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ORIGINAL ARTICLE

On the influence of low initial pressure and detonation stochastic nature on Mach reflection of gaseous detonation waves

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Abstract The two-dimensional, time-dependent and reactive Navier–Stokes equations were solved to obtain an insight into Mach reflection of gaseous detonation in a stoichiometric hydrogen-oxygen mixture diluted by 25 % argon. This mixture generates a mode-7 detonation wave under an initial pressure of 8.00 kPa. Chemical kinetics was simulated by an eight-species, forty-eight-reaction mechanism. It was found that a Mach reflection mode always occurs for a planar detonation wave or planar air shock wave sweeping over wedges with apex angles ranging from 5° to 50°. However, for cellular detonation waves, regular reflection always occurs first, which then transforms into Mach reflection. This phenomenon is more evident for detonations ignited under low initial pressure. Low initial pressure may lead to a curved wave front, that determines the reflection mode. The stochastic nature of boundary shape and transition distance, during deflagration-to-detonation transition, leads to relative disorder of detonation cell location and cell shape. Consequently, when a detonation wave hits the wedge apex, there appears a stochastic variation of triple point origin and variation of the angle between the triple point trajectory and the wedge surface. As the wedge apex angle increases, the distance between the triple point trajectory origin and the wedge apex increases, and the angle between the triple point trajectory and the wedge surface decreases exponentially.

Keywords Gaseous detonation wave · Mach reflection · Regular reflection · Transverse wave · Detailed chemical reaction model · Numerical simulation

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1 Introduction

Detonation is a complex phenomenon occurring in nature. It involves a supersonic precursor shock front followed by a reaction zone. When it interacts with a wedge, wedge geometry affects the leading shock strength, as well as the temperature and chemical reaction rates behind it. This leads to the occurrence of either regular reflection or Mach reflection. The reflection mode is determined mainly by the angle between the detonation wave front and the wedge surface (DW-angle). For a planar detonation wave, regular reflection occurs when DW-angle is less than the Mach reflection critical angle, Ω. Otherwise, Mach reflection occurs.

Mach reflection of gaseous detonation on a wedge is an important and fundamental topic. At the same time it is also a challenging aspect of such practical problems as the development of pulse detonation engines and explosion hazards in gas fuel pipelines. There is a large amount of literature focusing on this topic. Gvozdeva and Predvoditeleva [1] and Edwards et al. [2] reported that Mach reflection, as well as regular reflection, was observed in detonation phenomena. Zhang et al. [3] performed large-scale experiments of detonation reflection in acetylene–air mixtures, and observed transition from regular reflection to Mach reflection. Alkbar [4] employed laser photography to visualize the propagation of gaseous detonation waves on a wedge surface. It was found that detonation Mach reflection is self-similar and the angle between the triple point trajectory and the wedge surface is consistent with theoretical predictions. Ohyagi et al. [5] simulated detonation reflection for wedges with different wedge angles, using the Euler equations and a two-step induction parameter model. They concluded that the triple point trajectory is not a straight line but curves in space. Interaction between the transverse waves and the wedge surface determines the sizes and shapes of cells behind the detonation wave in the Mach stem region. Guo et al. [6] provided smoked foil experiment and cellular pattern proof that the triple point trajectory is not a straight line. They also concluded that the angle between the triple point trajectory and the wedge (TW-angle) is determined mainly by wedge angle and less by initial pressure. Zhang et al. [7] also used a two-step reaction model to simulate detonation Mach reflection. Trotsyuk et al. [8,9], using a high-order MUSCL scheme, demonstrated non-self-similarity of multifront CJ and overdriven detonation reflection from wedges with different angles, and studied carefully the effect of computational grid size, H_2–O_2 mixture reactivity and local perturbation on simulation results. Hu and Jiang [10] simulated wave dynamic processes in cellular detonation reflection from a wedge by employing the Euler equations and a detailed chemical reaction model. It has been found that transverse waves determine the cell size in the region swept by the Mach stem. Moreover, detonation self-similarity fails when the cell width is comparable to or larger than the Mach stem length.

Many studies have contributed to detonative Mach reflection; however, there are still some unanswered questions and unsolved problems. For example, it is well known that, due to the nonlinear dependence of chemical reactions on temperature, the detonation wave is both spatially and temporally unstable so that the detonation wave front develops a complicated three-dimensional time-dependent structure. The incident shock is wrinkled, consisting of alternative weaker shock and stronger shock (Mach stem) portions, joined at triple point by a reflected (transverse) wave. For a detonation wave ignited under a high initial pressure, the non-planar nature of its incident shock is not as prominent, so it can be regarded approximately as a planar wave. But for a detonation wave ignited under low initial pressure, where the cells are comparable to the Mach stem or channel width, the curved shape of the detonation wave front can no longer be ignored. Questions arise: When a detonation, with this 3D structure, is diffracted around a wedge apex, does the detonation wave exhibit a Mach reflection or regular reflection mode? Is it possible that the transition from regular reflection to Mach reflection exists? Does the detonation cell's stochastic nature affect triple point trajectory and TW-angle?

These problems are addressed in this paper by a numerical simulation of gaseous detonation Mach reflection. Other basic information is also analyzed, such as wave evolution and TW-angle variation.

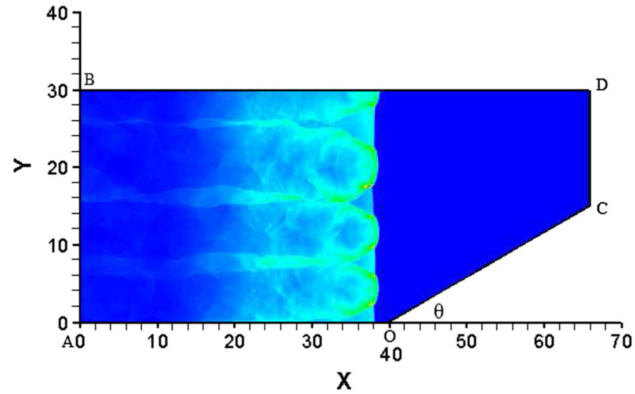


Fig. 1 Schematic of the computational domain

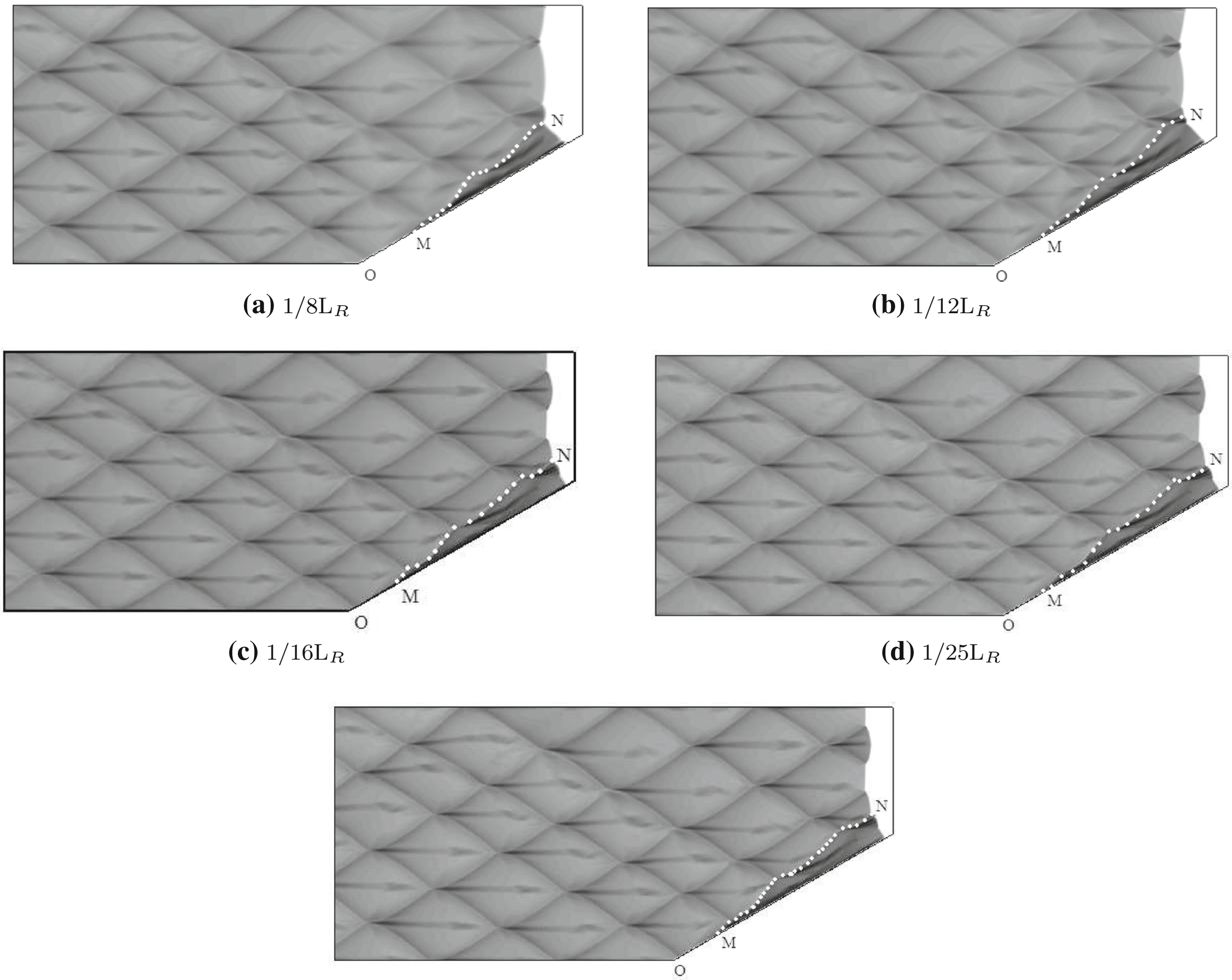
2 Numerical modeling

In this paper, the Navier–Stokes equations involving a detailed chemical reaction model are employed to describe detonation reflection phenomena. A second-order additive semi-implicit Runge–Kutta method is used to integrate the governing equations. This avoids the stiff problem of chemical sources [11]. An 8 species, 48 reaction mechanism [12] is used for chemical kinetics of a stoichiometric hydrogen–oxygen mixture diluted by 25 % Argon. Reacting species are H_2, O_2, H, O, OH, HO_2, H_2O_2 and H_2O. Convective terms are integrated by a fifth-order Weighted Essentially Non-Oscillatory scheme [13]. Viscous, heat and diffusion terms are evaluated by using second-order central finite differences.

Figure 1 presents the schematic of the computational domain. For comparing the wedge angle effect, wedge surface length OC is always kept constant (30 mm) for all wedge angles. The initial straight part extends 40 mm along x-direction and 30 mm along y-direction, respectively. Wedge angle θ ranges from 5° to 60° with an increment of 5°. To simplify the computational initialization process, a self-sustaining cellular detonation propagating towards the wedge is moving in the straight part of the tube. The boundary conditions are as follows. No-slip solid wall conditions are imposed on AO, DB and wedge OC. Non-reflecting boundary condition is used on AB. Since the computations are stopped before the detonation wave reaches the right boundary CD, gas flow near CD is quiescent, and, therefore, pressure outlet boundary conditions are imposed.

3 Grid resolution study

Sharpe [14] reported that more than 20 cells per reaction zone length is required to ensure convergence in the simulated phenomena. Many published papers reported that grid resolutions of 16–64 grid cells in the reaction zone are sufficient. The authors also tested the influence of grid resolution on det-



(e) 1/32L$_R$

Fig. 2 Cellular patterns with different grid resolution ($2H_2 + O_2 + Ar$, $p_0 = 8.00$ kPa, $\theta = 30°$)

onation Mach reflection. Under initial pressure of 8.00 kPa, five resolutions of 8, 12, 16, 25, and 32 grid cells per reaction zone length L_R were examined. Figure 2 presents cellular patterns with different grid resolution, for wedge angle of 30°. It shows that, for grid sizes of 1/8L_R and 1/12L_R, the Mach stem stays relatively planar, whereas for a finer grid, an obvious triple point, formed on the Mach stem, causes it to be curved. When grid size is equal to or finer than 1/16L_R, cellular patterns are essentially identical. This can also be proved by Table 1. TW-angle is 8.21° for grid sizes of 1/25L_R and 1/32L_R. For grid size of 1/16L_R, there is only 0.01 absolute difference or 0.12 % relative difference with the above-mentioned value, while for grid sizes of 1/8L_R and 1/12L_R, there is more than 26 % relative difference. Maximum pressure distributions along the wedge in Fig. 3 provide further information: with grid size equals to or larger than 1/16L_R, a relatively big difference appears; for grid size of 1/25L_R, the maximum pressure curve is much closer to that for grid size of 1/32L_R. Thus, the resolution of 25 grid cells within the reaction zone length was adopted for our computations.

Table 1 Effect of grid size on TW-angle

Grid size/reaction zone length	TW-angle (°)
1/8	10.36
1/12	11.07
1/16	8.22
1/25	8.21
1/32	8.21

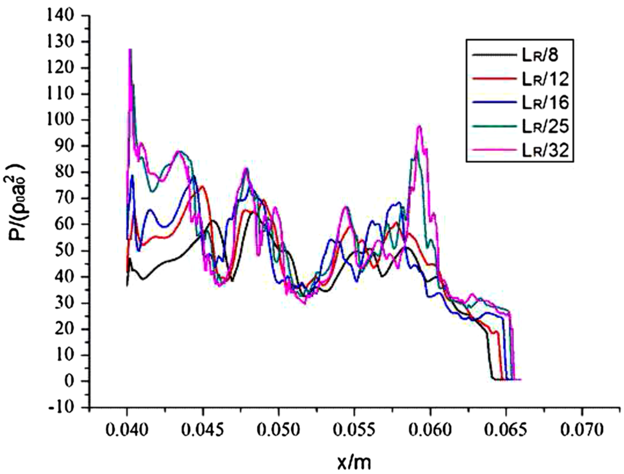
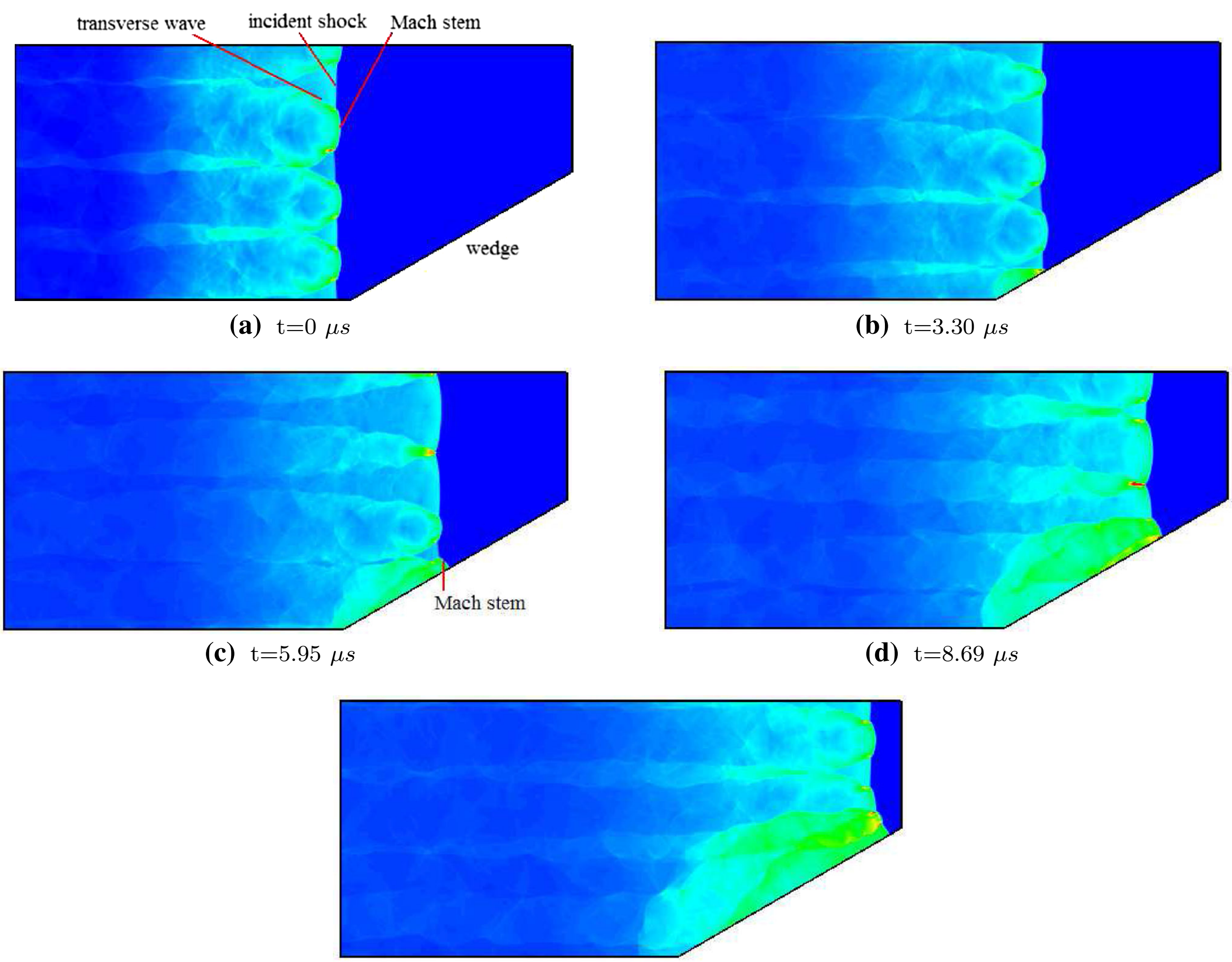


Fig. 3 Maximum pressure distributions along the wedge with different grid resolution

4 Results and discussion

4.1 Overall structure of detonation Mach reflection

Figure 4 presents a series of pressure contours of typical detonation Mach reflection on a wedge with wedge angle of 30°. Initial pressure and temperature are 8.00 kPa and 300 K, respectively. In the case of low initial pressure, detonation front structure including incident shock, Mach stem and reflected (transverse) wave is clearly observed. At an early stage, see Fig. 4a, a steadily repeating pattern of 7 triple points (a mode-7 detonation wave) is about to interact with the wedge. Its cell width and length are about 8.6 and 14.9 mm, respectively. It is easily identified that the Mach stem is stronger than the incident shock in the detonation structure. The Mach stem is slightly curved whereas the incident shock is straight. In Fig. 4b, Mach reflection just occurs with



(a) t=0 μs **(b)** t=3.30 μs **(c)** t=5.95 μs **(d)** t=8.69 μs **(e)** t=11.34 μs

Fig. 4 Pressure contours of typical detonation Mach reflection ($2H_2 + O_2 + Ar$, $p_0 = 8.00$ kPa, $\theta = 30°$)

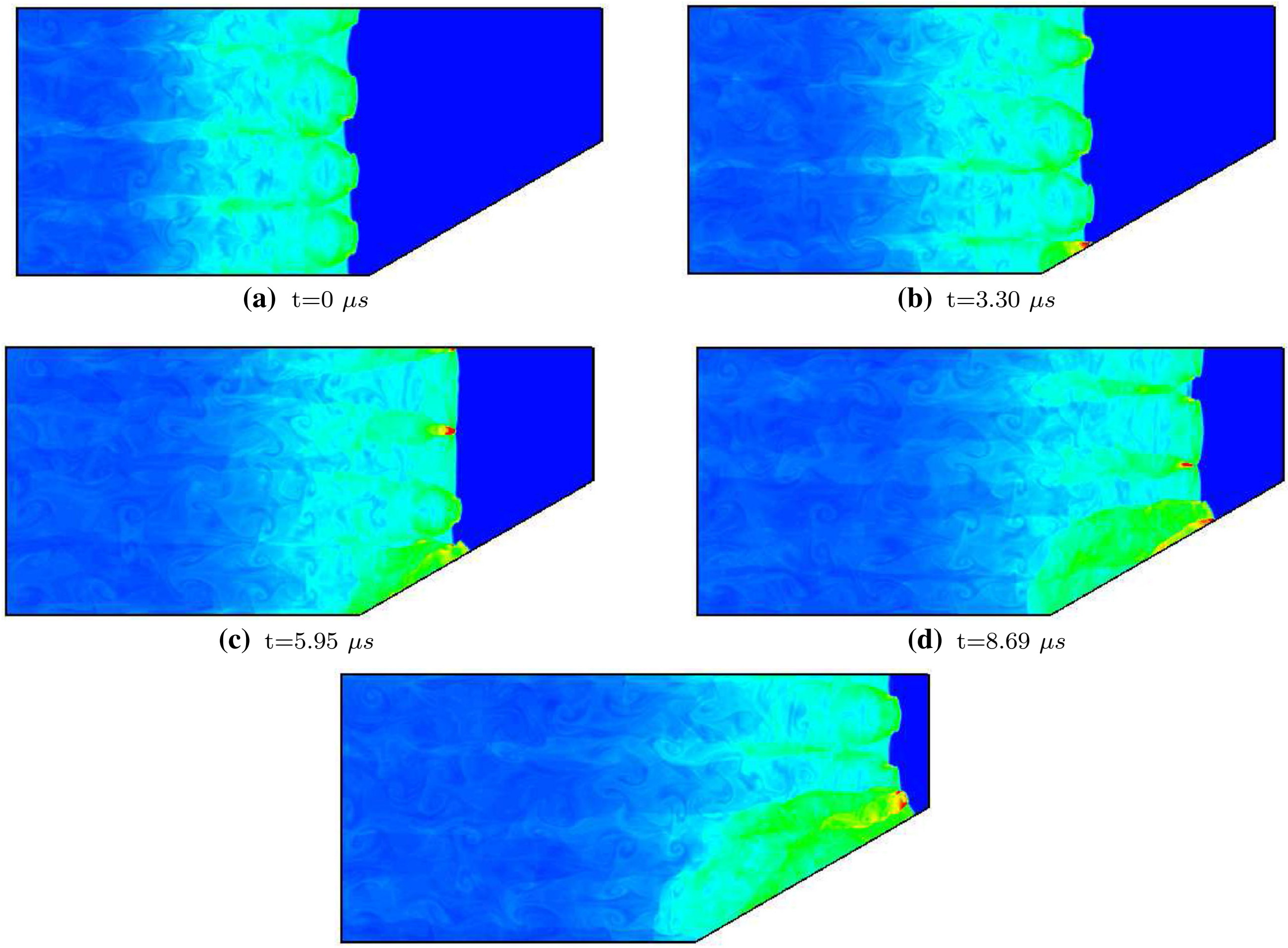


Fig. 5 OH contours of typical detonation Mach reflection ($2H_2 + O_2 +$ Ar, $p_0 = 8.00$ kPa, $\theta = 30°$)

a very short Mach stem appearing in the vicinity of the wedge surface. The undisturbed part of the incident detonation continues to propagate in a self-sustaining mode. In Fig. 4c, the height of the Mach stem further increases and one triple point has disappeared on the detonation front due to wedge surface contraction. In Fig. 4d, the detonation wave in the Mach stem region has developed with two triple points. At the trailing edge of the wedge, as shown in Fig. 4e, a cellular detonation wave is formed in the Mach stem region, but the incident detonation wave is not fully disturbed by wedge due to either not long enough wedge surface or not big enough wedge angle. Its self-sustaining propagation part has three remaining triple points.

Corresponding to pressure contours in Figs. 4, 5 presents OH contours of detonation Mach reflection under the same initial condition. In the gaseous detonation reflection process for hydrogen/oxygen gas mixture, OH appears as an intermediate product of chain-branching reactions; therefore, OH concentration indicates the state of chemical reaction. As shown in Fig. 5a, OH concentration behind the Mach stem is much higher than that behind the incident shock. It is well known that a higher OH concentration generates a shorter delay to the leading shock. The reaction zone is closely coupled with the Mach stem and is slightly separated from the incident shock. This implies that the incident shock is weaker than the Mach stem. In Fig. 5b, a very high OH mass fraction is produced behind the detonation wave in the short Mach stem region, and therefore the chemical reaction generates hardly any delay to the wave front. Based on the above results, it is concluded that behind the Mach stem the detonation wave is highly overdriven. It is noticed from Fig. 5c–e that high OH concentration occurs not only behind the detonation wave in the Mach stem region, but also behind the reflected shock due to high temperature and pressure after shock reflection.

4.2 Triple point trajectory characteristics

Figure 6 presents cellular patterns of detonation reflection on wedges with angle ranging from 5° to 60°. It is observed in every pattern that, when the wedge angle is less than or equal to 50°, there is always a sharp dividing line MN emerging from a certain point on the wedge surface and extending downstream. On both sides of it, the size, shape, and number of cells are obviously different. Usually, this line is regarded as the triple point trajectory. Above it, the detonation wave propagates undisturbed in a self-sustaining mode, whereas below it, the detonation wave in the Mach stem region travels in an overdriven mode. As wedge angle reaches or exceeds 53°, no Mach reflection occurs. Thus, it is estimated that the critical wedge angle corresponding to transition from Mach reflection to regular reflection is within the range from 50° to 53°, which is consistent with the value experimentally estimated by Guo et al. [6].

It is to be noted that the triple point trajectory is not a straight line, as also reported by Guo et al. [6]. The main reasons are as follows. Firstly, triple point trajectory is the detonation cell boundary. It is well known that for a whole detonation cell, convex curvature occurs in the first half cell cycle and concave curvature occurs in the second half cell cycle. Furthermore, the asymmetry of a detonation cell is developed in our channel. Secondly, collision between two transverse waves or between a transverse wave and wall results in new cell formation. Due to wedge slope contraction upward, the transverse wave collides with the upper wall on shorter and shorter spatial scale. This also leads to another fact that transverse waves close to wedge decay less. In other words, transverse waves in the Mach stem region turn stronger and stronger. When these stronger transverse waves interact with those in the undisturbed region, the influenced transverse space, such as the part above dividing line MN, is shortened and the detonation cell is accordingly smaller. It appears that interaction among transverse wave and reflected shock or wall causes the formation of a new cell. These factors combined support the argument that the tripe point trajectory in detonation Mach reflection is not a straight line.

Another striking phenomenon is that the triple point trajectory MN does not start from the wedge apex. Thus, what happens before Mach reflection? From Fig. 7, it can be deduced that regular reflection occurs initially which then transforms into Mach reflection. This is possibly attributable to low initial pressure. Under low initial pressure, relatively large transverse space is present between the wedge surface and the upper wall, and the wave front shape is continually adjusted. Therefore, its curvature at the interaction point with the wedge surface, determines the type of reflection. That is to say, for "averaged" or planar wave front, Mach reflection must occur. However, for detonation wave front under low initial pressure, it is possible that when the wave front hits the wedge apex Mach reflection does not occur at the apex, but appears further down the wedge surface in a transition from regular reflection to Mach reflection.

There are two aspects to be discussed in some detail:

- Wedge angle is less than critical angle of a planar detonation wave ($\theta < 90^\circ - \Omega$): in such a case, as shown in Fig. 8a, for a planar detonation wave, Mach reflection always occurs and starts from the wedge apex. Under low initial pressure, the detonation front consists of alternate weak incident shock and stronger Mach stem sections and the front is not planar. Therefore, the interaction between the curved front and wedge surface leads to variation of reflection type. If curvature is present, as shown in Fig. 8b, the bottom part of the wave front in a detonation cell may have an angle α with wedge surface, which is smaller than critical angle Ω, and therefore regular reflection occurs. As the wave front continues to move it interacts with the wedge, the reflection point moves up and α increases. When α at some point, such as M or B, of the top part of the curved wave front becomes larger than Ω, Mach reflection occurs. The detonation reflection process in Fig. 7 satisfies this condition. It is also possible that α at some point of the bottom part of the curved wave front becomes larger than Ω, as shown in Fig. 8c.
- Wedge angle is larger than critical angle of a planar detonation wave ($\theta > 90^\circ - \Omega$): as shown in Fig. 9a for the case of planar detonation wave, α is smaller than Ω, so that regular reflection occurs. As mentioned above, the bottom part of the curved wave front has an angle α with the wedge surface which is smaller than that in the case of planar detonation wave, so that regular reflection persists. It is possible that, within the top part of the curved wave front, some point, such as M or B, exists where α becomes larger than Ω, as shown in Fig. 9b, so that Mach reflection occurs.

Figure 10 presents the dependence between L and wedge angle θ, where L is the distance between the starting point M of the triple point trajectory and wedge apex O. It shows that when the wedge angle increases, L also increases. That is to say, the transition from regular reflection to Mach reflection occurs further and further away from the wedge apex.

4.3 Effect of detonation cell stochastic nature on reflection

Some calculations were done to obtain an insight into the effect of the detonation cell's stochastic nature on Mach reflection. Our shock tube has a cross-section of 40 × 40 mm, with smoked foils mounted on the side-walls. Figure 11 presents a critical state in the DDT process [15]. It shows that the boundary shape between no-cell region and cell region is

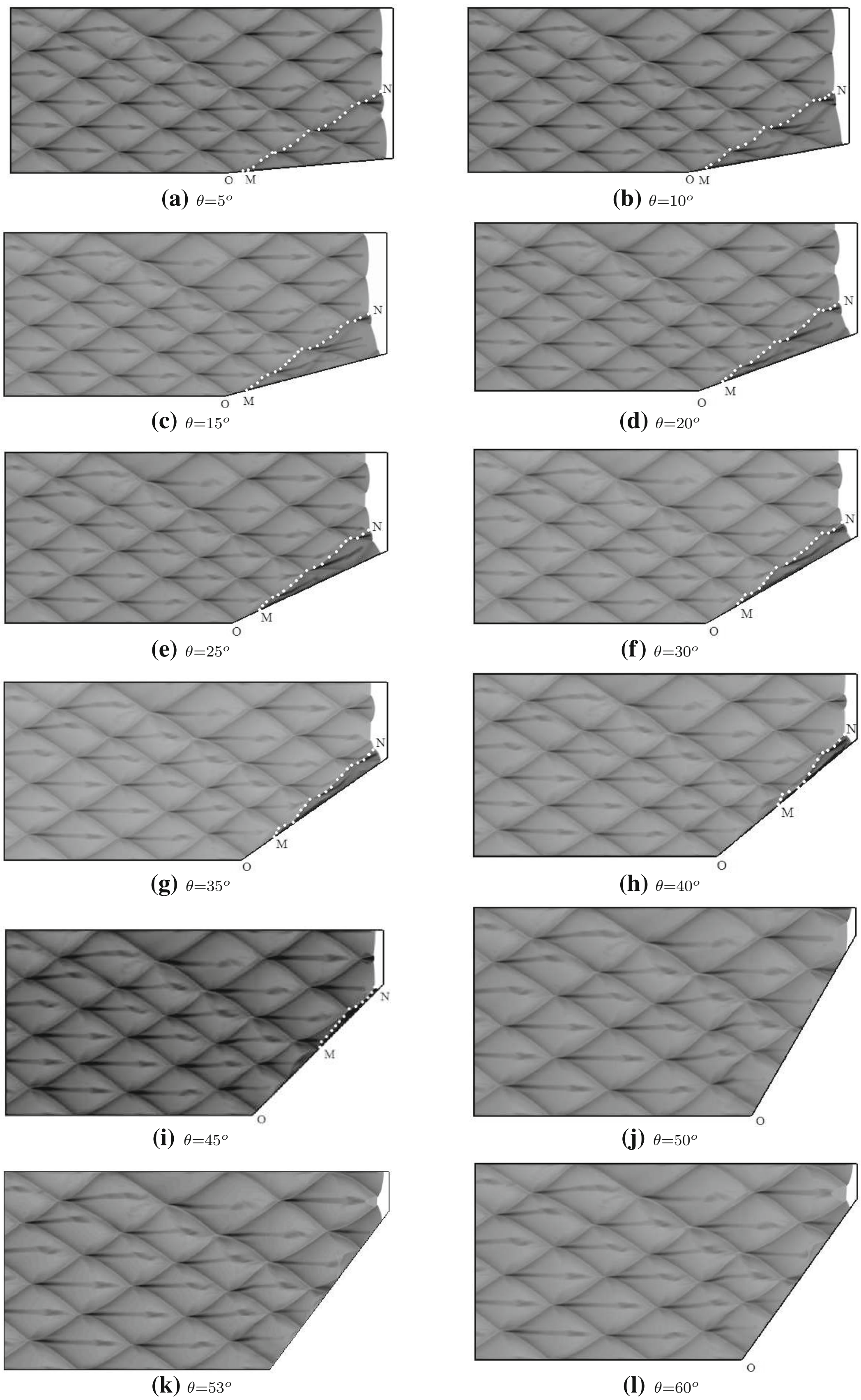


Fig. 6 Cellular patterns of detonation reflection for different wedge angles ($2H_2 + O_2 + Ar$, $p_0 = 8.00$ kPa)

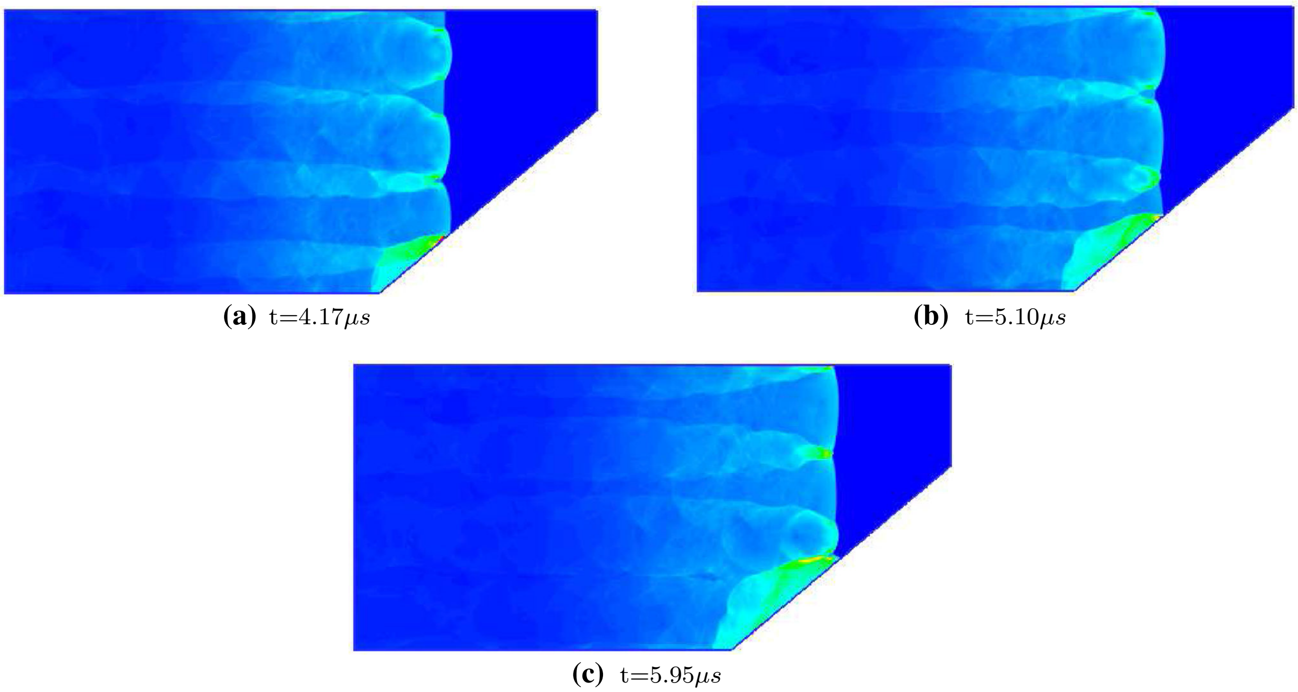


Fig. 7 Detonation reflection on a 40° wedge

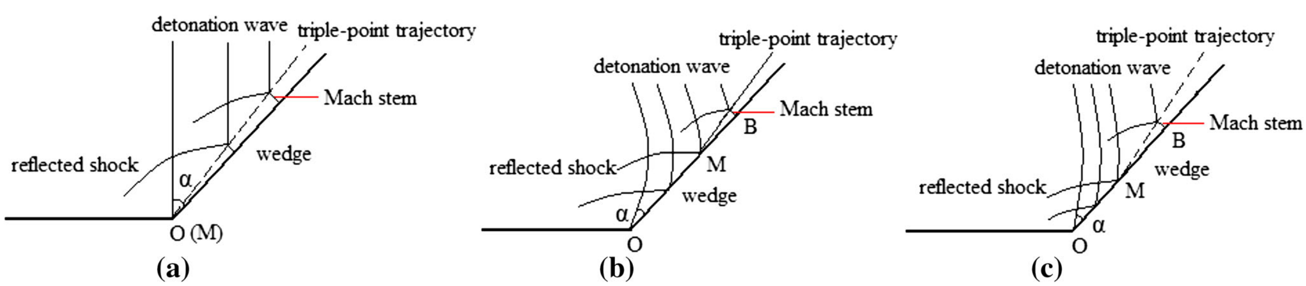
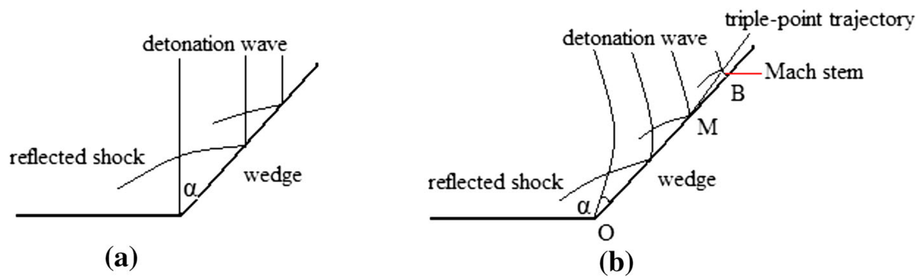


Fig. 8 Schematics of reflection patterns for the wedge angle less than the critical angle for a planar detonation wave ($\theta < 90° - \Omega$)

Fig. 9 Schematics of reflection patterns for the wedge angle larger than the critical angle for a planar detonation wave ($\theta > 90° - \Omega$)



stochastic. Under the same initial condition, it was impossible to obtain the same critical boundary in our experiments. Additionally, even though initial pressure and other conditions are kept the same, the DDT distance from ignition end to the critical boundary is still different for every experiment, as shown in Table 2. Therefore, for detonation diffraction around a wedge, detonation cell shape and cell location relative to wedge apex are stochastic, which may influence the cell shape in the Mach stem region and TW-angle. In the present numerical simulations, the detonation stochastic nature is modelled by specifying different cell locations relatively to the wedge apex. Four cases were calculated with the cell offsets to the left from the apex of 0 cell, 1/4 cell, 1/2 cell and 3/4 cell, so that representative offsets within the whole detonation cell length are considered. In fact, in every simulation, the same detonation front is imposed at the different locations mentioned above.

Figure 12 presents the cellular patterns of detonation Mach reflection for the four cases. It is observed that below the triple point trajectory, the cell shape, size and number are not

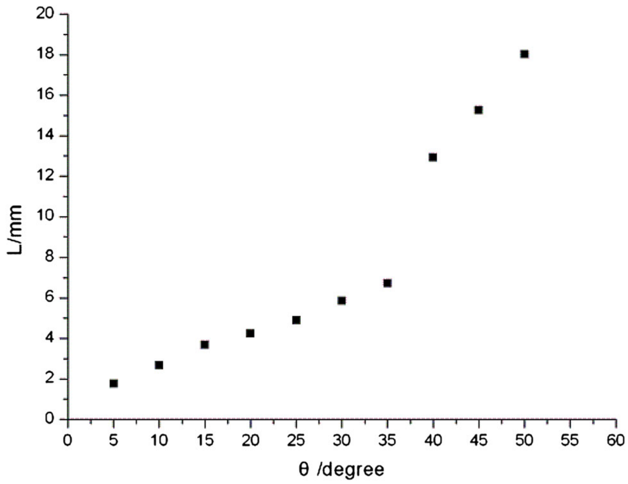


Fig. 10 Distance L between points M and O vs. wedge angle θ

identical due to different initial cell offset. This means that the detonation intensity in the Mach stem region is variable. In addition, the origin of the triple point trajectory MN is not the same. For 1/4 cell-length offset, it starts nearly from the wedge apex. For the other three cases, the origin point M is at different distances relatively to wedge apex O, which indicates that regular reflection appears first and Mach reflection happens later.

Table 3 shows the effect of detonation cell stochastic nature on TW-angle. Due to different triple point trajectories and their corresponding origin points, TW-angles have the following values: 8.22°, 7.30°, 7.25° and 9.77°. The maximum difference is 2.52° and is about 30 % of the average value.

Table 2 DDT distance vs initial pressure ($2H_2 + O_2 +$ Ar)

Initial pressure (kPa)	DDT distance (mm)		
	Shot1	Shot2	Shot3
26.67	2,097	2,142	2,151
33.33	2,012	2,006	1,976
40.00	1,645	1,657	1,611
46.67	762	746	739
53.33	682	702	716

Stochastic nature in DDT leads to relative discordance of detonation cell location and shape. The origin point of triple point trajectory is also stochastic on the wedge slope; moreover, the variation of TW-angle is evident.

4.4 Effect of wedge angle on TW-angle

As Guo et al. [6] reported, TW-angle is dependent mainly on the wedge angle and is not sensitive to initial pressure. Therefore, in the current study, only wedge angle variation is considered for a stoichiometric hydrogen-oxygen mixture diluted by 25 % Argon. Figure 13 presents the dependence

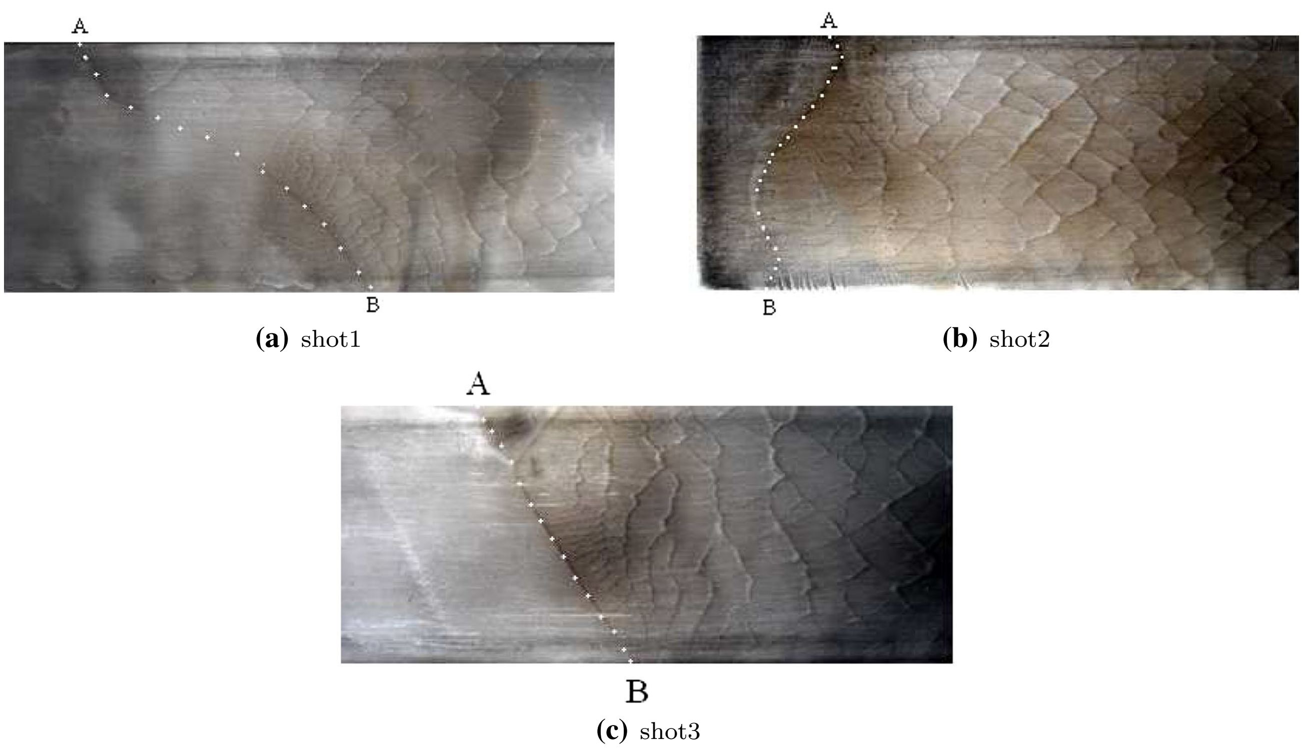
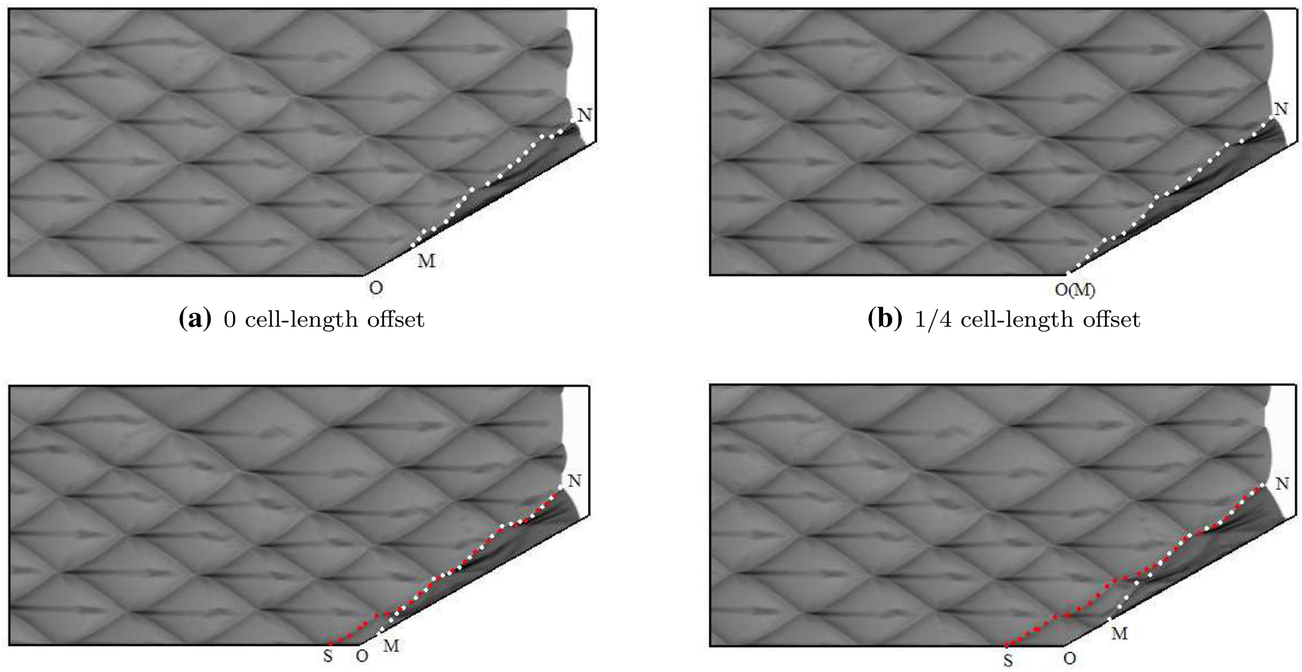


Fig. 11 Experimental cellular patterns in the critical state in DDT process. AB is the critical boundary between no-cell region and cell region



(a) 0 cell-length offset **(b)** 1/4 cell-length offset

(c) 1/2 cell-length offset **(d)** 3/4 cell-length offset

Fig. 12 Cellular patterns of detonation Mach reflection with different cell offsets

Table 3 Effect of detonation stochastic nature on TW-angle

Wave front location offset	TW-angle/degree
0 cell-length offset	8.22
1/4 cell-length offset	7.30
1/2 cell-length offset	7.25
3/4 cell-length offset	9.77

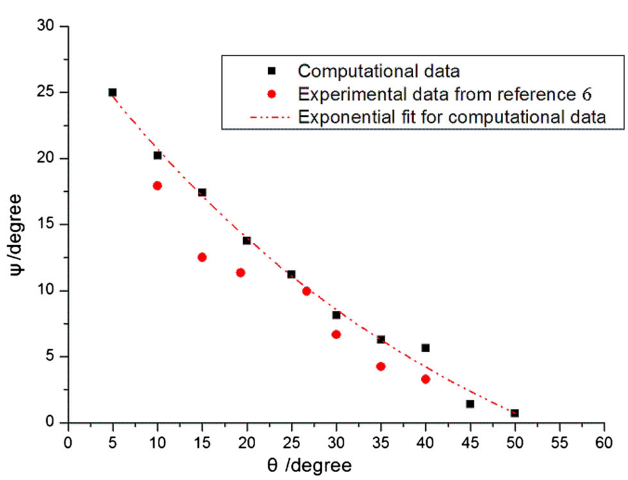


Fig. 13 TW-angle vs. wedge angle

between the TW-angle and the wedge angle. With wedge angle increasing, TW-angle rapidly decreases. When wedge angle is 5°, TW-angle has a maximum value of approximately 25°. When wedge angle reaches 50°, TW-angle drops to 0.69°. From these data, an empirical formula was deduced based on exponential fitting:

$$\psi = 42.66e^{(-\theta/45.69)} - 13.56 \tag{1}$$

where ψ is the TW-angle (in degrees), and θ ranges from 5° to 50°. This exponential fitting has correlation of 0.9938, and can be used to predict the TW-angle for other wedge angles. Since Guo et al. [6] experimentally demonstrated that initial pressure has little effect on TW-angle, it may be possible to extend the above formula to other cases, especially those involving hydrogen and oxygen mixtures at different initial pressures. This conjecture needs much more experimental and computational data for validation. In a comparison of computational data with Guo's experiments, it is found that both exponential relations between TW-angle and wedge angle are similar. The authors' computation is basically consistent with Guo et al.'s experiment: the computation slightly overestimates the experimental values. This is attributed to the following three reasons. Firstly, the experimental initial pressure is 16 kPa, whereas it is only 8 kPa in the computations. Secondly, the triple point trajectory selected for TW-angle in the experiment may be different from that in the computation. For example, as shown in Fig. 12, the same triple point trajectory is likely to be chosen in case (b). Nevertheless, for cases (c) and (d), line SN is possibly chosen in the experiments whereas line MN is selected in our computations. This may lead to different TW-angle values: 4.46°

instead of 7.25° for case (c) and 1.58° instead of 9.77° for case (d). Finally, the computation cannot exactly reproduce experimental phenomena without error, due to numerical modeling, smoked print technique and the above mentioned stochastic nature of detonation.

5 Conclusions

Numerical simulations presented in this paper provide detailed information about detonation wave Mach reflection phenomena on a wedge under low initial pressure. The main conclusions are as follows:

1. The non-planar nature of detonation waves becomes more evident at low initial pressures. When the wave front hits the wedge surface, its angle and curvature at the interaction point determine the subsequent reflection type. For different wedge angles ranging from 5° to 50°, regular reflection appears first and then Mach reflection occurs. This behavior is different from that for a planar detonation wave or an air shock wave. Even though the wedge angle is larger than the critical angle, detonation Mach reflection can emerge in local regions on these wedges at a lower initial pressure.
2. Due to DDT stochastic nature, cell shape and wave front location relative to the wedge apex are also stochastic. This leads to stochastic variation of the origin point of triple point trajectory and the variations of TW-angle.
3. The triple point trajectory starts at some point on the wedge surface and does not necessarily start from the wedge apex. As wedge angle increases, the distance between the origin point of triple point trajectory and the wedge apex increases.
4. With the increase of wedge angle, the TW-angle rapidly decreases. They satisfy the exponential relation $\psi = 42.66e^{(-\theta/45.69)} - 13.56$. The critical wedge angle for transition from Mach reflection to regular reflection is within the range from 50° to 53°, which is consistent with Guo et al.'s experiment [6].

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