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



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ABSTRACT

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.

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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 thermalcycle 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 fuelpoor 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 twodimensional 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:

$$\mathbf{U} = \begin{cases} \rho_1 \\ \vdots \\ \rho_n \\ \rho u \\ \rho v \\ e \end{cases}, \quad \mathbf{F} = \begin{cases} \rho_1 u \\ \vdots \\ \rho_n u \\ \rho u^2 + p \\ \rho u v \\ (e + p)u \end{cases},$$

$$\mathbf{G} = \left\{ \begin{array}{c} \rho_1 \mathbf{v} \\ \vdots \\ \rho_n \mathbf{v} \\ \rho u \mathbf{v} \\ \rho \mathbf{v}^2 + p \\ (e+p) \mathbf{v} \end{array} \right\}, \qquad \mathbf{S} = \left\{ \begin{array}{c} \omega_1 \\ \vdots \\ \dot{\omega}_n \\ 0 \\ 0 \\ 0 \\ 0 \end{array} \right\}. \tag{1}$$

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

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

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 (H₂, O₂, O, H, OH, HO₂, H₂O₂, H₂O, N₂, 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 H₂ 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 $\theta = 12.5^{\circ}$, 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.

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