of oblique detonations in hydrogen–air mixtures with various equivalence ratios

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Oblique detonations are simulated using Euler equations with the detailed chemical reaction models, and the initiation in hydrogen–air mixtures is studied. Different from most previous studies, inflow gas mixtures with low pressure and high temperature, derived from high altitude flight conditions of Oblique Detonation Wave Engines (ODWE), are used in this study. Numerical results demonstrate that the oblique shock-detonation surface is composed of three sections, including one section of quasi-detonation, demonstrating the weak coupling of shock and heat release. To study the inflow inhomogeneity effects derived from fuel injection, the simplified cases with different fuel–air equivalence ratios, from 0.1 to 2.0, are simulated and analyzed further. Results show that the dependence of characteristic length on fuel–air equivalence ratio is the classical U-shape curve with critical ratio 0.8. Their values are influenced by inflow Ma but keep the same shape regardless of the inflow Ma.

1. Introduction

Air-breathing hypersonic aircrafts attract more and more attention in recent years. One of the key problems is to develop the novel propulsion systems, because traditional aircraft engines cannot provide enough power when flight Ma increases. Then Scramjet is proposed to achieve combustion in supersonic flow. After tens of years study, practical engines have been tested operating between Ma 5–7 with hydrocarbon fuel. To achieve further higher Ma, it is necessary to develop oblique detonation wave engine (ODWE) [1]. As one kind of improved Scramjet, ODWE is also known as shock-induced combustion Ramjet, inheriting several main advantages of Scramjet. On the other hand, it has the advantages of detonation propulsion, mainly high thermal-cycle efficiency and fast combustion rate. Therefore, ODWE has the potential to become the engines of future hypersonic aircrafts.

Structure of oblique detonation waves need to be clarified first to develop the ODWE. In the early researches [2,3], oblique detonation waves are usually simplified to be the oblique shock waves and post-shock release zones. Further studies, both numerically [4] and experimentally [5], demonstrate that the oblique detonations are composed of a nonreactive oblique shock, an induction region, a set of deflagration waves, and the oblique detonation surface. Subsequent studies mainly focus on two issues, one is how the oblique detonation initiates, and the other is whether this structure is stable. On the initiation studies, two kinds of initiation structures have been shown [6], which are called as the abrupt transition and the smooth transition. One model based on numerical result and theoretical analysis is proposed by Teng and Jiang [7], attributing the formation of two initiation structures into the difference of oblique shock and detonation deflection angles. Due to independent on the chemical reaction parameters, Teng and Jiang's model provides a simple but powerful tool to predict the wave structure ODWE. On the stability studies [8–10], the whole structure is found to be resilient to inflow disturbance, but the interior instability of oblique detonation, characterized by fine scale structures on oblique detonation surfaces, has been studied recently. Furthermore, two successive destabilization processes are observed [11,12], one is the formation of left running transverse waves, and the other is characterized by the formation of right running transverse waves, like normal cellular detonations. Recent study [13] demonstrates two destabilization processes are both influenced by the activation energy, but the second process is more complicated and the quantitative studies are necessary in the future. To facilitate the application in the engines, the concept of multi-mode detonation engine [14,15], combining the oblique detonation with the pulsed normal detonation, is proposed, and oblique detonation waves in confined wedge are simulated and analyzed [16,17].

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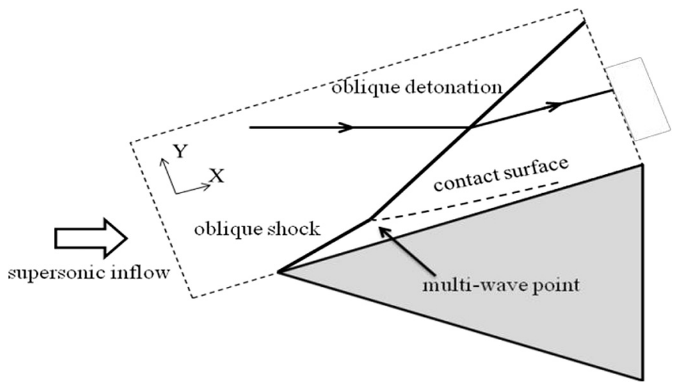

Fig. 1. Schematic of wedge-induced oblique detonations in the combustible gas mixtures.

Although both the initiation and structures have been studied widely, it is still not enough in the ODWE design. Previous studies usually use the ideal inflow conditions, e.g. well-premixed mixtures with 1.0 atm and about 300 K [18–20], deviates from the realistic flow in the ODWE. Our recent study [21] demonstrates that the high inflow temperature, derived from the high flight altitude, influences the structure and instability significantly. Based on these results, another problem related with the non-ideal inflow conditions is investigated further in this study. The fuel injection will induce the inflow mixtures inhomogeneous, fuel-rich or fuel-poor locally. The inflow inhomogeneity will influence the oblique detonation initiation, so its effects are studied in this paper to facilitate the ODWE design. Section 2 will introduce the numerical methods, and the main assumption. Section 3 will show the numerical results and analyze the results. Concluding remarks will be given in Section 4.

2. Mathematical and physical models

Sketch of oblique detonation wave induced by the wedge in the combustible gas mixtures is shown in Fig. 1. Supersonic combustible gas mixtures reflect on the two-dimensional wedge and generate an oblique shock wave first. The shock wave may induce the exothermic chemical reaction, and then a complicated detonation structure will form downstream. The computational simulation is carried out in the dashed zone shown in Fig. 1, whose coordinate is rotated to the direction along the wedge surface. Previous results [22] showed that the viscosity and boundary layer have little effects on this structure except changing the boundary layer thickness slightly, and most of the results use the inviscid calculation. Then the governing equations are simplified as two-dimensional multi-species Euler equations and can be written as follows:

$$\frac{\partial \mathbf{U}}{\partial t}+\frac{\partial \mathbf{F}}{\partial x}+\frac{\partial \mathbf{G}}{\partial y}=\mathbf{S}$$

where:

$$\mathbf{U}=\left\{\begin{array}{c}\rho_1\\ \vdots\\ \rho_n\\ \rho u\\ \rho v\\ e\end{array}\right\},\qquad \mathbf{F}=\left\{\begin{array}{c}\rho_1 u\\ \vdots\\ \rho_n u\\ \rho u^2+p\\ \rho u v\\ (e+p)u\end{array}\right\},$$

$$\mathbf{G}=\left\{\begin{array}{c}\rho_1 v\\ \vdots\\ \rho_n v\\ \rho u v\\ \rho v^2+p\\ (e+p)v\end{array}\right\},\qquad \mathbf{S}=\left\{\begin{array}{c}\dot{\omega}_1\\ \vdots\\ \dot{\omega}_n\\ 0\\ 0\\ 0\end{array}\right\}. \tag{1}$$

In above equations ρ_i $(i=1\cdots n)$ is the i-th specie density and the total density $\rho=\sum_{i=1}^{n}\rho_i$; u and v are the velocity in the x- and y-direction. Total specific energy e is calculated by

$$e=\rho h-p+\frac{1}{2}\rho\left(u^2+v^2\right)$$

where specific enthalpy can be written as $h=\sum_{i=1}^{n}\rho_i h_i/\rho$ and the i-th specie specific enthalpy h_i can be got by curve fitting; p stands for gas pressure and equation of state is

$$p=\sum_{i=1}^{n}\rho_i R_i T,$$

where R_i is the i-th specie gas constant and T is the gas temperature; $\dot{\omega}_i$ is the i-th specie specific mass production rate, which is decided by the chemical reaction model.

Governing equations are solved on adaptive unstructured quadrilateral grids [23] with MUSCL-Hancock scheme [24]. This scheme achieves the second-order accurate in space and time by constructing the Riemann problem on the intercell boundary, and the solution is computed by HLLC approximate Riemann solver. Hydrogen/air chemical reaction model [25] is selected from the widely used CHEMKIN package and 11 species (H_2, O_2, O, H, OH, HO_2, H_2O_2, H_2O, N_2, N, NO) and 23 reactions are account for in chemical reactions, with stiff solver for chemical reaction calculation by the DVODE package [26]. The slip reflecting boundary condition is used on the wedge surface, and the other boundaries are interpolated under the assumption of the zero first-order derivatives of all flow parameters. Default mixtures are stoichiometric hydrogen–air with H_2:O_2:N_2 = 2:1:3.76. This is ideal mixtures so defined as the fuel–air equivalence ratio 1.0. Changing the ratio of H_2 will vary the fuel–air equivalence ratio, such as H_2:O_2:N_2 = 1:1:3.76 corresponding fuel–air equivalence ratio 0.5. The detonation-induced wedge angle is fixed to be 15° in this study.

To simulate the flow dynamics in an ODWE, the flight conditions need to be prescribed to determine the inflow parameters. Air-breathing aircrafts equipped ODWE are supposed to fly on high altitude, but the study on the engine configuration has not been performed widely. Dudebout et al. [27] proposed two ODWE models, one of them assumes that the inflow is compressed twice by weak oblique shock wave before the detonation initiation. This two-shock compression configuration has been used in the later research [1,28,29], and adopted in this study. The inflow is supposed to be compressed twice by weak oblique shock wave. Following the implicit relation between the oblique shock angle β and deflection angle θ, the oblique shock angle β can be calculated and then used to decide the pressure and temperature. Supposing the flight altitude 25 km and Ma 10 with both the deflection angles $\theta=12.5°$, we get static pressure about 119 kPa and static temperature about 998 K, with corresponding Ma about 4.3. The fuel–air equivalence ratio varies between 0.1 and 2.0 to simulate the inflow inhomogeneity. Another bifurcation parameter in this study is inflow Ma, with has complicated relations with the flight Ma, flight attitude and attach angle. In this study, the flow is simplified that Ma varies between 4.0 and 5.0 without considering the change of static pressure and temperature.

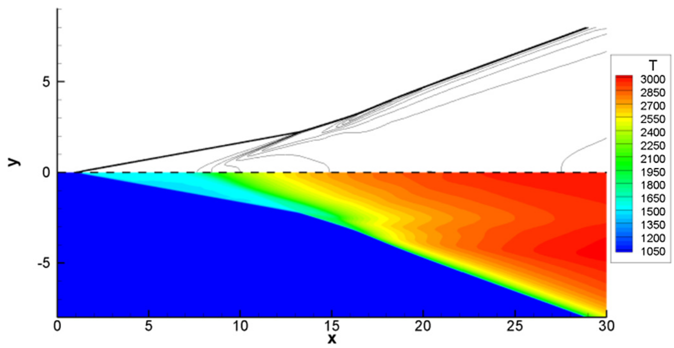

Fig. 2. Pressure (upper) and temperature (lower) of oblique detonation with ideal fuel–air equivalence ratio in the case of Ma 4.3.

3. Numerical results and discussion

Oblique detonation structure with the incident Ma 4.3 is shown in Fig. 2. The computational domain is 30 mm × 10 mm, and the finest grid is 0.05 mm by adaptive mesh refinement (AMR) method. Referring previous studies [10,29], this grid resolution can capture not only the wave structure but also the surface instability, although the later is not triggered in this study. The wedge starts from $x = 1.0$ and the length scale dimension is mm in the figures shown later. It can be observed the oblique shock to detonation transition is different from the sketch shown in Fig. 1. Generally the oblique shock-detonation surface has three sections. The first one is the oblique shock, which compresses the inflow gas to achieve the self-ignition. Then the deflagration starts before $x = 10$ near the wedge, and intersects with the oblique shock around $x = 13$. The intermediate structure from $x = 13$ to 16 is not oblique detonation yet, characterized as the complex of shock and flame. The surface becomes the oblique detonation after $x = 16$, where the shock and flame couples together closely and smoothly.

The intermediate structure shows a quasi-steady phenomenon in the oblique detonation initiation. In this region, the oblique shock is stronger than upstream one but weaker than downstream one, as shown in Fig. 2. The heat release influences the oblique shock, inducing the large oblique angle. However, the heat release is slower than that behind the oblique detonation, so the temperature gradient is small here. Our recent study [21] shows the induction zone length of chemical reactions decreases after the detonation initiation, but a quasi-steady plateau appears in this region. This weak coupling of shock and heat release resembles the quasi-detonation in rough tubes [30], so it can be viewed as quasi-detonation in oblique detonation waves.

Oblique detonations with different fuel–air equivalence ratio are simulated. Because the variation of fuel–air equivalence ratio will change the sound speed, keeping both the inflow velocity and Ma the same is impossible. Considering the characteristics of hypersonic engines, fixing the inflow velocity rather than Ma is a better choice. With ideal fuel–air equivalence ratio 1.0, Ma 4.3 corresponds to inflow velocity 3205 m/s, which is used in various equivalence ratio cases.

Oblique detonation structures with fuel–air equivalence ratio 0.5 and 2.0 are shown in the Fig. 3. Results show that basic structures are similar, but the ratio variation changes the structures. The length of quasi-detonation is large in the case of low ratio, while small in the case of high ratio. Moreover, post-detonation average temperature is low and the reaction is not drastic in the case of low fuel–air equivalence ratio. This is because the low ratio decreases the heat release, meaning less fuel density, so both the amount of heat and its release process are weakened. However, the heat release starting position with low ratio moves upstream, derives from the variation of post-oblique-shock temperature. The

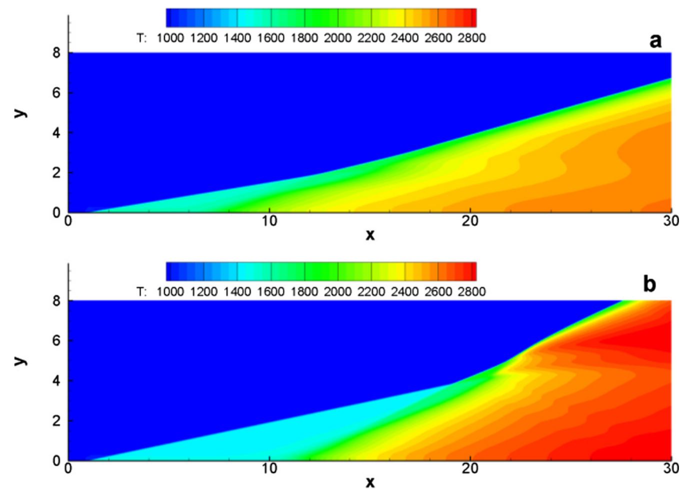

Fig. 3. Temperature of oblique detonation with fuel–air equivalence ratio 0.5 and 2.0 in the case of inflow velocity 3205 m/s.

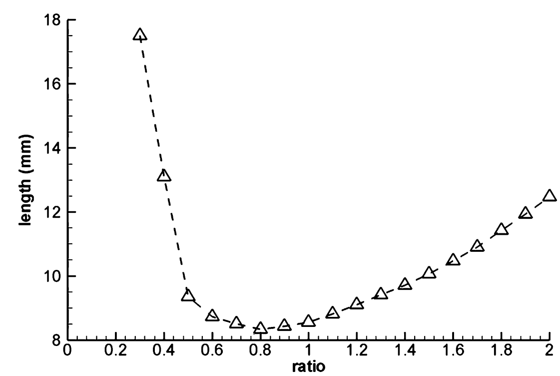

Fig. 4. Characteristic length as function of fuel–air equivalence ratio with inflow velocity 3205 m/s.

temperature is about 1540 K in Fig. 3a and 1430 K in Fig. 3b. This results from the different inflow Ma to keep the same inflow velocity. With the same inflow velocity, the low ratio case has low sound speed, and then its inflow Ma is higher than the high ratio case.

To carry out the quantitative analysis, it is necessary define the characteristic length of initiation process. Given the same gas mixtures with the same detailed chemical reaction mechanisms, we can get its ZND structure of CJ detonation with CHEMKIN package [25]. Results show that the temperature at the end of induction zone is about 2200 K. Hence we define the initiation length starts from the oblique shock and terminates when temperature rises to 2200 K. The lengths are dependent on their distances from the wedge. The mixtures close to the wedge surface are nearly self-ignition, so we choose it as the initiation characteristic length.

Fig. 4 shows the characteristic length as function of fuel–air equivalence ratio. With ratio 0.0 without any fuel in the inflow, the length is infinite. By increasing the equivalence ratio, the length first decreases and then increases, with the minimum value corresponding to the ratio 0.8. This ratio-length curve, the classic U-shape curve, is similar to those of the initiation energy or cell width dependence on the fuel–air equivalence ratio [31]. Theoretically the minimum characteristic length should appears in the case of ideal ratio 1.0, but critical ratio 0.8 is not a surprising result because the critical ratios in initiation energy or cell width are also deviates from idea ratio 1.0 slightly. Some possible reasons have been discussed [32], but it is still an open problem in the detonation research.

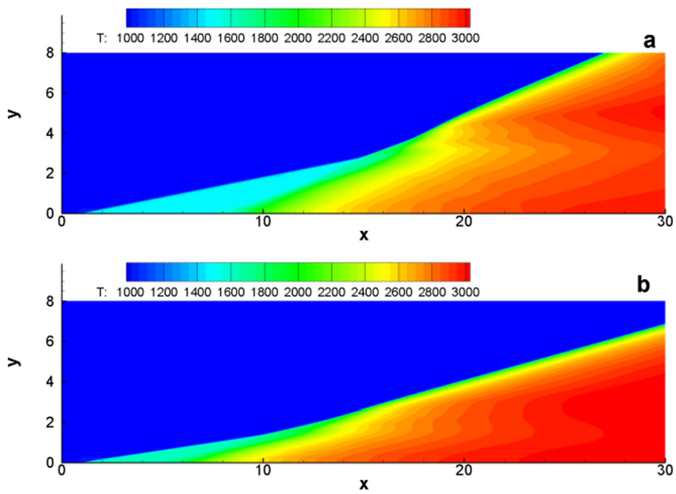

Fig. 5. Temperature of oblique detonation with fuel–air equivalence ratio 1.0 in the case of Ma 4.0 (a) and 5.0 (b).

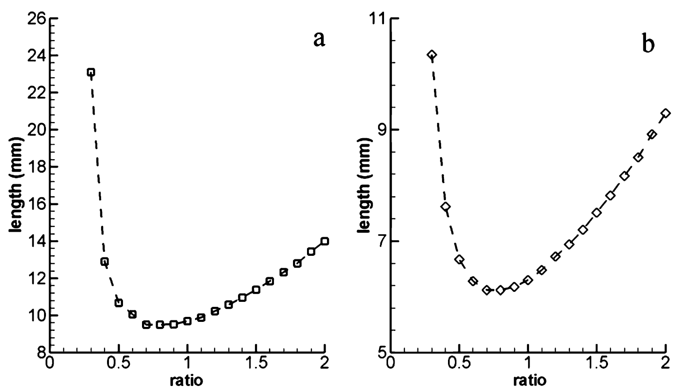

Fig. 6. Characteristic length as function of fuel–air equivalence ratio with inflow velocity 2982 m/s (a) and 3727 m/s (b).

To study the effects of different inflow Ma, oblique detonations with inflow Ma 4.0 and 5.0 are simulated and shown in Fig. 5. The static pressure is 119 KPa and static temperature is 998 K, with ideal fuel–air equivalence ratio 1.0. Numerical results show that the oblique angles of shock and detonations in the case of Ma 4.0 are large, while the angles in the case of Ma 5.0 are small. Furthermore, the detonation initiates early in the case of high inflow Ma. These phenomena are the same as previous studies qualitatively. The oblique detonation structures shown in Fig. 5 are both composed of three sections, with quasi-detonations similar to those shown in Fig. 2. Although their positions are different, the length projections on the x-axis are all about 3 mm, demonstrating the length of oblique quasi-detonation surface is not sensitive to inflow Ma.

For both the inflow Ma 4.0 and 5.0 cases, oblique detonations with different fuel–air equivalence ratios are simulated, and the characteristic lengths dependent on the ratios are shown in Fig. 6. Generally both the curves are similar to that shown in Fig. 4, demonstrating the U-shape curves. Numerical results show that the length is strongly dependent on the inflow velocity, as shown in Fig. 6. The length of velocity 2982 m/s cases are much higher than those of velocity 3727 m/s cases, but the critical ratios in call cases are about 0.8, corresponding to the minimum characteristic length.

Because the inflow inhomogeneity is unavoidable in ODWE, these results are helpful for the engine design. The fuel–air equivalence ratio 0.8 induces the minimum characteristic length, demonstrating the weak fuel-poor mixtures are the best from the viewpoint of oblique detonation initiation. However, the length increases drastically in all cases when the ratio decreases below 0.5, providing a constraint condition for the fuel injection system design. From Figs. 4 and 6, we observe that the length increase is slow in the region of fuel-rich region, meaning fuel-rich is better than fuel-poor for the initiation. It is probably both fuel-rich and fuel-poor regions appear in the realistic flow field, so initiating the detonation in the fuel-rich region is a better choice based on these results.

4. Concluding remarks

Oblique detonations are simulated to study the initiation in hydrogen–air mixtures with various equivalence ratios. Inflow gas mixtures with low pressure and high temperature, derived from high altitude flight conditions of Oblique Detonation Wave Engines (ODWE), are used in this study. Numerical results show that the oblique shock-detonation surface is composed of three sections, including one section of quasi-detonation, demonstrating the weak coupling of shock and heat release. To study the inflow inhomogeneity effects derived from fuel injection, several simplified cases with different fuel–air equivalence ratios are simulated. Results show that the characteristic length dependence on fuel–air equivalence ratio is the classical U-shape curve with critical ratio 0.8. The lengths are found to be influenced by inflow Ma but keep the same shape regardless of the inflow Ma.

Conflict of interest statement

No conflict of interest.

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