Available online at www.sciencedirect.com

ScienceDirect

Procedia Engineering 126 (2015) 209 – 213

Procedia Engineering

www.elsevier.com/locate/procedia

7th International Conference on Fluid Mechanics, ICFM7

Oblique shock to detonation transition in hydrogen-air mixtures

Tao Wang[a], Yining Zhang[b], Honghui Teng[a,*], Zonglin Jiang[a]

[a]State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, Chinese Academy of Sciences, Beijing, 100190, China
[b]State Key Laboratory of Laser Propulsion & Application, Beijing Power Machinery Research Institute, Beijing, 100074, China

---

Abstract

Oblique detonation waves in hydrogen-air mixtures are simulated with detailed chemical reaction models to study the initiation process. To mimic the flow in Oblique Detonation Wave Engines (ODWE), the combustible gas mixtures, with low pressure and high temperature, are derived from flight condition and used in the simulations. Numerical results show the initiation is achieved through the smooth transition from oblique shock to detonation, different from the abrupt transition studied widely before. The mechanism of forming the smooth transition is discussed, which is consistent with previous theory. To perform quantitative analysis, the characteristic length of initiation process is defined, and then the length dependences on detonation-induced wedge angle, incident Ma and flight Ma are listed.

Peer-review under responsibility of The Chinese Society of Theoretical and Applied Mechanics (CSTAM)

Keywords: oblique detonation; hydrogen; oblique shock

---

1. Introduction

High efficient propulsion systems attract more and more attention in recent years to develop air-breathing hypersonic aircrafts. One of the propulsion concepts uses oblique detonation waves, which derive into Oblique Detonation Wave Engines (ODWE) and Ram Accelerators [1]. This kind of propulsion system not only has the advantages of the Scramjet (Supersonic combustion ramjet), but also achieves the high thermal cycle efficiency through the detonation [2]. However, it is difficult to form the steady oblique detonations in high speed combustible mixtures, and more studies on the oblique detonation structure and instability need to be performed.

---

* Corresponding author. Tel.:.+86-10-82544011
*E-mail address:*hhteng@imech.ac.cn

Peer-review under responsibility of The Chinese Society of Theoretical and Applied Mechanics (CSTAM)
doi:10.1016/j.proeng.2015.11.222

In the early research, oblique detonation waves are usually simplified to be oblique shock waves and post-shock release zones attached on the wedge. Further studies demonstrate the realistic structure near the wedge front tip is complicated. Li et al. [3] simulated the oblique detonation numerically, and observed the structure composed of a nonreactive oblique shock, an induction region, a set of deflagration waves, and the oblique detonation surface. This structure is verified experimentally [4] and then considered to be the standard structure used widely in later studies. Choi et al. [5] observed the fine scale structures characterized with “saw tooth” flame on oblique detonation surfaces, whose formation is attributed to the instability of oblique shock and combustion coupling. Teng et al.[6,7] found out that oblique detonation surfaces are unstable unconditionally, like multi-dimensional cellular detonations, although the formation of triple points will be suppressed by high overdrive degrees.

Previous studies mainly focus on the instability of oblique detonation surfaces, but the oblique shock to detonation transition does not attract enough attention. Two kinds of transition structures, the abrupt one and the smooth one, have been observed [8]. The abrupt one is achieved by a multi-wave point connecting the oblique shock and detonation surfaces, as shown in Fig. 1, while the smooth one has an arc shock instead of the multi-wave point. Teng & Jiang [9] studied the structure differences in the cases of different chemical and aerodynamic parameters, and the criterions on the transition type are proposed. Furthermore, transient structures are observed dependent on the inflow Ma and activation energy [10], demonstrating the realistic oblique detonations are more complicated.

Transition from the oblique shock to detonation is actually the oblique detonation initiation, so its research is crucial in the ODWE design. Recent studies [11] on the normal detonation initiation have demonstrated that both the aerodynamic and mixture thermodynamic properties greatly influence the initiation of detonation. However, a deep knowledge of the oblique structure in the ODWE is still lacking and needs to be addressed. Most of previous studies use simplified chemical reaction models, mainly one-step irreversible model. Moreover, the inflow parameters are usually set artificially, deviating far from those in ODWE. In this study, oblique detonation waves in hydrogen-air mixtures are studied with detailed chemical reaction models. The inflow parameters are chosen to simulate the flow in ODWE with high altitude, and numerical results show the initiation is achieved by the smooth one. The mechanism of forming on the smooth transition is discussed, and the initiation position variation as function of incident Ma and wedge angle is analyzed quantitatively.

2. Mathematical and physical models

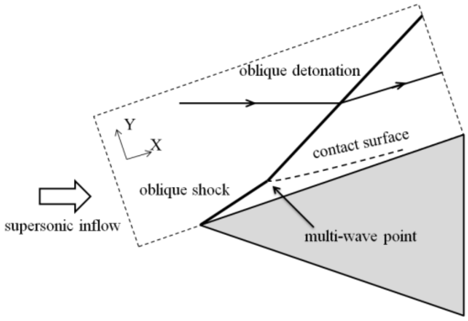

Fig. 1. Schematic of wedge-induced oblique detonations in the combustible gas mixtures.

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 two-dimensional wedge and generate an oblique shock wave first. The shock wave may trigger exothermic chemical reaction, and then induce oblique detonation wave 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 showed that the viscosity and boundary layer have little effects on this structure except changing the boundary layer thickness slightly, and almost all previous simulations use the inviscid calculation. Governing equations are solved on adaptive unstructured quadrilateral grids [12] with MUSCL-Hancock scheme. Hydrogen/air chemical reaction model [13] 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. Stoichiometric hydrogen-air mixtures with H2:O2:N2= 2:1:3.76 are used. 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.

3. Numerical results and discussion

To simulate the flow in ODWE, the flight conditions need to be prescribed first to decide the inflow pressure and temperature. Air-breathing aircrafts equipped ODWE are supposed to operate on high altitude 25-35 km, and a wide range of Ma can be covered theoretically. The realistic flow is very complicated concerning the fuel mixing in supersonic flow, so this study assumes the inflow is well-premixed to focus on the oblique detonation structure. Considering the flight altitude 30 km and Ma 10, the inflow is supposed to be compressed twice by weak oblique shock wave. Supposing the deflection angle $\theta = 12.5°$, we can get static pressure about *56 kPa* and static temperature about *1021 K*, with the corresponding Ma about *4.3*. In this study, the detonation-induced wedge angle varies between 11°-20°. The flight Ma and attitude have complex effects on pre-detonation inflow parameters. Roughly the flow is simplified that Ma varies between *4.0* and *5.0* without considering the change of static pressure and temperature. Finally the effects of inflow pressure and temperature, associated with Ma variation, are simulated and discussed.

3.1. Structure of oblique detonation waves

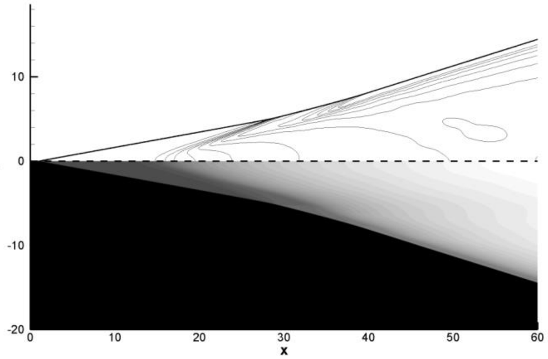

Fig. 2. Pressure (upper) and temperature (lower) in the case of incident Ma 4.3 and wedge angle 15°

Oblique detonation structure with the incident Ma 4.3 and wedge angle 15° is shown in Fig. 2. The computational domain is 60mm×20mm, and the primary mesh 0.2mm×0.2mm can be refined into the finest grid 0.05 mm by adaptive mesh refinement. The wedge starts from x=1.0 and the length scale is mm in the figures shown later. It can be observed this structure is different from the abrupt transition shown in Fig. 1, which appears in most of previous studies. The transition is smooth with an arc shock, and there is no obvious contact surface in the combustion product. Oblique detonation structure in Fig. 2 shows the smooth transition, different from the abrupt transition, although the later attracts much more attention. Oblique shock and detonation surfaces are connected by a multi-wave turning point in the abrupt transition, while surfaces in the smooth transition are connected by an arc shock. However, these results are consistent with the previous theory on the formation mechanism of different structures [9]. In this study, gas mixtures deduced from the ODWE flight conditions have high temperature and low pressure. Hence, the density of incident flow is rather low, and the heat release is limited. This induces the difference of oblique shock and detonation angle is small, so the smooth transition forms in ODWE.

3.2. Effects of wedge angle and incident Ma

Oblique detonation structures in ODWE are influenced by several factors. First of all, we study effects of two key parameters, the wedge angle and the incident Ma. To study effects of wedge angles, two cases with wedge angle 13° and 17° are simulated and shown in Fig. 3. Obviously, the initiation position moves downstream when wedge angle decreases, and moves upstream when wedge angles increases. In the case of wedge angle 13°, 15°, 17°, corresponding initiation positions are about x=45, 30, 20 mm, respectively. Structures in the cases of different incident Ma with the same wedge angle 15° are not shown here because the initiation positions in both cases locate around *x=30 mm*. Although the difference can be observed, the variation of initiation position is not significant.

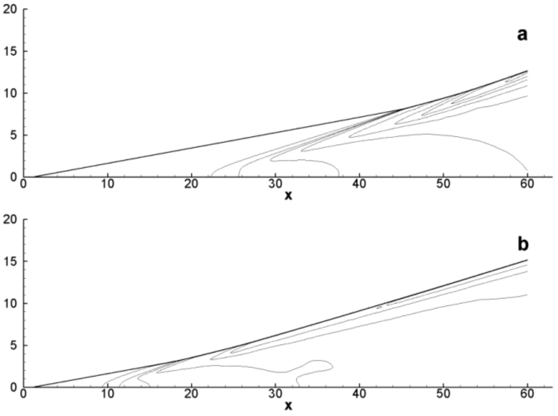

Fig. 3. Pressure in the case of incident Ma 4.3, wedge angle 13° (a) and 17° (b)

3.3. Quantitative analysis on the characteristic length

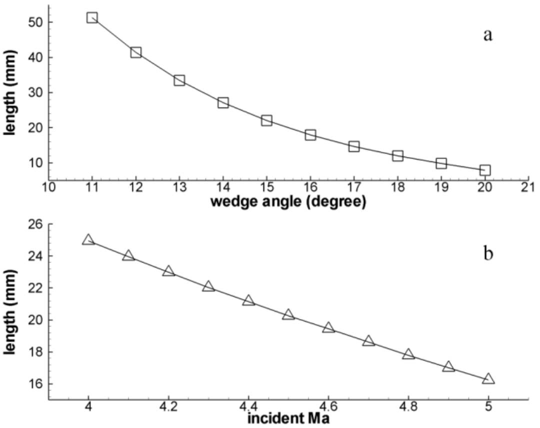

Fig. 4. Characteristic lengths as function of wedge angle with incident Ma 4.3 (a) and incident Ma with wedge angle 15°(b)

To get the quantitative results, 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. Results show that the temperature at the end of induction zone, whose length is about 2150 K. Hence this temperature is chosen to denote the end of induction zone in this study. The initiation length starts from the oblique shock and terminates at the end of induction zone. The lengths are different along different flow stream lines, dependent on their distances from the wedge. We define the initiation characteristic length by the maximum one of each case, which locates on the wedge surface. Figure 4 shows the characteristic lengths as function of wedge angle and incident Ma. With incident Ma 4.3, the length decreases when the wedge angle increases, and increases when the wedge angle decrease, as show in Fig. 4(a). Similar relation between the length and incident Ma can be also observed in Fig. 4(b), with wedge angle 15°. However, it can be observed that the length dependences on the wedge angle and incident Ma are different. The length on the wedge angle varies nonlinearly, while the length on the Ma varies and almost linearly. There's no doubt that Ma itself varies in a narrow range, compared with the wedge angle. However, Ma variation is different from wedge angle because the former is limited by the flight condition, but the later can be chosen freely as a detonation-induced parameter. This induces different variation range, and different length dependence relations can be observed.

4. Conclusion

Oblique detonation waves in hydrogen-air mixtures are simulated with detailed chemical reaction models to study the initiation process. To mimic the flow in Oblique Detonation Wave Engines (ODWE), the combustible gas mixtures, with low pressure and high temperature, are derived from flight condition and used in the simulations. Numerical results show the initiation is achieved through the smooth transition from oblique shock to detonation, different from the abrupt transition studied widely before. The mechanism of forming the smooth transition is discussed, which is found to be consistent with previous theory. Based on the characteristic length of initiation process, quantitative analysis is performed, demonstrating the different initiation length dependences on the wedge angle and incident Ma.

Acknowledgements

The research is supported by NSFC No. 11372333 and 51376165.

References

[1] K. Kailasanath, Review of propulsion applications of detonation waves, AIAA J. 41 (2003) 145-159.
[2] P. Wolanski, Detonation propulsion, Proc. Combust. Inst. 34(1) (2013) 125-158.
[3] C. Li, K. Kailasanath, E.S. Oran, Detonation structures behind oblique shocks, Phys. Fluids 6 (1994) 1600–1611.
[4] C. Viguier, L. Figueira da Silva, D. Desbordes, B. Deshaies, Onset of oblique detonation waves: comparison between experimental and numerical results for hydrogen-air mixtures, Proc. Combust. Inst. 26 (1996) 3023-3031.
[5] J. Y. Choi, D. W. Kim, I. S. Jeung, F. Ma, V. Yang, Cell-like structure of unstable oblique detonation wave from high-resolution numerical simulation, Proc. Combust. Inst. 31 (2007) 2473-2480.
[6] H. H. Teng, Z. L. Jiang, H. D. Ng, Numerical study on unstable surfaces of oblique detonations, J. Fluid Mech. 744 (2014) 111-128.
[7] H. Teng, H.D. Ng,, K. Li, et al., Cellular structure evolution on oblique detonation surfaces, Combustion and Flame 162 (2015) 470-477.
[8] L. F. Figueira da Silva, B. Deshaies, Stabilization of an oblique detonation wave by a wedge: a parametric numerical study. Combust. Flame 121 (2000) 152-166.
[9] H. H. Teng, Z. L. Jiang, On the transition pattern of the oblique detonation structure, J. Fluid Mech. 713 (2012) 659-669.
[10] H. Teng, Y. Zhang, Z. Jiang, Numerical investigation on the induction zone structure of the oblique detonation waves, Computers & Fluids 95 (2014) 127-131.
[11] B. Zhang, N. Mehrjoo, H.D. Ng, et al., On the dynamic detonation parameters in acetylene-oxygen mixtures with varying amount of argon dilution, Combustion and Flame 161(2014) 1390-1397.
[12] M. Sun, K. Takayama, Conservative smoothing on an adaptive quadrilateral grid, Journal of Computational Physics 150 (1999) 143-180.
[13] R. J. Kee, F. M. Rupley, E. Meeks, et al., Chemkin-II: a fortran chemical kinetics package for the analysis of gas-phase chemical and plasma kinetics, UC-405, SAND96-8216, Sandia National Laboratories, 1996.