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Numerical study of oblique detonation initiations with chain branching kinetics

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Oblique detonations induced by semi-infinite wedge are simulated by solving Euler equations with chain branching kinetics. Numerical results show the initiation can be triggered by either the abrupt transition or smooth transition, dependent on incident Ma M_{in} and wedge angle θ, and then their effects on the oblique detonation angle β and initiation length L_{ini} are analyzed. When θ increases, L_{ini} decreases monotonically but β has a minimum value, corresponding to θ = 29 ° in this study. When M_{in} decreases, both L_{ini} and β increases monotonically until M_{in} decreases below certain critical value, M_{in} = 9.2 in this study. Then low inflow Ma effects generate the maximum L_{ini}, with the complex of ODW (oblique detonation wave), SODW (secondary oblique detonation wave) and SIDW (self-ignition deflagration wave). The transient process is observed, demonstrating the structure can self-adjust to find a proper position. The wave structure suggests two wave/heat release process determining the detonation initiation. In the cases with high M_{in} featured by SIDW, the oblique-shock induced self-ignition dominates, and L_{ini} increases when M_{in} decreases. In the cases with low M_{in} featured by SODW, the interaction of ODW and SODW dominates, and L_{ini} decreases when M_{in} decreases.

Nomenclature

e	=	total energy
E_I	=	activation energy of the induction zone
E_R	=	activation energy of the heat release process
k_I	=	reaction rate constant of the induction zone
k_R	=	reaction rate constant of the heat release process
L_{ini}	=	initiation length
M_{in}	=	incident Mach number
p	=	pressure
Q	=	heat release of chemical reaction
T_s	=	post-shock temperature
u	=	velocity in the x- direction
v	=	velocity in the y- direction
β	=	oblique detonation angle
γ	=	ratio of specific heats
ξ	=	induction reaction index
θ	=	wedge angle
λ	=	heat release index
ρ	=	density

I. Introduction

GASEOUS detonations, featured by its pressure gain combustion, attract more and more attention in high speed air breathing propulsion.[1,2] One of the propulsion systems uses oblique detonation wave, including oblique

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detonation wave (ODW) engines and ram accelerators. Because it is difficult to initiate the oblique detonation fixed in hypersonic combustible flow, further research on oblique detonation is necessary in the propulsion engineering.

Oblique detonations can be triggered by many ways, but the ideal way, which brings less total pressure loss, is by wedge-induced oblique shock. In the literature a wealth of research studies on oblique detonations can be found. For instance, Li et al.[3] revealed that the multi-dimensional oblique detonation structure consists of a non-reactive oblique shock, an induction region, a set of deflagration waves, and an oblique detonation surface. The instability of oblique detonation surface has been studied widely, demonstrating the cellular structure formation and evolution [4,5,6,7]. Another research direction is the oblique shock-to-detonation transition, which can be viewed as the initiation process of oblique detonation. Vlasenko & Sabelnikov [8] showed that the shock-to-detonation transition may occur smoothly by curved shock rather than by one multi-wave point. A number of parametric studies were carried out numerically to investigate the dependence of the transition type on various initial conditions and flow parameters such as the incoming flow Mach number, wedge angle and the reactivity of the mixture [9,10]. Besides the transition type, the wave structures near the transition region have been simulated, and several kinds of shock systems are observed[11,12,13]. These structures are found to become complicated when the incident Ma decreases, but it is still lack of theory to predict its formation and characteristic length scale.

The ODW formation is simulated with chain branching kinetics, focusing on the initiation mechanism influenced by the inflow Ma. To study the initiation, one-step irreversible heat release model used in previous studies[14,15,16] is over-simplified because it can't model the induction zone. Some studies[11,17] use the detailed chemical kinetics, which are much expensive. Multi-step chain branching kinetics has been proposed, inheriting the simplicity of global kinetics but enough to model the initiation, and used in the detonation instability research[18,19,20]. In this study, this kinetics is used to simulate the ODW. Parametric study on the detonation oblique angle and initiation length is performed, and two initiation mechanisms related with the inflow Ma are discussed.

II. Numerical model and methods

A typical ODW induced by a wedge in a combustible gas mixture is shown schematically in Fig. 1. The presence of a wedge in supersonic inflow induces first an oblique shock wave (OSW). For a high inflow Mach number causing a high post-shock temperature behind the OSW, an exothermic chemical reaction begins, leading to the ODW formation. For the computation, the coordinate is rotated to the direction along the wedge surface. Hence, the Cartesian grid in the rectangular domain enclosed by the dashed line is aligned with the wedge surface, like our previous studies[6,7].

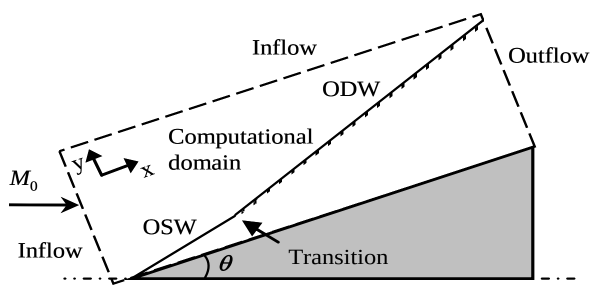

Figure 1. Schematic of a typical oblique detonation wave.

Similar to most previous studies, Euler equations are used as governing equations. Two additional reaction indexes are introduced, one is the induction reaction index ξ, and the other is the heat release index λ. For the new variables, the equations are

$$\frac{\partial\rho\xi}{\partial t}+\frac{\partial(\rho u\xi)}{\partial x}+\frac{\partial(\rho v\xi)}{\partial y}=H(1-\xi)\rho k_I\exp[E_I(\frac{1}{T_S}-\frac{1}{T})]. \quad (1)$$

$$\frac{\partial\rho\lambda}{\partial t}+\frac{\partial(\rho u\lambda)}{\partial x}+\frac{\partial(\rho v\lambda)}{\partial y}=[1-H(1-\xi)]\rho(1-\lambda)k_R\exp[-\frac{E_R}{T}]. \quad (2)$$

with the Heaviside step function

$$H(1-\xi)=\begin{cases}1, & \text{if } \xi\le 1\\ 0, & \text{if } \xi>1\end{cases}. \quad (3)$$

Then the equation of state is changed to be

$$e = \frac{p}{\rho(\gamma - 1)} + \frac{1}{2}\left(u^2 + v^2\right) - \lambda Q. \tag{4}$$

In this study, the main parameters are set to be Q = 50, γ = 1.2, $E_I = 8.0T_s$, $E_R = 1.0T_s$, where T_s is post-shock temperature. The bifurcation parameter used in previous study k_R, which controls the heat release rate, is fixed to be 0.95 in all cases. This set of parameters corresponds to the stable 1D detonation and more details are available in reference[21]. Dispersion Controlled Dissipation (DCD) scheme[22] and 3nd order Runge-Kutta algorithm are used in this study.

III. Numerical results and discussion

A. Resolution study

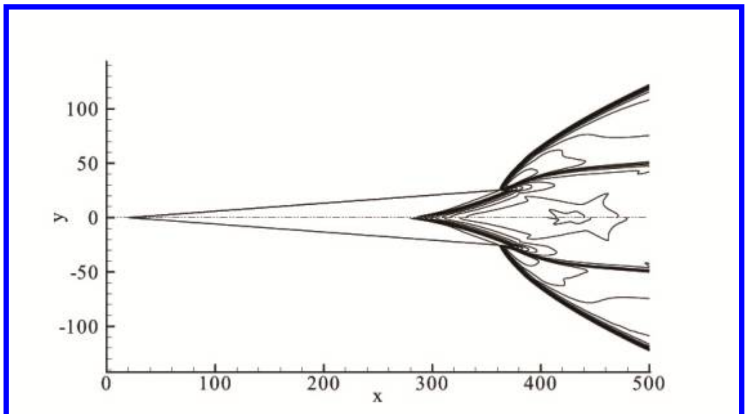

Figure 2. Temperature of oblique detonation with θ = 26 ° and M_{in} = 10, grid scale 0.2 (upper) and 0.4 (lower).

Resolution study is performed in the case of wedge angle θ = 26 °and incident Ma M_{in} = 10, as shown in Fig. 2. The wedge starts from x = 20, from where the oblique shock is initiated. The upper half shows the results from the grid scale 0.2, while the lower half shows the results from the grid scale 0.4. It can be observed that the oblique shock-to-detonation transition forms around x = 370 in both simulations, whose difference is hard to observed. Actually the region beneath the oblique shock can be viewed as the induction zone, which is terminated by the obvious heat release after x = 300. Due to the enlarged induction region, it is not surprised that the oblique initiation needs less grid per unit length scale. Generally, the grid scale 0.4 is enough to simulate the oblique detonation structure, and used in the later study.

B. Parametric study on detonation structures

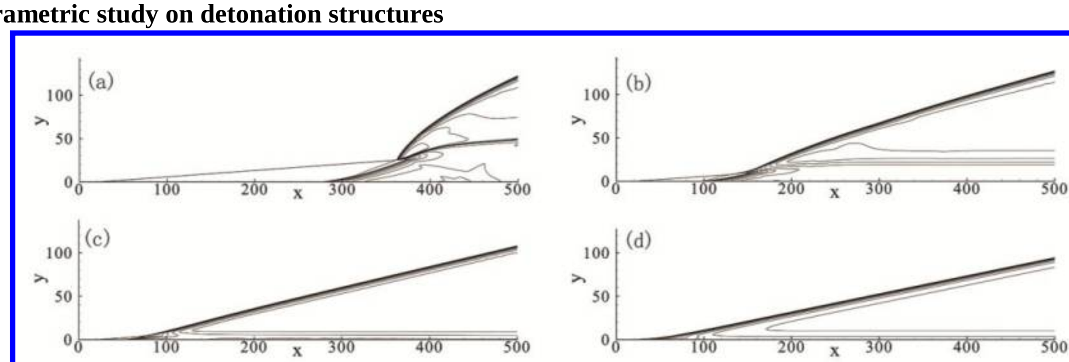

Figure 3. Temperature of oblique detonations with θ = 26 °and M_{in} = 10(a), 11(b), 12(c), 13(d).

Detonation structures influenced by both incident Ma M_{in} and wedge angle θ, are simulated and shown in Fig. 3 and 4. It can be observed that the oblique shock-to-detonation transition moves upstream when increasing M_{in} or θ, illustrating the detonation initiates is easy to be triggered. This is physically reasonable because of high post-shock temperature derived from increasing M_{in} or θ. Furthermore, it can be observed that the transition type of shock-to-detonation changes, from the abrupt transition to the smooth transition by the curved shock, which is accordant with previous study qualitatively[10].

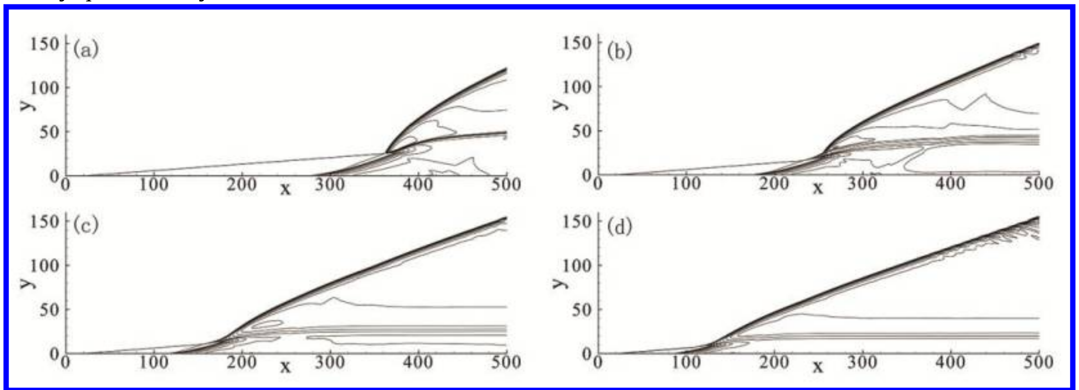

Figure 4. Temperature of oblique detonations with M_{in} = 10 and θ = 26°(a), 27°(b), 28°(c), and 29°(d).

In the engineering, the length of initiation region and oblique detonation angle are important parameters for ODW design. Therefore, we perform the parametric study of the initiation length L_{ini} and oblique detonation angle β as function of M_{in} and θ. L_{ini} is defined from the wedge tip to the starting point of oblique detonation surface along the x-axis, and θ is measured on the detonation surface excluding the initiation region with curved shock. Figure 5 shows L_{ini} and β with difference M_{in}, and Fig. 6 shows L_{ini} and β with difference θ. When M_{in} increases, both L_{ini} and β decrease monotonically, while when θ increases, only L_{ini} decreases monotonically. As shown in Fig. 6, β-θ has a minimum value and increases slightly when θ increases above 29°. Although β-θ increases weakly, the β increase will be pronounced considering the θ change. The formation of the minimum β demonstrates that the dependence of β on θ is complicated, deserving more attention in the further study.

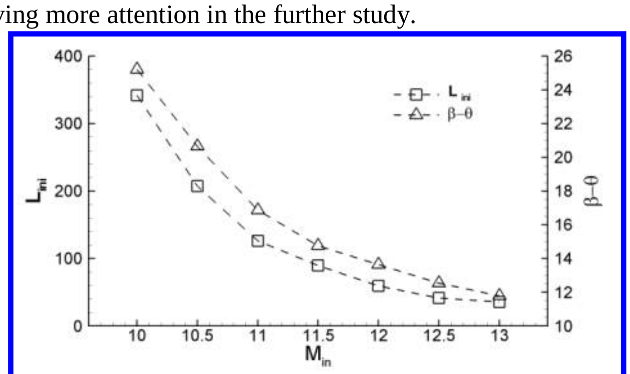

Figure 5. Variation of L_{ini} and β-θ as function M_{in}.

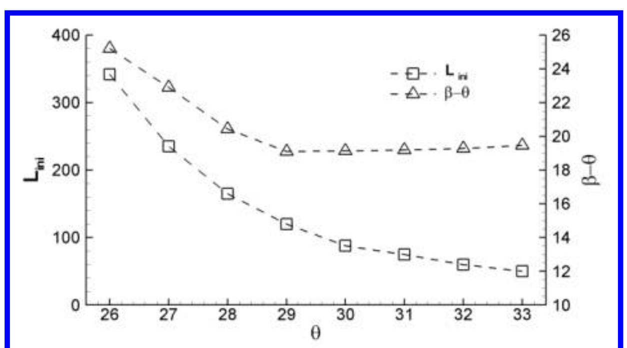

Figure 6. Variation of L_{ini} and β-θ as function of θ.

C. Discussion on low M_{in} phenomena

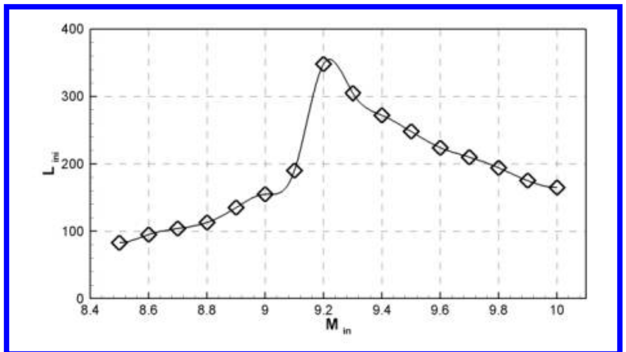

Figure 7. Variation of L_{ini} as function of M_{in} with θ = 28 °.

Previous study has demonstrated that the structures near the initiation region become more complicated when the incident Ma decreases, called low M_{in} effects. These effects are crucial in the ODWE design, for it's the scientific basis to decide the low flight Ma limit of engines. To study the low M_{in} phenomena, numerical simulations are performed with θ = 28 °, whose L_{ini} as function of M_{in} is shown in Fig. 7. Clearly, L_{ini} increases when M_{in} decreases until the critical value M_{in} = 9.2, below which L_{ini} decreases when M_{in} decreases further. The phenomenon above M_{in} 9.2 is similar to that shown in Fig. 3 and 5, but there exists the different dependence of L_{ini} on M_{in}. This generates the maximum initiation length around M_{in} = 9.2, which can be observed in Fig. 7.

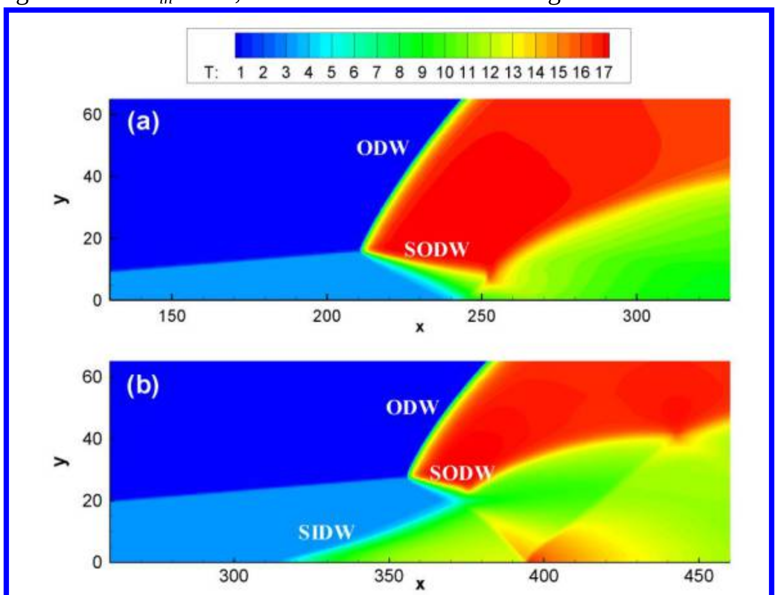

Figure 8. Temperature of oblique detonations with θ = 28 °, M_{in} = 9.1(a) and 9.2(b).

The wave structures around the initiation regions in the case of M_{in} 9.1 and 9.2 are shown in Fig. 8. In the case of M_{in} = 9.1, the flow fields are different from those shown above. Besides the main ODW surface, the second oblique detonation wave (SODW) appears in the shocked gas, with a regular reflection on the wedge. Similar structure has been observed except with the Mach reflection of SODW on the wedge [11,13]. Increasing M_{in} into 9.2, one more complicated structure form as shown in Fig. 8b. There are not only the ODW and SODW, but also the self-ignition deflagration wave (SIDW). Actually, this structure can be viewed as the combination of classical structure shown in Fig. 3 and 5, and the low M_{in} structure shown in Fig. 8a.

Furthermore, the low M_{in} effects also induce the transient process shown in Fig. 9. The simulation starts with uniform flow field, and soon the oblique shock and detonation form. The detonation initiates downstream first and then move upstream. The black contours show the extreme upstream position, and then the structure turn around to move downstream at time 1210 μs. Before reaching the final position shown by pink contours, the structure moves over it from upstream to downstream first, reaching the extreme position at time 1500 μs shown by red contours, and then from downstream to upstream, reaching the extreme position at time 1870 μs shown by blue contours. It can also be seen the movement speed is very slow at the final stage. The movement demonstrates the structure can self-adjust to find a proper position, which is dependent on the interaction of ODW and SODW.

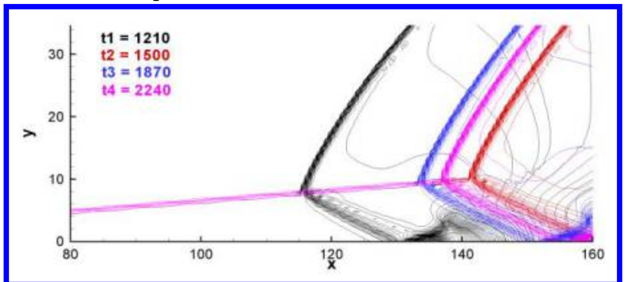

Figure 9. Transient process of the shock-to-detonation transition region.

The structure evolution influenced by low M_{in} effects has been observed before, but the mechanism of several complicated structures has not been discussed deeply. Usually the SODW has the Mach reflection on the wedge, generating the so called "Y" bifurcation shock [11,12]. Its interaction will induce the Mach stem between the SODW and SIDW, bringing several wave configurations hard to be analyzed. In this study, the SODW bends downstream significantly, benefiting from the high heat release and then relatively high M_{in}. Then the interaction of SODW and SIDW can be observed clearly, as shown in Fig. 8, to distinguish the wave origin. The complex of ODW, SODW ad SIDW is hard to be observed because it only exists with certain critical M_{in}, demonstrating the transition of two different structures in the initiation regions. Actually it suggests two wave/heat release process deciding the structure of initiation region, one is the oblique-shock induced self-ignition, and the other is the interaction of ODW and SODW. In the case of high M_{in}, the oblique-shock induced self-ignition dominates, generating the SIDW first and then triggers the detonation, whose initiation moves downstream when M_{in} decreases. While in the low M_{in} cases, the interaction of ODW and SODW determines the balance initiation position, which moves upstream when M_{in} decreases, and vice versa.

IV. Conlcusion

Oblique detonations induced by semi-infinite wedge are simulated by solving Euler equations with chain branching kinetics. Numerical results show the initiation can be triggered by either the abrupt transition or smooth transition, dependent on M_{in} and θ, and then their effects on β and L_{ini} are analyzed. When θ increases, L_{ini} decreases monotonically but β has a minimum value, corresponding to $\theta = 29°$ in this study. When M_{in} decreases, both L_{ini} and β increases monotonically until M_{in} decreases below certain critical value, $M_{in} = 9.2$ in this study. Then low inflow Ma effects generate the maximum L_{ini}, with the complex of ODW, SODW and SIDW. The transient process is observed, demonstrating the structure can self-adjust to find a proper position. The wave structure suggests two wave/heat release process determining the detonation initiation. In the cases with high M_{in} featured by SIDW, the oblique-shock induced self-ignition dominates, and L_{ini} increases when M_{in} decreases. In the cases with low M_{in} featured by SODW, the interaction of ODW and SODW dominates, and L_{ini} decreases when M_{in} decreases.

Acknowledgments

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