Initiation characteristics of wedge-induced oblique detonation waves in a H2-O2 mixtures with Ar dilution

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1 Introduction

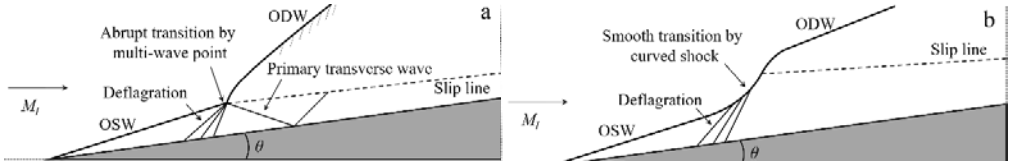

Fig. 1 Sketch of ODW structures, abrupt transition (a) and smooth transition (b).

The oblique detonation engine [1], also called shock-induced combustion ramjet, is one kind of propulsion devices based on oblique detonation wave (ODW). In early researches [2], both abrupt and smooth transition structures has been found, as shown in Fig. 1. One is referred to as the abrupt transition, featured by a multi-wave point, and the other is the smooth transition featured by the curved shock. Detailed chemical reaction models are beneficial for the study of different fuels. Recently, several numerical studies are performed using detailed chemistry to look at the effects of initiation mechanism [3], and illustrate the ODW characteristics in hydrogen-air, i.e., H2-O2-N2, mixtures.

In this study, H2-O2 mixtures with Ar dilution are used to study the ODW structure. The present numerical results reveal that the ODW structures in H2-O2-Ar mixtures are sensitive to inflow static pressure, different those in H2-O2-N2 mixtures and never been reported before. Based on serial simulations, the ratio of induction and heat release zone lengths is proposed to model the difference, and how different dilution gases influence the ODW structures are discussed.

2 Physical and mathematical models

Following our previous studies, e.g., [3,6], a schematic of typical ODWs induced by a two-dimensional, semi-infinite wedge is given in Fig. 2. The coordinate is rotated to the direction along the wedge surface

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and the Cartesian grid in the rectangular domain enclosed by the dashed line in Fig. 2 is aligned with the wedge surface.

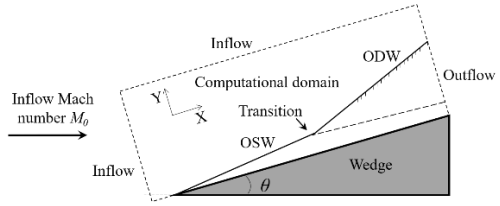

Fig. 2 Sketch of wedge-induced oblique detonation simulation

Neglecting the viscosity and diffusion effects, the governing equations are the unsteady reactive Euler equations, i.e.:

$$\frac{\partial \mathbf{U}}{\partial t}+\frac{\partial \mathbf{F}}{\partial x}+\frac{\partial \mathbf{G}}{\partial y}=\mathbf{S} \tag{1}$$

where:

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

The total density and total energy are calculated by:

$$\rho=\sum_{i=1}^{n}\rho_i,\ e=\rho h-p+\frac{1}{2}\rho\left(u^2+v^2\right) \tag{3}$$

The chemical kinetic model used in this study is taken from a comprehensive H2/O2 kinetic model for high pressure combustion [4]. This mechanism involves 27 reversible, elementary reactions among the 8 species H2, O2, H2O, H, O, OH, HO2, and H2O2, with 5 inert species, N2, Ar, He, CO, and CO2. Thermodynamic properties of the chemical species are evaluated from the 9-coefficient NASA polynomial representation. The governing equations are discretized on Cartesian uniform grids and solved with the DCD scheme with Strang's splitting.

Unless specified, 2H2+O2+7Ar is used as the default stoichiometric mixture with wedge angle 25º. In this study, the inflow temperature is 298.15 K for all cases, while inflow static pressure P_0 varies below 1 atm as an important parameter. 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. On the lower computational boundary, the wedge starts from x = 0.512 mm. Initially, the entire flow fields are uniform, and the simulation does not stop until the flow fields reach the steady state. Due to the multi-scale nature of the phenomena, the computational domain and mesh scale are each adjusted from 4 μ m to 128 μ m.

3 Numerical results and discussion

3.1 Effects of Mach number M0 on the ODW structure

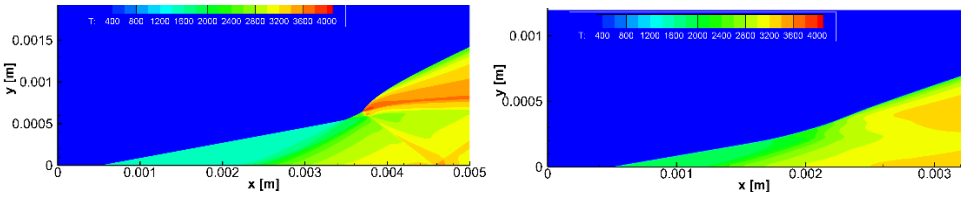

Fig. 3 Temperature fields in the cases of M_0 =7.0 (a), 8.0 (b), P_0 = 1.0 atm

As shown in Fig. 3. Results show that wave structures are sensitive to M_0, and the initiation length changes significantly. By increasing M_0, the structure changes from abrupt transition of Figs. 3a, into smooth transition of Figs. 3b. These results are the same qualitatively as those in previous studies [3], despite of different chemical reaction models used among those.

3.2 Effects of P_0 on the ODW structure

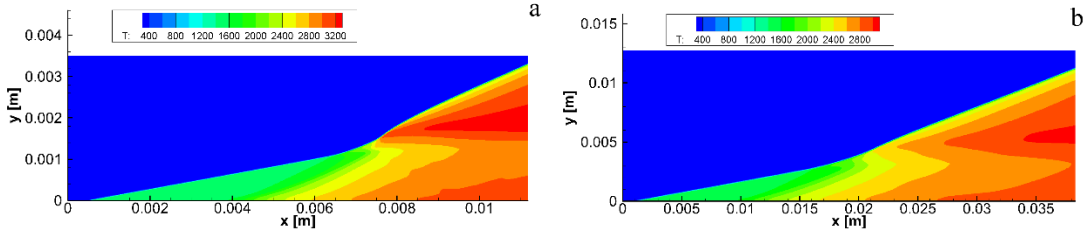

Fig. 4 Temperature fields in the cases of M_0 = 7.0, left: P_0 = 0.5 atm and right: P_0=0.2 atm

As shown in Fig. 4, it is observed that the wave structures are also sensitive to P_0, similar to the effects of M_0. With relatively high P_0, the structure tends to be an abrupt transition, and decreasing P_0 results into a smooth transition. The smooth structure is simpler than the abrupt structure, lack of the secondary oblique shock and contact surface. Generally, effects of decreasing P_0 are similar to effects of increasing M_0, so the results of Fig. 3d and Fig. 4b are comparable, although the initiation length of Fig. 4b is about ten times of the initiation length of Fig. 3c.

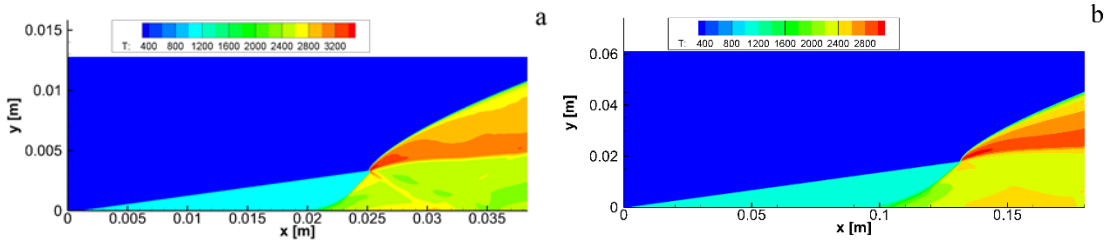

Fig. 5 Temperature fields in the cases of M_0 = 7.0, Left: P_0 = 1.0 atm and right: P_0=0.2 atm in the mixtures of 2H2+O2+7N2

Although P_0 is found to be an important parameter in the ODW formation, most of the previous studies only concern the effects of M_0. Our recent study [3] addressed effects of P_0 in stoichiometric H_2-Air mixtures, concluding that those structures are not sensitive to P_0, different from the present results of Fig. 5. Considering both studies uses the same set of codes, including the same shock-capturing scheme and detailed chemistry model [4], the difference should be derived from the combustion characteristics of mixtures. It is noted that previous study [3] uses the mixture of $2H_2+O_2+3.76N_2$, so additional simulations are performed with the mixtures of $2H_2+O_2+7N_2$ to confirm and exclude possibly the effects of N_2 dilution ratio. As shown in Fig. 5, clearly, the structures change only a little and are not sensitive to P_0, demonstrating the abrupt structures with similar wave configurations. In other words, the structure is sensitive to P_0 in H_2-O_2-Ar mixtures, but not sensitive in H_2-O_2-N_2 mixtures.

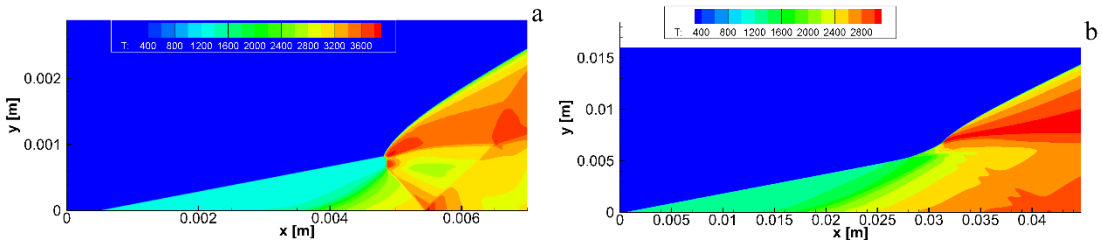

Fig. 6 Temperature fields in the cases of M_0 = 6.5, P_0 = 1.0 atm (a) and 0.2 atm (b)

As shown in Fig. 6. The structures may be abrupt or smooth in the cases of M_0 = 6.5, depending on P_0, similar to those in the cases of M_0 = 7.0. Similar phenomena can be observed in in the cases of M_0 = 7.5. Therefore, it appears that the structure sensitivity to P_0 is a universal phenomenon in H_2-O_2-Ar mixtures regardless of M_0.

3.3 Analysis on the structure characteristics

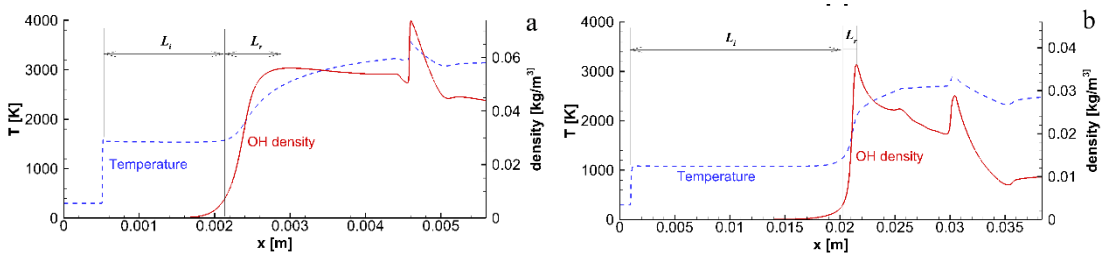

Fig. 8 Temperature and Oh density profiles along the wedge in the case of M_0 = 7, P_0 = 1.0 atm, 2H2+O2+7Ar (a) and 2H2+O2+7N2 (b)

To explain above phenomena, two characteristic lengths, L_i and L_r, are defined as the induction zone length and heat release zone length. As shown in Fig. 8, OH density curves are used to define L_i and L_r. The former starts from the shock, and ends when obvious OH density variation is observed. Compared with temperature curve, the position is chosen at where 15% of the maximum OH density is achieved. This is also the starting point of the heat release zone, which ends at the location of 95% of the maximum OH density. It should be noted that the criteria of the length definitions, 15% and 95%, are not universal and other close values can be used. At such, the detailed values shown in Table 2 may vary, but the conclusions should remain the same. Numerical results illustrate that with the same M_0 and P_0, e.g., M_0 = 7, P_0 = 1.0 atm, the heat release processes are different significantly in H_2-O_2-Ar and H_2-O_2-N_2 mixtures. The former mixture results into higher post-

oblique shock temperature, so the heat release process is easy to start but modest. Contrarily, the heat release is hard to start but with a sharp profile in H_2-O_2-N_2 mixtures. Table 1 shows the length ratio R_L, defined by L_i/L_r, as a function of M_0 and P_0 in both mixtures. ODWs in H_2-O_2-Ar mixtures have small R_L, while in H_2-O_2- N_2 mixtures have large R_L. Therefore, R_L provides a good criterion to determine whether the structures of ODW are sensitive to P_0.

Table 1 R_L with different mixtures and M_0

P_0 (atm)	M_0 = 6.5		M_0 = 7.0		M_0 = 7.5	
	7Ar	7N_2	7Ar	7N_2	7Ar	7N_2
1.0	4.76	53.3	3.49	24.4	3.17	17.1
0.8	3.86	43.3	3.33	22.4	2.75	14.1
0.6	3.31	42.7	2.55	22.2	2.13	12.5
0.4	2.41	38.9	1.96	20.4	1.57	11.4
0.2	1.41	28.7	1.22	15.0	1.06	8.16

Before analyzing why R_L varies so significantly, it should be noted that a similar parameter χ has been proposed to quantify the sensitivity of normal detonations [5]. That study revealed that unstable detonations with irregular oscillation patterns and cellular structures generally have large χ values. Because the effects of activation energy have been considered there, the parameters R_L and χ cannot be compared directly. Drawing from the previous study [5], normal detonations with high R_L should be more unstable with irregular cellular structures and vice versa. That finding seems incongruent with the present study because ODW structures with high R_L seem more stable. The discrepancy is attributable to different definitions of sensitivity and the role of the induction zone. For normal detonations, the relatively long induction zone and correspondingly high R_L favor the amplification of a disturbance and result in strong sensitivity. For oblique detonations, the long induction zone is the post-oblique shock region in which the flow is supersonic. High R_L indicates that the induction is much longer than the heat release zone, so difficult to change via heat release processes. This induces stable structures independent of P_0. Therefore, this study on steady, oblique detonations does not oppose the previous study on unsteady, normal detonations [5].

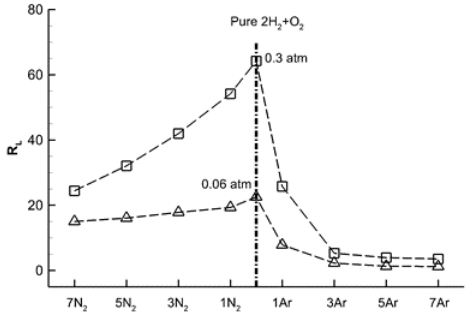

Fig. 9 RL with different dilution ratio of Ar and N2 dilution, keeping same amount of 2H2+O2

Following the idea of keeping the same amount of 2H2+O2, more cases were simulated with different dilution ratios (i.e., 10%, 30%, and 50%) in both mixtures. Fig. 9 displays the length ratio R_L variation, whose maximum values appear in cases of no dilution. On the left branch, increasing N2 dilution causes R_L

to decline, which occurs more quickly in cases of high pressure. On the right branch, RL declines with increasing Ar dilution, showing an exponential-like profile. R_L first declines rapidly from 0 Ar to 3 Ar and then approaches a constant asymptotically

L_r changes a little, and the dominant variation of R_L should be attributed to the change of L_i. These results demonstrate how the type and amount of dilution gas change the combustion process of ODWs. Regarding the effects of dilution gas, two patterns are expected: accelerating chemical reactions through the third-body effects and changing the mixture properties. Due to third body effects, L_i and L_r each decline but L_i varies more substantially regardless of the dilution gas, so that R_L declines when the dilution gas increases. However, different properties of dilution gas play important roles on the right branch (when including Ar). As a single-atom gas with a molecular weight of 40, Ar is not similar to O2 as is N2. The inclusion of Ar changes the mixture properties, such as the average molecular weight and specific heat capacity ratio, so a rapid decline in R_L appears on the right branch. For cases with more than 3 Ar, the effects of adding more dilution are weaker, and R_L hence approaches a constant.

4 Concluding remarks

Two types of combustible mixtures, H_2-O_2-Ar and H_2-O_2-N_2, are widely used in detonation research, but only the latter is studied in the oblique detonation wave (ODW) studies before. This study addresses ODWs in H_2-O_2-Ar, demonstrating some special characteristics which have never elucidated before. Similar to the ODWs in H_2-O_2-N_2 mixtures, the structures vary with different M_0. However, it is found that the structures are also sensitive to P_0 in $2H_2$+O_2+7Ar mixtures. Based on the analysis of the flow fields, the ratio of induction and heat release zone lengths, R_L, is proposed to model the difference induced by the dilution gas. Generally, R_L is found to be large in N_2 diluted mixtures, while small in Ar diluted mixtures. The variation rule of R_L is analyzed, demonstrating how different dilution gases determine the ODW structures.

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