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Numerical Study on Critical Wedge Angle of Cellular Detonation Reflections *

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The critical wedge angle (CWA) for the transition from regular reflection (RR) to Mach reflection (MR) of a cellular detonation wave is studied numerically by an improved space-time conservation element and solution element method together with a two-step chemical reaction model. The accuracy of that numerical way is verified by simulating cellular detonation reflections at a 19.3° wedge. The planar and cellular detonation reflections over 45°–55° wedges are also simulated. When the cellular detonation wave is over a 50° wedge, numerical results show a new phenomenon that RR and MR occur alternately. The transition process between RR and MR is investigated with the local pressure contours. Numerical analysis shows that the cellular structure is the essential reason for the new phenomenon and the CWA of detonation reflection is not a certain angle but an angle range.

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Detonation reflection on a wedge is a very complicated phenomenon, and it is one of the fundamental problems of detonation propagation in complex channels. Similar to the shock wave situation, regular reflection (RR) or Mach reflection (MR) occurs when a detonation wave encounters a wedge.[1]

Studies on detonation reflections are still tentative, especially for the critical wedge angle (CWA) for the transition from RR to MR. The CWAs in different studies may be quite different even under the same research conditions. The commonest study conditions of detonation reflections are the H_2–O_2 detonation waves whose properties are familiar to researchers. Table 1 shows the CWAs in the stoichiometric H_2–O_2 detonation reflections. The CWAs are ranged from 32° to 83° in theoretical analysis because there is no appropriate theory for detonation reflections. The experimental results are also uncertain (39°–50°) for the limitations of the equipment and measurement methods. Thus the numerical simulations become important in research on detonation reflections.[2–4]

Table 1. The CWAs of H_2-O_2 detonation waves by different means.

Researchers	Means		
	Theory analysis	Experiments	Numerical simulations
Meltzer *et al.*[5]	32°	40°–45°	
Gavrilenko *et al.*[6]	34°	39°–41°	
Akbar.[1]	33°	45°–50°	
Li *et al.*[7]	42°, 83°		
Yu.[3]			50°
Hu *et al.*[4]			∼ 48.5°

Numerical simulations of detonations have improved immensely in the recent 25 years with the development in both computational methods and available computer facilities. There are two main challenges in detonation simulations. One is the calculation of the process of energy release in the reaction flows; the other is the strategy of capturing the strong discontinuity in detonation waves. Successful solutions of the two challenges depend on the developments of chemical reaction models and numerical schemes, respectively. In this study, we adopt an improved space-time conservation element and solution element (CE/SE) scheme[8,9] and a two-step chemical model.[10]

The CE/SE method originally proposed by Chang[11] in 1995 is a new numerical framework for solving conservation laws. The CE/SE method substantially differs from the existing well-established computational fluid dynamics (CFD) methods. The CE/SE method has many features such as a unified treatment of space and time, satisfying both local and global flux conservation in space and time and simple treatments under boundary conditions. Because of its simplicity, generality and accuracy, the CE/SE method has been successful applied to fluid problems and engineering practices. However, the original two-dimensional CE/SE method[12] is complicated by the special design of solution elements (SEs) and conservation elements (CEs). Thus, we have proposed an improved two-dimensional CE/SE scheme by adopting a general rectangle mesh to construct SEs and CEs (shown in Fig. 1)[8] and high-order accuracy Taylor expansions.[13] Moreover, we have extended the improved CE/SE scheme to detonation simulations and verified its accuracy.[8,9]

Many chemical reaction models such as the C-J model, the one/two-step reaction model, Sichel's two-step reaction model and the detailed chemical reaction

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model have been applied to numerical simulations of detonation waves. The one/two-step chemical reaction model can describe the chemical reaction process and does not need many computing resources.[14,15] Thus, we adopt the two-step reaction model in this study.

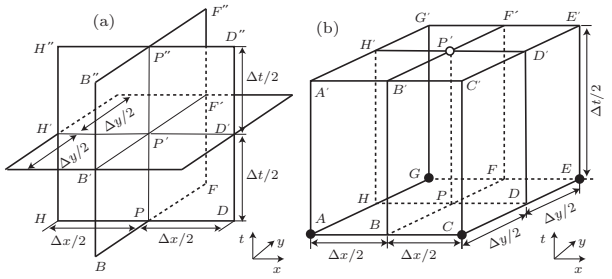


Fig. 1. Space-time geometry of the improved two-dimensional CE/SE scheme.

The two-step reaction model simplifies the complicated chemical reactions to an induction reaction and an exothermic reaction. The progress parameters α and β, for the induction reaction and the exothermic reaction, respectively, are both unity first, followed by decrease of α to zero, then β decreases until the equilibrium state is reached. The rates of α and β, ω_α and ω_β, are given as follows:[10]

$$\omega_\alpha = \frac{d\alpha}{dt} = -k_\alpha \rho \exp\Big(-\frac{E_a}{RT}\Big), \tag{1}$$

$$\omega_\beta = \frac{d\beta}{dt} = \begin{cases} 0, & (\alpha > 0), \\ -k_\beta p^2 \big[\beta^2 \exp\big(-\frac{E_\beta}{RT}\big) - (1-\beta)^2 \\ \cdot \exp\big(-\frac{E_\beta + Q}{RT}\big)\big], & (\alpha \le 0), \end{cases} \tag{2}$$

where ρ is the mass density, T the temperature, R the gas constant, Q the heat release parameter, k_α and k_β the constants of reaction rates, and E_α and E_β the activation energies.

The governing equations for a detonation problem are the two-dimensional Euler equations

$$\frac{\partial \boldsymbol{Q}}{\partial t} + \frac{\partial \boldsymbol{E}}{\partial x} + \frac{\partial \boldsymbol{F}}{\partial y} = \boldsymbol{S}, \tag{3}$$

where $\boldsymbol{Q} = (\rho, \rho u, \rho v, E, \rho\alpha, \rho\beta)^T$, $\boldsymbol{E} = (\rho u, \rho u^2 + p, \rho uv, (E+p)u, \rho\alpha u, \rho\beta u)^T$, $\boldsymbol{F} = (\rho v, \rho uv, \rho v^2 + p, (E+p)v, \rho\alpha v, \rho\beta v)^T$, $\boldsymbol{S} = (0, 0, 0, 0, \omega_\alpha, \omega_\beta)^T$, in which u and v are velocity components, p the pressure. E is the total energy density and defined as

$$E = \frac{p}{\gamma - 1} + \frac{\rho(u^2 + v^2)}{2} + \rho\beta Q, \tag{4}$$

where γ is the specific heat ratio.

In order to verify the accuracy of the improved CE/SE scheme and the two-step reaction model in cellular detonation reflections, we simulate a stoichiometric H_2-O_2 cellular detonation propagating in a channel with a 19.3° wedge. The initial pressure and temperature are 1 atm and 298 K, respectively. The ignition condition of pressure in the channel left is 40 atm. The computing parameters of the two-step reaction model for the stoichiometric H_2–O_2 gas mixture are given as $Q = 1.33 \times 10^7$ J/kg, $k_\alpha = 3.0 \times 10^8$ m^3/kg/s, $k_\beta = 1.875 \times 10^{-5}$ m^4/N^2/s, $E_\alpha = 2.261 \times 10^7$ J/kg, $E_\beta = 4.6151 \times 10^6$ J/kg.[10]

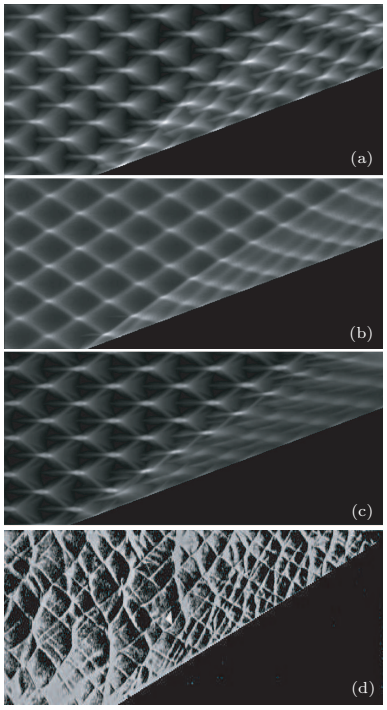


Fig. 2. Cellular patterns of detonation waves over the 19.3◦ wedge: (a) Numerical simulation (400×200 meshes), (b) Sichel's two-step reaction model (400 × 200 meshes), (c) detailed chemical reaction model (400 × 200 meshes), (d) experiment of Guo *et al.* in 2001.

Figure 2 shows the cellular patterns by the numerical simulation (using the two-step reaction model, Sichel's two-step reaction model[16] and the detailed chemical reaction model[17] respectively) and the corresponding experiment.[18] The numerical cellular patterns by the three chemical reaction models all can obtain clear cellular structure and can describe the basic phenomena of the cellular detonation reflection, e.g., the triple-point trajectory is not a straight line and the cell sizes between the triple-point trajectory and the wedge become smaller. Table 2 shows the characteristic parameters of cellular patterns and detonation reflections under different computing meshes and different chemical reaction models. We can find that the numerical parameters by the two-step reaction model can agree well with the experimental ones at the five mesh types. The numerical parameters by Sichel's two-step reaction model and the detailed chemical reaction model can also agree well with the experimental ones, but they cost more computing resources, such as memory ($M_{\text{two-step}} : M_{\text{Sichel's}} : M_{\text{detailed}} = 1.0 : 1.4 : 3.1$)

and computing time ($t_{\text{two-step}} : t_{\text{Sichel's}} : t_{\text{detailed}} = 1.0 : 2.5 : 3.2$).

Table 2. Characteristic parameters of cellular patterns and detonation reflections. Here a is the ratio of cell width to cell length, ϕ is the exit angle, χ is the entrance angle, ψ is the angle of the transverse wave trace, ξ is the angle between the triple-point trajectory and the wedge.

	a	ϕ(deg)	χ (deg)	ψ (deg)	ξ (deg)	Meshes
Experiment	0.5–0.6	5–10	32–40	~ 30	11.5–13.0	
Two-step	0.59	9.2	38.0	30.5	~ 13.1	400×200
Two-step	0.56	9.0	36.2	29.24	~ 13.0	600×300
Two-step	0.53	8.5	33.3	29.12	~ 12.9	800×400
Two-step	0.53	8.5	33.2	29.10	~ 12.9	1000×500
Two-step	0.53	8.5	33.2	29.08	~ 12.9	1200×600
Sichel's	0.60	11.2	31.5	29.0	~ 11.3	400×200
Detailed	0.51	9.5	38.2	28.5	~ 12.2	400×200

We simulate the planar and cellular detonation reflections at different wedge angles (ranging from 45° to 55° with 0.5° interval). The grid sizes are 1200×750 and the CFL number equals 0.5. Similar to reflections of shock waves,[19] the reflection of planar detonation is a self-similar phenomenon. The CWA of the planar detonation is 49.5°. However, the reflection of cellular detonation is not a self-similar phenomenon for the complex wave system in the detonation front. Summarizing the numerical results of cellular detonation reflections, we can find the following phenomena: (1) MR occurs when the cellular detonations are over the wedges whose angles are less than 49.5°. (2) RR occurs when the cellular detonations are over the wedges whose angles are greater than 50.5°. (3) RR and MR occur alternately when the cellular detonation wave is over the 50° wedge.

The phenomenon of RR and MR occurring alternately under steady environment conditions (a steady detonation wave and a wedge with fixed angle) does not occur in the shock wave reflections. That phenomenon has not been observed because of the limitations of the measurement equipment and methods. In this study, we describe and analyze the phenomenon by the numerical results.

Figure 3 shows the transition process from RR to MR of the cellular detonation over the 50° wedge by describing the local pressure contours every 20 steps between steps 2800 (56.65 μs) and 3860 (60.88 μs). In order to distinguish the Mach stem in the precursor shock wave (see step 2800), we call the Mach stem between the wedge and the precursor shock wave the MSWP (see step 2860). At step 2800, RR occurs because there is no MSWP, though the wave system behind the detonation front is complex. We can also find that one transverse wave has collided with the wedge and that enhances the pressure between the wedge and the reflection wave of the detonation wave. The reflected wave of the transverse wave also begins to interact with the reflected wave of the detonation wave. Both the facets strengthen the reflected wave of the detonation wave. Thus at step 2820 a MSWP begin to form at the detonation front near the wedge. At step 2840 we can find the MSWP near the wedge. At step 2860 the MSWP can be distinguished more clearly.

Figure 4 shows the transition process from MR to RR. MR occurs between steps 2960 (62.76 μs) and 3020 (64.04 μs). At step 2980 the transverse wave interacts with the reflected wave of the detonation wave and that also weakens the reflection wave of the detonation wave. At step 3000 the MSWP disappears before the reflection wave of the transverse wave interacts with the reflection wave of the detonation wave. At step 3200 RR occurs though the reflection wave of the transverse wave has interacted with the reflection wave of the detonation wave. The numerical results show the transition cycle time is about 4 μs.

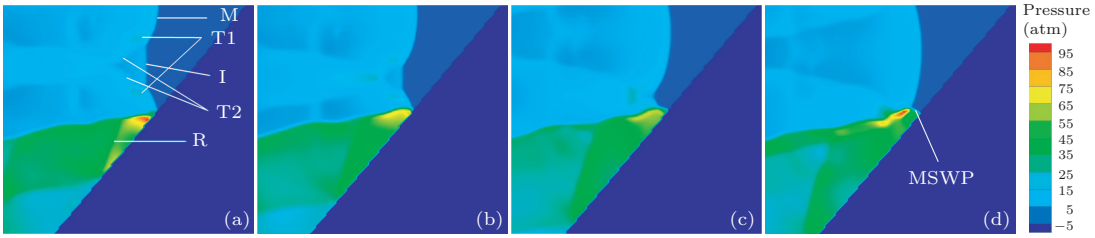
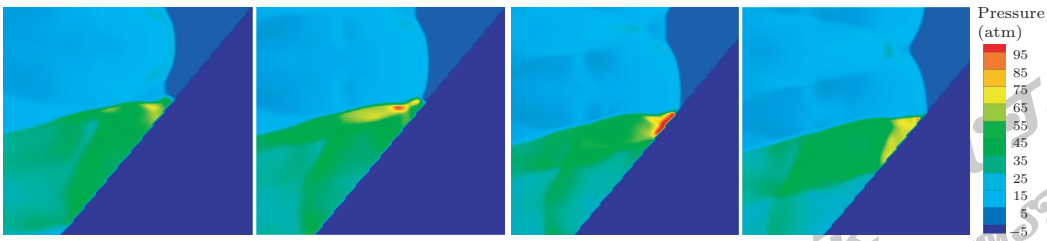


Fig. 3. Local pressure contours every 20 steps between steps 2800 and 2860 (M: Mach stem in the precursor shock wave, I: incident wave, T1: triple points, T2: transverse wave, R: reflected wave of transverse wave, MSWP: Mach stem between the wedge and the precursor shock wave).



(a) Step 2960 62.76 μs (b) Step 2980 63.16 μs (c) Step 3000 63.58 μs (d) Step 3020 64.04 μs

Fig. 4. Local pressure contours every 20 steps between steps 2960 and 3020.

Figure 5 shows that the velocity profiles of planar and cellular detonation waves at different times. The maximum particle velocities in the planar detonation front keep the same value (1910 ± 10 m/s) at different times. The self-similar distribution of physical quantities is the reason for the self-similar phenomena of planar detonation reflections. The maximum particle velocities in the cellular detonation front range from 1387.5 m/s to 2415.6 m/s at different times. The sound velocity in the initial H_2-O_2 gas mixture is 536.6 m/s. Thus the Mach numbers in the planar and cellular detonation fronts are 3.56 and 2.59–4.50, respectively. From the theory of shock wave[19] and planar detonation[7] reflections we know that the reflection types are decided by the Mach number if the wedge angle is fixed. Akbar's experiments[1] also show that reflection types of the detonation wave and shock wave have the same trend, though the detonation waves and shock waves have different waveforms. For planar detonation waves, the CWA is 49.5° in our study. This means that RR will occur if the Mach number is less than 3.56, and MR will occur if the Mach number is greater than 3.56 when the detonation wave encounters the 49.5° wedge. The Mach number of the cellular detonation wave ranges from 2.59 to 4.50, so RR and MR can occur alternately in the same wedge.

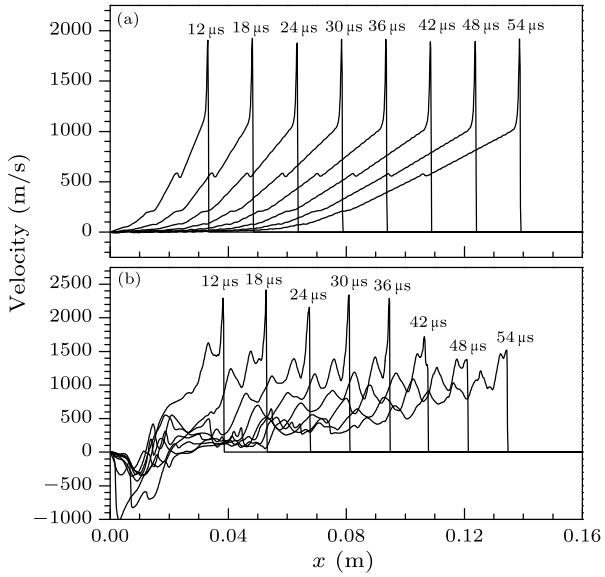


Fig. 5. Velocity profiles at different times: (a) planar detonation wave, (b) cellular detonation wave.

From the description we can find that the transverse waves play an important role in the transition process between RR and MR. From the analysis we know that the non-self-similarity of physical quantities is the reason for RR and MR occurring alternately. The mechanism of cellular structure is still a disputed problem, though some researchers thought that the transverse waves are the key character of cellular detonations.[20] However, it is widely accepted that the cellular structure is an inherent characteristic of detonation waves. Thus we believe that RR and MR can occur alternately with a steady detonation over a wedge with an appropriate angle and the CWA of detonation reflections is not a certain angle but an angle range.

In conclusion, the improved CE/SE scheme and the two-step chemical model have been introduced and verified for studying the CWA of cellular detonation reflections. We find that RR and MR occur alternately when the stoichiometric H_2–O_2 cellular detonation wave encounters the 50° wedge. The phenomenon of RR and MR occurring at the same wedge is essentially different from the reflections of planar detonation waves and shock waves. We describe the transition process between RR and MR aided by the local pressure contours. We analyze the reason for RR and MR occurring alternately using the numerical data and the theory of planar detonation reflections. The results show that the cellular structure of detonation waves induces the new phenomenon and the CWA of detonation reflection is not a certain angle but an angle range.

The CWA of the stoichiometric H_2–O_2 cellular and planar detonation reflection is 49.5°–50.5° and 49.5°, respectively. The CWA of the planar detonation reflection, which is approximately equal to that of the cellular detonation reflection, can be used in engineering designs.

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