Experimental study and numerical simulation of cellular structures and Mach reflection of gaseous detonation waves

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Abstract. In this paper the Deflagration to Detonation Transition (DDT) process of gaseous H_2-O_2 mixture and Mach reflection of gaseous detonation wave on a wedge have been conducted experimentally. The cellular pattern of DDT process and Mach reflection were obtained from experiments with wedge angle $\theta = 10^0 \sim 40^0$ and initial pressure of gaseous mixture 16kPa $\sim$ 26.7kPa. The 2-D numerical simulations of DDT process and Mach reflection of detonation wave were performed by using the simplified ZND model and improved space-time conservation element and solution element (CE/SE) method. The numerical cellular structures were compared with the cellular patterns of soot track. Compared results were shown that it is satisfactory. The characteristic comparisons on Mach reflection of air shock wave and detonation wave were carried also out and their differences were given.

1 Introduction

The Mach reflection will occur when a stable C-J detonation wave encounters obstacles, such as a wedge. In an academic sense, compared with the reflection of air shock waves, the reflection phenomena of detonation wave have not been studied extensively. A lot of fundamental questions are still unanswered up till now. However, it has received much attention over last decade due to the application in supersonic propulsion and the recognition of universality of the cellular structures from the detonation of chemical systems to thermonuclear supernovae. An increasing number of experimental study and numerical simulation have been devoted to this physical problem[1-5].

In this paper the Deflagration to Detonation Transition (DDT) process and Mach reflection of gaseous detonation wave on a wedge have been conducted experimentally by using a detonation tube. The recent cellular patterns based on soot track measurement were presented. The cellular structures before and after Mach reflection were obtained from experiments with wedge angle $\theta = 10^0 \sim 40^0$ and initial pressure of gaseous mixture 16kPa $\sim$ 26.7kPa. The phenomena and characteristics of cellular structures of detonation wave were described and analyzed symmetrically. The 2-D numerical simulations of the cellular structures before and after Mach reflection of detonation wave have been performed by using the simplified ZND model of two-step chemical reaction and improved space-time conservation element and solution element (CE/SE) method. The cellular structures before and after Mach reflection of detonation wave were given numerically. The numerical cellular structures were compared with the cellular patterns of soot track. Compared results were shown that it is satisfactory. The characteristic comparisons on Mach reflection of air shock wave and detonation wave were carried also out and their differences were given.

Fig. 1. Cellular pattern without wedge

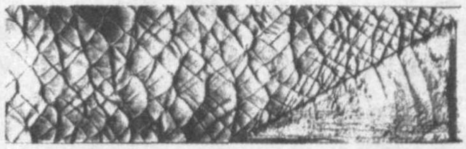

Fig. 2. Cellular pattern with $\theta = 19.3^0$ wedge

Fig. 3. Cellular pattern with $\theta = 30^0$ wedge

Fig. 4. Cellular pattern with $\theta = 40^0$ wedge

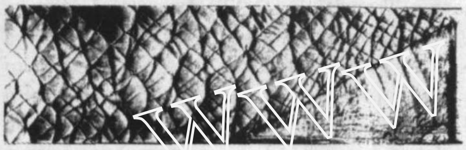

Fig. 5. Cellular pattern(P_0=20kPa,$\theta = 19.3^0$)

Fig. 6. Cellular pattern(P_0=26.7kPa,$\theta = 19.3^0$)

2 Experimental study of cellular patterns

Hydrogen-oxygen mixtures diluted with 25% argon ($2H_2+O_2+Ar$, γ=1.45, M_{Cj}=1.52) were used in present experiments. To show the relation of angle χ, which is between the trajectory of triple-point and wedge surface, and wedge angle θ, one test series were performed under identical initial pressure 16.0kPa and different wedge angles 10^0, 15^0, 19.3^0, 26.6^0, 30^0, 35^0 and 40^0 respectively. To show the relation between angle χ and initial pressure P_0, the second test series were performed under same wedge with $\theta = 19.3^0$ and different initial pressures 16.0, 20.0, 24.3, 26.3 and 40.0kPa respectively [6].

The cellular pattern of soot tracks for a detonation wave going through a tube without wedge was put into Fig.1. The cellular patterns of soot tracks for a detonation wave reflecting on a wedge with $\theta = 19.3^0, 30^0, 40^0$ were shown into Fig.2 to Fig.4.

The cellular patterns of soot tracks for a detonation reflecting on same wedge with 19.3^0 wedge angle under the different initial pressures 16.0, 20.0, and 26.7kPa were shown into Fig.2, Fig.5 and Fig.6.

The experimental results were primarily analyzed. It was known that the changes of cellular structures before and after Mach reflection are marked and they are relative to wedge angle of wedge and initial condition of gaseous mixture. The characteristic scales of cellular structures after Mach reflection will be diminished and the density of cells will be getting denser with the increase of initial pressure and wedge angle. When the wedge angle is larger more than 35^0 and initial pressure is larger more than 26.7kPa, the cellular structures after Mach reflection will no appear. The angle χ will be diminished with the increase of wedge angle. However the angle χ will only be slightly change with the increase of initial pressure of gaseous mixture.

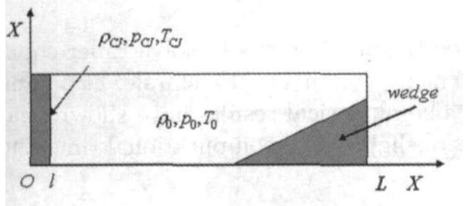

Fig. 7. Sketch of reflection of a detonation wave on a wedge

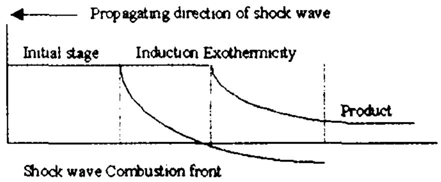

Fig. 8. Sketch of ZND model of two-step chemical reaction

3 Numerical simulation of cellular structures

3.1 Physical problem and simplified model

To simulate numerically cellular structures of reflection process of detonation wave on a wedge, the physical problem can be simplified as the sketch into Fig.7.

In the present simulation the following assumptions were made: flow is a 2-D problem; Gaseous hydrogen-oxygen mixtures diluted with 25% argon are perfect gas; the dissipative effects, such as viscous, heat conductive and diffusive effects etc, are neglected.

The chemical reaction is modeled by the following ZND model of two-step chemical reaction proposed by Korobeinikov et al. (1972) [7]. In the ZND model the complex chemical reactions are simplified by two reaction progresses: induction reaction and exothermic reaction.

In the ZND model there are two progress parameters of chemical reaction: α for induction reaction and β for exothermic recombination reaction, respectively. The parameter α is set equal to unity before detonation wave front and then decreases to zero from 1, when the induction reaction terminates. The parameter β is set to equal to unity when the parameter α is not equal to zero and it will approach a particular value, when the second chemical reaction reaches equilibrium. The ZND model of two-step chemical reaction is shown into Fig.8.

3.2 CE/SE method and its improvement

The space-time conservation element and solution element (CE/SE) method is a new numerical framework for solving the equations of conservation laws. This new approach differs substantially both concept and methodology from the well-established methods, i.e. finite difference, finite volume and finite element method.

In the CE/SE method the computational region is divided into conservation elements (CE) and solution elements (SE). They are staggered to cover on computational region. The solution elements (SE) represent the neighboring domain affected by the certain grid, in which the physical variables and numerical flux are the relation of certain simple function with physical qualities and numerical flux of this grid. The conservation elements (CE) ensure the conservation properties of physical variables and numerical flux in the local domain of conservation elements and total computational domain. Since time and space coordinates have fundamentally a property in computation, so the space and time are unified and treated on the same footing.

The CE/SE method proposed by S. C. Chang [8] originally has to use three solution elements to solve three equations, in which the element structure and the calculation of CE/SE method are very complex. Besides, if discontinuity is occurred in flow field, it needs to add a new auxiliary equation. Therefore it has not already accord with original time-space conservation idea. Here we adopt directly four elements to solve Euler equations. Although it increases a computational element, but it can be simple, clear and direct to solve the flow field with discontinuity. The numerical results have shown that our improved CE/SE method has the advantages of slightly less computational time and good computational results.

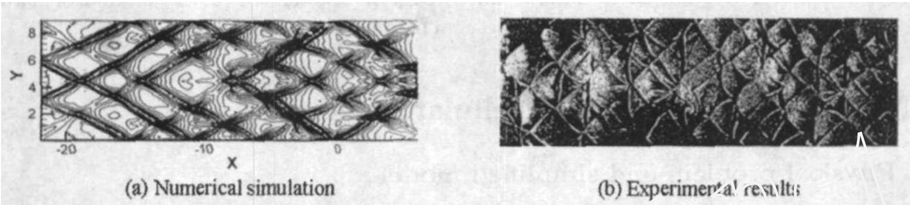

Fig. 9. Comparison of numerical simulation with experimental cellular pattern of DDT process for combustible hydrogen-oxygen mixture ($2H_2+O_2+Ar$, initial pressure 16kPa)

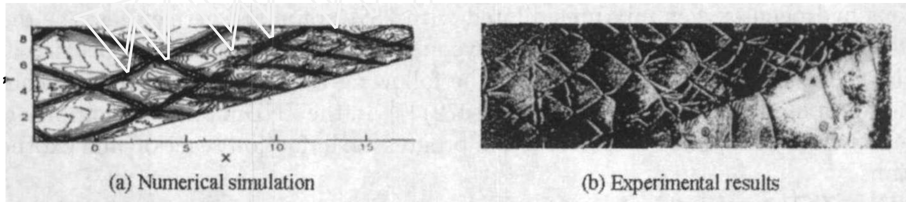

Fig. 10. Comparison of numerical simulation with experimental cellular pattern of Mach reflection for a detonation wave on a wedge (wedge angle 19.3^0)

3.3 Numerical results

The 2-D numerical simulations of the cellular structures before and after Mach reflection of detonation wave have been performed by using the simplified ZND model and improved (CE/SE) method. The cellular structures before and after Mach reflection have also been given numerically. Numerical cellular structure of the DDT process was put into Fig.9(a). Numerical cellular structure before and after Mach reflection of detonation wave on a wedge with 19.3^0 wedge angle was put into Fig.10(a).The numerical cellular structures were compared with the experimental cellular patterns by using soot track technique in Fig.9(b) and Fig.10(b). Compared results were shown that it is satisfactory. From numerical cellular structure in Fig.10(a) we can be seen that the changes of cellular structures before and after Mach reflection are very marked and the characteristic scales of cellular structures after Mach reflection will be diminished and the density of cells will be getting denser.

The numerical cellular structures with different wedge angles 10^0, 15^0, 19.3^0, 26.6^0, 30^0, 35^0, 40^0 and with different initial pressures 16.0, 20.0, 24.3, 26.3, 40.0kPa have been also simulated numerically. Numerical results pointed out that the numerical cellular structures are relative to wedge angle and initial pressures of gaseous mixture. The changes of numerical cellular structures before and after Mach reflection are basically consistent with experimental cellular patterns. It was shown that our numerical simulations of Mach reflection of gaseous detonation wave by using the improved CE/SE methods are successful.

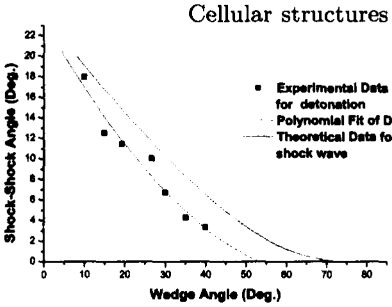

Fig. 11. $\chi-\theta$ relation for air shock wave and detonation wave

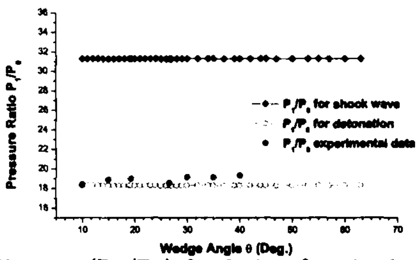

Fig. 12. (P_1/P_0)-θ relation for air shock wave and detonation wave

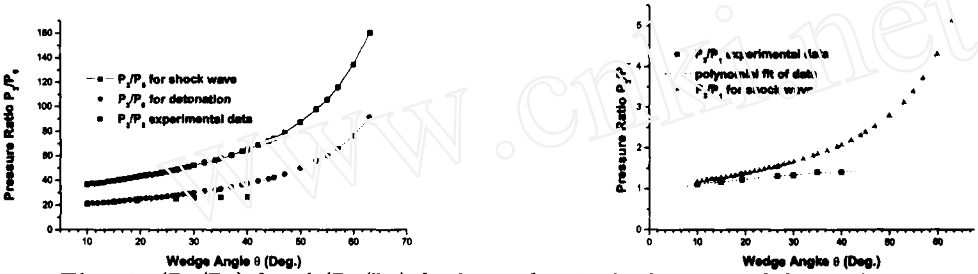

Fig. 13. (P_3/P_0)-θ and (P_3/P_1)-θ relation for air shock wave and detonation wave

4 Comparisons of the characteristics of Mach reflection between air shock wave and gaseous detonation wave

In order to understand deeply the mechanism of forming and developing process of the cellular structures and reflection properties of gaseous detonation wave, the analyses and comparisons of Mach reflection of air shock wave and gaseous detonation wave are very valuable. The characteristics of Mach reflection of air shock wave and gaseous detonation wave are different. Their main differences are as follows:

(1) In the flow-field of gaseous detonation wave there are complex cellular structures, but no cellular structures are exited in the flow-field of air shock wave. The cellular structures have a shape of lozenge pattern and during the detonation process of H_2-O_2 mixture with 16kPa initial pressure the mean scale of lozenge pattern is about 15mm. Under different conditions the mean scale of lozenge pattern can be different.

(2) The trajectory of the triple-point of Mach reflection of air shock wave is straight, but that of gaseous detonation wave is broken line. The angle χ between the trajectory of triple-point and wedge surface changes with the change of wedge angle. For both air shock wave and gaseous detonation wave, the change trend of angle χ is similar. However angle χ of air shock wave is larger more than that of gaseous detonation wave.

(3) Critical angle χ_{crit} for the transition from regular reflection to Mach reflection of air shock wave is larger than that of gaseous detonation wave. Angle χ_{crit} of air shock wave is $70^0 \sim 75^0$, that of gaseous detonation wave is $50^0 \sim 55^0$(see Fig.11).

(4) The ratios P_1/P_0 and P_3/P_0 of pressure behind incident shock wave and of pressure behind Mach reflection to initial pressure are changed with the change of wedge angle. The ratios P_1/P_0 and P_3/P_0 of air shock wave are larger more than those of gaseous detonation wave respectively. At M=5.12, The ratio values P_1/P_0 and P_3/P_0 of air

shock wave are 1.7 times more than those of gaseous detonation wave respectively (see Fig.12 ~ Fig.13).

5 Conclusions

1. The cellular structures before and after Mach reflection of gaseous detonation wave have been performed from experiments and numerical simulations. The numerical cellular structures were compared with the experimental cellular patterns. Compared results are satisfactory.
2. The changes of cellular structures before and after Mach reflection are marked. The cellular structures after Mach reflection will be diminished with the increase of wedge angle and initial pressure. When the wedge angle is larger more than 35^0 and initial pressure is larger more than 26.7kPa, the cellular structures after Mach reflection will no appear.
3. Critical angle χ_{crit} for the transition from regular reflection to Mach reflection of gaseous detonation wave is $50^0 \sim 55^0$.
4. The characteristics of Mach reflection of air shock wave and gaseous detonation wave are marked different.

6 Acknowledgement

This work was sponsored by NSFC & CEPA through NSAF foundation project with Grant No. 10276035.

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