The Role of Activation Energy on the Formation and Stability of Gaseous Oblique Detonation Waves

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1 Introduction

In recent years, high efficiency propulsion systems have been sought for their use in the development of air-breathing hypersonic aircrafts [1]. The concept of oblique detonation waves has given rise to the development of Oblique Detonation Wave Engines (ODWE) and Ram Accelerators [2]. This class of propulsion systems not only has the advantages of the supersonic combustion ramjet (Scramjet), but also achieves a high thermal cycle efficiency through the detonation mode of combustion. The oblique detonation wave is induced by a wedge in an incoming reactive flow. An oblique shock wave (OSW) first forms upon the flow interaction with the wedge igniting the combustible flow mixture, and subsequently transits into an oblique detonation wave (ODW) [3]. Due to the strong coupling sensitivity between fluid dynamics and chemical reactions, as well as the inherent unstable nature of the detonation wave [4], it remains technically challenging to establish the steady oblique detonations in high-speed combustible mixtures for practical propulsion applications, and such success requires fundamental understanding of the oblique detonation structure and instability.

With the advance in scientific computing using parallel CPU and Graphics Processing Units GPU computing, there has been significant advance in investigating in detail the unsteady oblique detonation waves. Using high-resolution numerical simulations, various formation structures of wedge-induced oblique detonation waves, i.e., the transition from the oblique shock wave (OSW) to ODW, have been revealed in recent investigations e.g., [5-10]. Notably, the two key transition types are the abrupt transition from OSW to ODW where a nonreactive oblique shock, a set of deflagration waves, and the oblique detonation surface, all united on a multi-wave point, and the smooth transition characterized by a smooth curved shock. It is well established that both the physical flow conditions and chemical properties of the combustible mixture determine the possible transition type. Although qualitatively it is found that the smooth transition usually appears in the cases of high Mach number and weak chemical sensitivity with low activation energy of the reactive mixture, the quantitative conditions are yet to be fully determined.

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In this work, a parametric numerical study is presented to address the effect of chemical reaction sensitivity on the ODW initiation structure. Following previous studies, the ODW phenomena are simulated using an ideal reactive flow model given by the inviscid Euler equations with one-step irreversible Arrhenius reaction kinetics. In the one-step reaction kinetic model, the temperature sensitivity is controlled by the activation energy E_a. For a fundamental study, this idealized model is shown to provide crucial results elucidating the underlying physics of the ODW dynamics. Computations were carried out with a very wide range of dimensionless E_a from 20 to 60, three wedge angle values θ and different inflow Mach number M_0. It is worth noting that the high E_a regime considered in this work has not been explored thoroughly in any previous studies due to the numerical resolution requirement. A boundary separating the two aforementioned transition types is obtained and salient features resulted from the effect of high activation energy on the flow structure at the vicinity of the ODW initiation and the fully developed ODW unstable surface are discussed in detail.

2 Numerical Setup

The schematic shown in Fig. 1 describes details of the computational setup. The computational domain bounded by the dashed lines is rotated to the direction along the wedge surface. A supersonic flow with Mach number M_0 enters the domain from the left and reflects on the two-dimensional wedge with angle θ. An OSW is generated and triggers the chemical reaction. After an induction period, transition to the oblique detonation occurs. Neglecting the viscous and diffusion, effects which are shown to have little influence on the overall ODW structure [11], the governing equations for the ODW flow dynamics are simplified into the reactive Euler equations. The single-step irreversible chemical reaction with an Arrhenius rate law is used to model the chemistry in which the reaction sensitivity is controlled by E_a. All the flow variables have been made dimensionless by reference to the uniform unburned state ahead of the detonation front and the pre-exponential factor k in the single-step Arrhenius rate law is chosen to define the spatial and temporal scales, so the ZND half reaction zone length of the corresponding Chapman-Jouguet (CJ) detonation is unit. Following previous studies, e.g., [12-16], the normalized heat release Q is chosen as 50 and the isentropic exponent $\gamma = 1.2$. The solutions to this equation system are obtained numerically using a 2nd order MUSCL-Hancock scheme with a HLLC Riemann solver [17, 18], with a CFL number of 0.90. To accelerate the simulation run-time, the entire flow solver was implemented using NVIDIA CUDA programming language (NVIDIA Corp.) and run on a NVIDIA Tesla K40 graphics processing unit (GPGPU). The simulation code based on GPU computing platform is also used in [18-20]. Three different computational domains are used to adjust the computational cost (i.e., 80 x 30, 160 x 60 or 220 x 80) depending on the initial flow and mixture conditions. Three wedge angle values θ are considered in study, i.e., 26°, 28° and 30°.

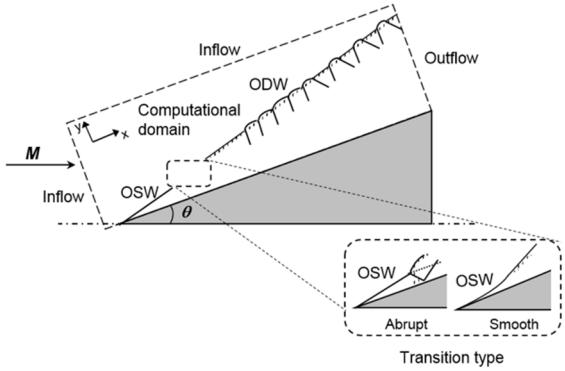

Figure 1. A schematic of the computational details and ODW phenomena

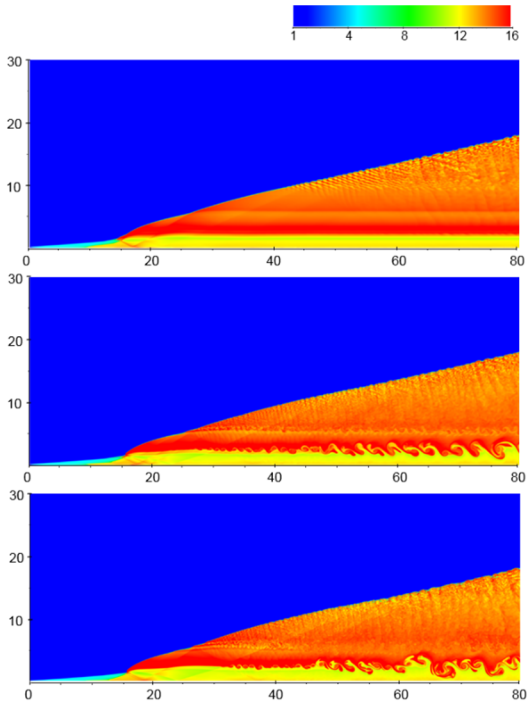

Figure 2. Temperature contours: 32 (upper), 64 (middle) and 128 (lower) pts/$l_{1/2}$ for M_0 = 12.5, E_a = 60 and θ = 26°

An important numerical issue we need to pay attention is that, in most of the former researches, a numerical resolution of 32 pts (or less) per half reaction zone length of a CJ ZND detonation $l_{1/2}$ is used in computations. However, when activation energy reaches a higher value, a much higher numerical resolution is required to achieve "converged" solutions [12, 13, 15]. Figure 2 shows the different temperature contours for the case of M_0 = 12.5, θ = 26° and high E_a = 60 with increasing grid resolution from 32, 64 to 128 pts per half reaction zone length $l_{1/2}$. It is clear that from Fig. 2 for E_a = 60, 32 pts/$l_{1/2}$ is not sufficient. The fore part of the unstable ODW structure and the Kelvin Helmholtz (K-H) vortex-rolling along the shear layer cannot be revealed. Only when the resolution is increased to 64 pts/$l_{1/2}$, the global features converge as those compared well with the results obtained using 128 pts/$l_{1/2}$. Taking this issue into account, the default resolution considered in this work is 64 pts per $l_{1/2}$ for E_a less than 30 and 128 pts per $l_{1/2}$ for higher E_a values.

3 Results and Discussion

Figure 3 shows the ODW formation structures obtained with θ = 26°, M_0 = 12.5 and 10, and E_a = 30. Consistent with the finding in [6, 10, 14], the transition is characterized by a smooth curved shock at M_0 = 12.5, while at low M_0 the transition is given by the classical abrupt structure. For the case with M_0 = 10, the multi-wave points connecting the deflagration wave, induction OSW, ODW and transverse compression waves can be clearly seen. A slip line extending downstream from the abrupt point can also be observed. Equivalently, Fig. 4 elucidates the two types of transitions with a fixed inflow M_0 = 10 and θ = 26° but with varying activation energy E_a from 20 to 30. Clearly, these results demonstrates that not only the inflow condition controls the transition process, the chemical sensitivity is another dominant parameter governing the initiation evolution. The smooth transition can be achieved only by a mixture with very low temperature sensitivity or small E_a.

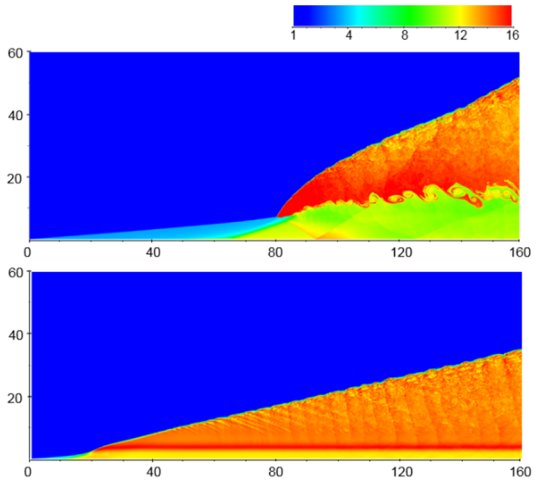

Figure 3. Temperature contours with $E_a = 35$ and $\theta = 26°$ for $M_0 = 10$ (upper) and $M_0 = 12.5$ (lower)

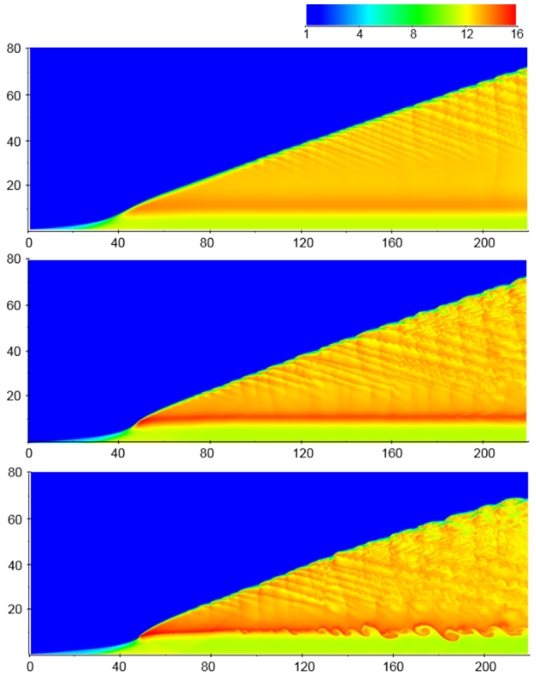

Figure 4. Temperature contours with $M_0 = 10$ and $\theta = 26°$ for $E_a = 20$ (upper) 24 (middle) and 30 (lower)

By carrying a parametric study boundary curves in $E_{a,cr}$–M_0 space distinguishing the two types of OSW-ODW transition for different wedge angles θ are obtained, see Fig. 5. For all θ a nearly linear relationship in most part between M_0 and the corresponding critical transition $E_{a,\,cr}$ is achieved. Only at high M_0 regime the curve for the high wedge angle $\theta = 30°$ begins to deviate. It can be observed from this plot that at low M_0 regime, all three curves collapse, i.e., the critical $E_{a,cr}$ for the transition is independent of the wedge angle. In other words, the chemical kinetics is thus the controlling factor on the transition pattern of the ODW. Only when M_0 increases to very high value, the boundary curves for the three wedge angles deviate from each other. This can be explained by the fact that at high M_0 regime, the resulting overdrive effect by the presence of the wedge with higher angle θ becomes the controlling factor on the transition type.

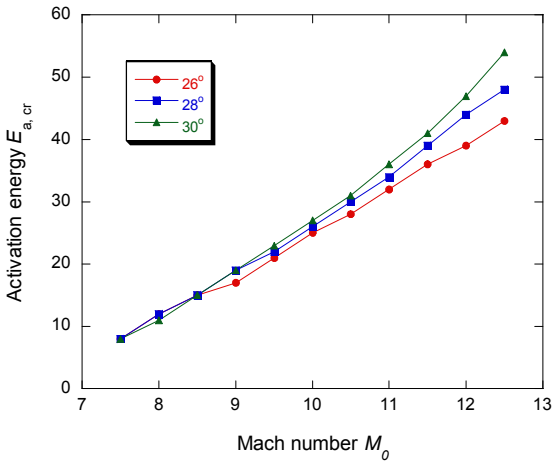

Figure 5. The conditions for smooth and abrupt transitions below and above the boundary respectively in the E_a–M_0 plane for three different wedge angles θ

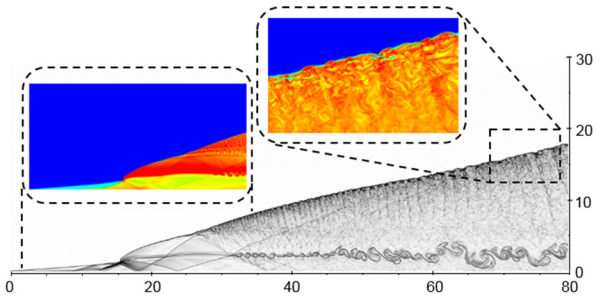

Figure 6. Schlieren and temperature contour (sub-plot) with 128 pts/$l_{1/2}$ for M_0 = 12.5, E_a = 60 and θ = 26°

The focus of previous studies on the high Mach number regime considers mostly moderately low E_a. In fact, by increasing E_a further at the high M_0 regime, besides the ODW flow field becomes more unstable, interesting complex features arise. Figure 6 shows the results obtained for θ = 26° and M_0 = 12.5 with a large activation energy E_a = 60, under which the transition is given by the abrupt type. At high E_a limit, more unstable characteristics begin to appear on the downstream fully-developed ODW surface. The increase of E_a makes the ODW cellular surface more irregular. For high E_a, the slip line also becomes unstable and the classical roll-up behavior of the K-H instability in the detonation product becomes more apparent. Similar to normal cellular detonation [21], for high E_a, the ODW cellular surface also becomes highly irregular with unburned pockets behind the leading ODW front [15, 22]. Another key feature is revealed near the initiation region. It is shown that the transverse compression wave resulted from the initiation point and reflected between the wall and the slip line become stronger as E_a increases. The reflected compression wave from the wall further adjusts the gas parameters of the combustion products and penetrates the slip line and influence the initially smooth ODW surface. The result of this interaction is the formation of another multi-wave points similar to the first initiation point. A second slip line, although faint, can be seen downstream, which eventually becomes unstable far downstream within the combustion product due to the K-H instability. At E_a = 60, this second multi-wave point appears to be close to the first appearance of transverse waves after another segment of smooth ODW from the main initiation location.

4 Concluding Remarks

In summary, this work investigates using high resolution numerical simulations the effects of activation energy over a large condition range on the ODW initiation and provides quantitatively critical conditions distinguishing the two known ODW formation types in the M_0-E_a plane. Interesting flow features are clearly revealed at the high activation energy limit including the presence of second multi-wave point and the apparent rolled-up vortex instabilities in the combustion product along each slip line extending downstream from the multi-wave points near the initiation region.

Acknowledgement

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