



Full Length Article

Numerical investigation of oblique detonations induced by a finite wedge in a stoichiometric hydrogen-air mixture



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ABSTRACT

Two-dimensional, oblique detonation waves (ODWs) in a stoichiometric hydrogen-air mixture are simulated using the reactive Euler equations with a detailed chemical reaction model. This study focuses the effects of expansion waves on the initiation, which is modeled by a finite-length wedge. Numerical results demonstrate that the expansion wave may quench the ODW if it interacts with the initiation region, and the critical position is found to be dependent on the incident Mach number M_0 . The critical position moves upstream in the case of high M_0 , and downstream in the case of low M_0 . Furthermore, ODW structures show different behaviors when the expansion wave is near its critical position. In the case of $M_0 = 10$, the structure is featured by a stationary but decoupled shock and reactive surface, while a transient downstream-moving ODW is observed in the case of $M_0 = 7$. By decreasing the turning angle, the former one keeps the same, while the later one becomes also stationary. These differences are related with the initiation mechanisms of two ODW structures, demonstrating that the structure of wave-controlled initiation is more sensitive to the expansion waves than the kinetic-controlled initiation.

1. Introduction

Detonations are supersonic combustion waves travelling in pre-mixed combustible mixtures, in which the strong leading shock and heat release are closely coupled [1,2]. The detonation research is useful and crucial for automotive internal combustion engines to prevent the super-knock phenomena [3,4]. More importantly, detonation engines used in the future aircrafts attract more and more attention due to the high thermal cycle efficiency. There are three kinds of detonation engines, which are pulse detonation engines [5], rotating detonation engines [6,7] and oblique detonation engines [8], respectively. Oblique detonation engines are one kind of ramjet engines in which oblique detonation wave (ODW) is triggered to achieve the fast and high efficient combustion. It has the potential to be used in the hypersonic propulsion, operating at the higher flight Mach number than Scramjet (supersonic combustion ramjet). In order to develop the practical ODW-based engines, it is necessary to get more fundamental understanding of the oblique detonation structure and instability.

ODW structures were usually simplified to be the oblique shock waves and post-shock release zones [9] initially, but further studies [10–14] demonstrate that the surface of ODW is composed of a

nonreactive oblique shock before the oblique detonation surface forms. There are several studies on surface instability of ODW recently [15–20], illustrating and quantifying the formation of fine-scale structures on oblique detonation surfaces. For simplicity, most of the previous numerical studies [10–20] used simplified chemical reaction models, mainly the one-step irreversible Arrhenius kinetic model, which has interior flaws in the initiation study. Recent studies [21–24] demonstrate that the complicated chemistry has obvious effects on the detonation characteristics, so ODW studies based on detailed chemistry model are necessary to be performed. Current studies mainly use the hydrogen-air mixtures, whose detailed chemical mechanisms are widely studied for tens of years. ODW structures influenced by the inflow Mach numbers and gas-dynamic parameters, such as inflow pressure and temperature, are simulated and discussed [25]. To study the ODW influenced by the fuel injection, the inflow inhomogeneity is modeled and simulated, demonstrating the distorted reaction surfaces and morphology variation of the ODW structures [26,27]. Our recent study demonstrated that there are two initiation mechanisms of ODW in the wedge-induced structures in hydrogen-air mixtures [28]. In the case of high incident Mach number, the temperature behind the oblique shock is high enough to achieve the self-ignite, so it is called the

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kinetics-controlled mechanism. On the other side, in the case of low incident Mach number, the temperature is not high enough so that the initiation position is determined by the interaction of the oblique shock and oblique detonation, which is called wave-controlled mechanism. The initiation length of kinetics-controlled ODW can be calculated from the constant-volume combustion theory, but the initiation length of wave-controlled ODW is still lack of theoretical model, which requires more knowledge on the wave dynamics of ODW structures.

To deepen our understanding on the ODW initiation, this study simulated the ODW using a finite-length wedge, replacing the semi-infinite wedge in the previous study [28]. Due to the effects of expansion waves, the initiation features of ODW structures may change and induce complicated phenomena. In the detonation instability and structure evolution [29–31], effects of expansion waves have been simulated and discussed. Papalexandris [32] found out that the expansion wave may quench the ODW, but it is still lack of the detailed study on the effects of expansion wave on ODW initiation. In this study, the ODW structures influenced by the expansion waves are simulated. By analyzing two typical cases, the interaction of expansion wave and ODW are studied to further our understanding on the ODW initiation.

2. Physical and mathematical models

A schematic of the oblique detonation wave induced by the wedge in a combustible gas mixture is shown in Fig. 1. The wedge in supersonic inflow induces an oblique shock wave (OSW) first. If the inflow is combustible mixtures with high incident Mach number M_0 , an exothermic chemical reaction may begin and result in oblique detonation. The computational domain is shown in region enclosed by the dashed line, and the Cartesian grid is aligned with the wedge surface. Similar to previous numerical studies on oblique detonations [28], the present analysis is based on the two-dimensional multi-species Euler equations written as follows:

$$\frac{\partial \tilde{U}}{\partial t} + \frac{\partial \tilde{F}}{\partial \xi} + \frac{\partial \tilde{G}}{\partial \eta} = \tilde{S} \quad (1)$$

where

$$\tilde{U} = \frac{U}{J}, \tilde{F} = \frac{1}{J}(\xi_x F + \xi_y G), \tilde{G} = \frac{1}{J}(\eta_x F + \eta_y G), \tilde{S} = \frac{S}{J} \quad (2)$$

with

$$U = \begin{pmatrix} \rho_1 \\ \vdots \\ \rho_n \\ \rho u \\ \rho v \\ e \end{pmatrix}, F = \begin{pmatrix} \rho_1 u \\ \vdots \\ \rho_n u \\ \rho u^2 + p \\ \rho uv \\ (e + p)u \end{pmatrix}, G = \begin{pmatrix} \rho_1 v \\ \vdots \\ \rho_n v \\ \rho uv \\ \rho v^2 + p \\ (e + p)v \end{pmatrix}, S = \begin{pmatrix} \omega_1 \\ \vdots \\ \omega_n \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (3)$$

and

$$\frac{1}{J} \frac{\partial(\xi, \eta)}{\partial(x, y)} = \begin{vmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{vmatrix} = \xi_x \eta_y - \xi_y \eta_x \quad (4)$$

In the above equations, the total density and total energy are

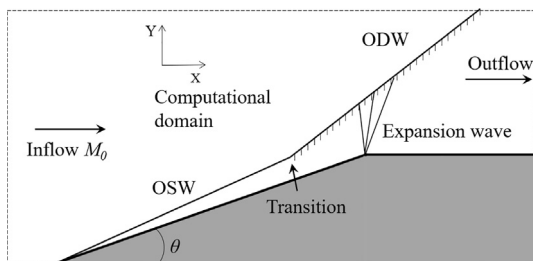


Fig. 1. Sketch of the oblique detonation simulation.

calculated by

$$\rho = \sum_{i=1}^n \rho_i, \quad e = \rho h - p + \frac{1}{2} \rho (u^2 + v^2) \quad (5)$$

where specific enthalpy can be written as $h = \sum_{i=1}^n \rho_i h_i / \rho$ with h_i obtained from thermodynamic data of each individual specie. The equation of state is

$$p = \sum_{i=1}^n \rho_i \frac{R_0}{w_i} T \quad (6)$$

where w_i is the molecular weight and T is the gas temperature; ω_i is the species' specific mass production rate, which is dictated by the chemical reaction model.

The governing equations are discretized on Cartesian grids and solved with the DCD scheme [33] with Strang's splitting, and the algorithm has been used to study the complicated flows [34,35]. The latest H₂/O₂ kinetic model for high-pressure combustion [36–38] is used here, which involves 27 reversible elementary reactions among the 8 species (H₂, O₂, H₂O, H, O, OH, HO₂, and H₂O₂) with 5 non-reacting species (N₂, Ar, He, CO, and CO₂). Thermodynamic properties of the chemical species are evaluated from the 9-coefficient NASA polynomial representation [39]. A stoichiometric hydrogen-air mixture with H₂:O₂:N₂ = 2:1:3.76 is used, with the temperature 300 K and the pressure 101,325 Pa. The uniform flow is set as the initial condition, whose velocities are calculated from the incident Mach number M_0 . The slip reflecting boundary condition is used on the wedge surface and the other boundaries are interpolated under the assumption of zero first-order derivatives of all flow parameters. Since the characteristic lengths of chemical reactions vary in a wide range, both the computational domain and mesh scale are adjusted. For each case, the results are examined to assure the mesh scale effects are trivial enough. Unless specified, a wedge angle θ is fixed to be 25° and the turning angle inducing the expansion waves is also 25°, so the outflow is paralleled with the inflow.

3. Numerical results and discussion

3.1. ODW influenced by the expansion waves

The flow fields of ODW structures with $M_0 = 10$ and 7 are shown in Fig. 2, with the upper displaying results from low resolution and the lower from high resolution. In the low-resolution simulations, the grid of the left boundary is 0.005 mm * 0.005 mm in the case of $M_0 = 10$, and 0.05 mm * 0.05 mm in the case of $M_0 = 7$. The grid 500 * 400 is employed in both cases, so the grid scale around the initiation points becomes about 0.005 mm * 0.003 mm in the case of $M_0 = 10$ and 0.05 mm * 0.03 mm in the case of $M_0 = 7$, respectively. Obvious differences can be observed between the flow fields shown in Fig. 2a and b. The smooth transition appears in Fig. 2a, while the abrupt transition appears in Fig. 2b, which is physically reasonable according to our previous study [13]. Because of the difference of incident Mach number M_0 , the initiation length of inert shock in the case of $M_0 = 7$ is almost 10 times of that in the case of $M_0 = 10$.

Resolution tests are performed and the results are compared in both frames in Fig. 2. The computational domain of the case $M_0 = 10$ is 2.5 mm * 2.0 mm, while the domain of the case $M_0 = 7$ is 25 mm * 20 mm. In the both cases, the high-resolution simulation uses the grid 1000 * 800, doubling the grid numbers in both directions. Obviously, the general ODW structures of two cases are similar to each other, although some slight differences can be observed. Low resolution induces the initiation moving downstream a little in Fig. 2a, while moving upstream a little in Fig. 2b. However, it should be noted that the low resolution is not adequate to resolve all the chemical kinetic scales, such as the behaviors on the slip line instability observed shown in Fig. 2b. Despite of the observed differences, for the purpose of this

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