# Wave Dynamic Process in Detonation Reflection from Wedges

### Zonglin Jiang, Zongmin Hu and John Lee\*

LHD, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China \*Mechanical Engineering Dept., McGill University, Montreal, Quebec H3B 4L8, Canada zljiang@imech.ac.cn

### Introduction

Many studies exist on shock reflection from wedges and more recently an increasing number of investigations have also been undertaken on detonation reflection. Yet, for the detonations reflection, some questions still remain unanswered, for example, the detonation front structure influenced by the reflection; the difference between shock and detonation reflections; the wave dynamic phenomena occurring in reflection processes; and the level of pressure enhancement due to different detonation reflection models.

Zhang *et al.* reported a large scale experiment on the detonation reflection in acetyleneair mixture, and the transition from regular to Mach reflection was found to take place in the Mach reflection regime predicted with three-shock theory. Guo *et al.* 2001 and Thomas *et al.* 2002 experimentally visualized detonation reflection from wedges and the smaller detonation cell behind Mach stem was demonstrated by using smoked foil. Ohyagi *et al.* 2003 simulated Mach reflection of detonation front, and the trajectory of a triple point was compared with experiments. Hu *et al.* 2004 computed various cases of detonation reflection from wedges and demonstrated the triple-point trajectory difference between shock waves and detonations. In this paper, the detonation reflection from wedges are investigated aiming at the wave dynamic process occurring in the wave front, including transverse shock motion and detonation cell variations behind the Mach stem.

### **Governing equations**

Assuming that viscosity effect on detonation propagation is negligible, the governing equations of gaseous detonations are the two-dimensional multi-component Euler equations with chemical reaction source terms. The equations can be written in conservation form with *ns* continuity equations for a perfect gas in Cartesian coordinates:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{i}{y} S_g = S$$

$$U = \begin{bmatrix} \rho C_1 \\ \rho C_2 \\ \vdots \\ \vdots \\ \rho C_{ns} \\ m \\ n \\ E \end{bmatrix} \quad S_g = \begin{bmatrix} nC_1 \\ nC_2 \\ \vdots \\ \vdots \\ nC_{ns} \\ mn/\rho \\ n^2/\rho \\ (E+p)n/\rho \end{bmatrix} \quad S = \begin{bmatrix} \frac{w_1}{w_2} \\ \vdots \\ \vdots \\ \vdots \\ \frac{w_{ns}}{w_{ns}} \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad F = \begin{bmatrix} mC_1 \\ mC_2 \\ \vdots \\ \vdots \\ mC_{ns} \\ m^2/\rho + p \\ mn/\rho \\ (E+p)m/\rho \end{bmatrix} \quad G = \begin{bmatrix} nC_1 \\ nC_2 \\ \vdots \\ \vdots \\ nC_{ns} \\ mn/\rho \\ n^2/\rho + p \\ (E+p)m/\rho \end{bmatrix}$$

where U is unknown variable, F and G numerical flux, Sg and S source and chemical reaction terms.  $C_i (i = 1, \dots, ns)$  are mass concentration,  $m = \rho u$ ,  $n = \rho v$ , u and v are velocity component in x- and y-direction,  $\rho = \sum_{i=1}^{n_s} \rho_i$ , the density of each species is

denoted by  $\rho_i$  (i = 1, ..., ns), the total energy per specific volume E is defined as

$$E = \rho h - p + \rho v^2 / 2 \tag{2}$$

According to Dalton's law, pressure p is the sum of the partial pressure for each species, and can be calculated with the equation of state for a perfect gas.

$$p = \sum_{i=1}^{n_s} \rho_i R_i T \tag{3}$$

where,  $R_i$  is the gas constant of species *i*, and *T* the temperature of gas mixture. For chemical reaction, all species are usually assumed to be thermally perfect gases, and the specific heat  $c_{vi}$  could be computed as following:

$$\frac{c_{pi}}{R_i} = a_{1i} \frac{1}{T^2} + a_{2i} \frac{1}{T} + a_{3i} + a_{4i} T + a_{5i} T^2 + a_{6i} T^3 + a_{7i} T^4 .$$
(4)

The enthalpies  $h_i$  per unit mass for each species are written as

$$\frac{h_i}{R_i T} = -a_{1i} \frac{1}{T^2} + a_{2i} \frac{1}{T} \ln T + a_{3i} + \frac{a_{4i}}{2} T + \frac{a_{5i}}{3} T^2 + \frac{a_{6i}}{4} T^3 + \frac{a_{7i}}{5} T^4 + \frac{b_{1i}}{T}.$$
 (5)

The constants  $a_{1i}, \dots, a_{7i}$  and  $b_{1i}$  can be found in Ref.[3]. As to the enthalpy of the gaseous mixture *h*, the following relation holds

$$h = \sum_{i=1}^{n_s} Y_i h_i , \quad Y_i = \rho_i / \rho$$
(6)

The chemical production rates  $\dot{w}_i$ , derived from a reaction mechanism that consists of *NR* chemical reactions, can be calculated by

$$\dot{w}_{i} = W_{i} \sum_{k=1}^{NR} (v_{ik}'' - v_{ik}') \left( K_{f,k} \prod_{j=1}^{n_{s}} (M_{j})^{v_{jk}'} - K_{b,k} \prod_{j=1}^{n_{s}} (M_{j})^{v_{jk}''} \right)$$
(7)

where, *i* and *j* denote the species in the *k* th chain reaction for reactants and products, *NR* stands for the total number of elementary reactions; the molecular weight of each species is denoted by  $W_i$ ;  $v'_{ik}$  and  $v''_{ik}$  are stoichiometric coefficients of species *i*, appearing as a reactant and as a product. The molecular concentration of each species is denoted by  $M_j$ .  $K_{f,k}$  and  $K_{b,k}$  denote the forward and the backward reaction rates, respectively. The forward reaction rate of each reaction is calculated by the Arrhenius law, and the corresponding backward reaction rate can be derived from the equilibrium constant. A nine species and 19 reactions model is accepted to account for hydrogenoxygen combustion in the present study. The reacting species are chosen to be  $H_2$ ,  $O_2$ , H, O, OH,  $H_2O_2$ ,  $HO_2$ ,  $H_2O$ , and a certain percentage of Argon.

### Numerical Algorithms

For numerical simulations, the second-order explicit difference equations of Eq.(1) discretized both in space and time by using the dispersion-controlled dissipative scheme proposed by Jiang *et al.* 1995 for shock wave capturing can be given as follows:

$$U_{j,k}^{n+1} = U_{j,k}^{n} - \frac{\Delta t}{\Delta x} \left( \overline{F}_{j+1/2,k}^{n} - \overline{F}_{j-1/2,k}^{n} \right) - \frac{\Delta t}{\Delta y} \left( \overline{G}_{j,k+1/2}^{n} - \overline{G}_{j,k-1/2}^{n} \right) - \frac{\Delta t}{y} S_{g_{j,k}}^{n} - \Delta t S_{j,k}^{n}$$
(9)

where 
$$\begin{cases} \overline{F}_{j+1/2}^{n} = F_{j+1/2L,k}^{+} + F_{j-1/2R,k}^{-} \\ \overline{G}_{j,k+1/2}^{n} = G_{j,k+1/2L}^{+} + G_{j,K-1/2R}^{-} \\ \end{cases}$$
$$\begin{cases} F_{j+1/2L,k}^{+} = F_{j,k}^{+} + \frac{1}{2} \Phi_{A}^{+} \min \operatorname{mod}(\Delta F_{j-1/2,k}^{+}, \Delta F_{j+1/2,k}^{+}) \\ F_{j+1/2R,k}^{-} = F_{j+1,k}^{-} - \frac{1}{2} \Phi_{A}^{-} \min \operatorname{mod}(\Delta F_{j+1/2,k}^{-}, \Delta F_{j+3/2,k}^{-}) \\ \end{cases}$$
$$\begin{cases} G_{j,k+1/2L}^{+} = G_{j,k}^{+} + \frac{1}{2} \Phi_{B}^{+} \min \operatorname{mod}(\Delta G_{j,k-1/2}^{+}, \Delta G_{j,k+1/2}^{+}) \\ G_{j,k+1/2R}^{-} = G_{j,k+1}^{-} - \frac{1}{2} \Phi_{B}^{-} \min \operatorname{mod}(\Delta G_{j,k-1/2}^{-}, \Delta G_{j,k+1/2}^{-}) \\ \end{cases}$$
$$\begin{cases} \Delta F_{j+1/2,k}^{\pm} = F_{j+1,k}^{\pm} - F_{j,k}^{\pm} \\ \Delta G_{j,k+1/2}^{\pm} = G_{j,k+1}^{\pm} - G_{j,k}^{\pm} \end{cases}, \quad \begin{cases} F^{\pm} = A^{\pm}U \\ G^{\pm} = B^{\pm}U \end{cases}, \quad \begin{cases} \Phi_{B}^{\pm} = I \mp \beta \Lambda_{B}^{\pm} \\ \Phi_{B}^{\pm} = I \mp \beta \Lambda_{B}^{\pm} \end{cases}$$

In these equations,  $(\cdot)^+$  and  $(\cdot)^-$  superscript signs denote flux vector splitting according to the Steger and Warming method. The time-marching integration was performed using a Runge-Kutta algorithm of second-order accuracy. In computation, the contribution from fluid dynamic terms is first calculated to obtain an intermediate value of U. This is followed by a calculation accounting for chemical reaction contributions to evaluate Ufor the next step. The approach allows separately solving fluid dynamic terms and chemical reaction terms with different time steps. The implication means that the fluid dynamic terms can be integrated during  $\Delta t$  being consistent with the *CFL* condition, and the chemical reaction terms are integrated with its own required time accuracy.

## Numerical results and discussion



Fig.1 CFD code verification

To verify the numerical code, a detonation propagating in a straight tube was calculated. After a steady state detonation develops, the detonation speed was found agrees well with experiment data and the detonation profile is similar to the self-similar law, as shown in Fig.1.

By setting a wedge of  $\alpha$ =19.3° and selecting a mixture of 2H<sub>2</sub>+O<sub>2</sub>+Ar at initial state conditions of  $P_0$ =16kPa and  $T_0$ =298K, the second case is carried out and some results are presented in Fig.2. Figure 2a shows a numerically calculated smoked foil record along a side wall, which demonstrates different detonation cells behind the detonation front. Figure 2b shows the maximum pressure at the detonation front both along the wedge surface and the upper wall at a series of time steps. The pressure indicates transverse shock reflection and triple-point collision. Figure 2a shows that the triple-point passes into the reflection region, moves faster downstream, and then reflects from wedge surface, and again moves faster toward no reflection region, which results in the smaller detonation cell behind March stem. The phenomenon is demonstrated more clearly in Fig.2b, where more pressure pecks indicating triple-point collisions are recorded on the wedge surface than on the upper wall. The reason is that the detonation reflection induces a Mach stem being an over-driven detonation front, so the transverse shocks travel faster.



(a) Detonation cell (b) Maximum pressure distributions Fig.2 Multi-wave detonation front reflecting from a wedge of  $\alpha$ =19.3° at initial pressure of 16*kPa* 

By increasing the initial pressure to 24kPa, the third case was carried out to show how transverse shock triple-points pass into no-reflection region. The results similar to Fig.2 are presented in Fig.3. Figure 3a show that as a transverse shock triple-point from the wedge passes into no-reflection region, a weak reflection is back into the reflection region, which results in detonation sub-cells. The small peaks observable late in the maximum pressure distribution on lower (wedge) wall indicate sub-triple point collisions. The main triple-point of the detonation reflection will catches up with adjacent transverse shock triple-points that move toward the upper wall, but the interaction effect is not visible in Fig.3. More cases were done on transition on regular to Mach reflection, and the critical angle was found to be 48°, which is smaller than most of the experimental data of 50°-53°, but agrees with that predicted with CCW (Chester-Chisnell-Whitham) theory. The detonation regular to Mach reflection results in even more higher pressure increase. In conclusion, detonation cells and transverse shock interaction occurring near the main triple-point play an important role in detonation reflection.



Fig.3 Multi-waves detonation front reflecting from a wedge of  $\alpha$ =19.3° at initial pressure of 24kPa

## References

- F. Zhang, S.B. Murray, P.A. Thibault: Transition from regular to Mach reflection of detonation waves in acetylene-air mixture. Proc. of the ISSW21, Australia, July 20-25, 1997, 339-341.
- [2] C.M. Guo, D.L. Zhang, and W. Xie: The Mach reflection of a detonation based on soot track measurements. Combustion and Flame, 127:2051-2058, 2001.
- [3] G.O. Thomas and R.L.Williams: Detonation interaction with wedges and bends. Shock Waves, 11: 481–492, 2002.
- [4] S. Ohyagi *et al.*: A numerical simulation of reflection processes of a detonation wave on a wedge. 19th ICDERS, Hakone, Japan, July 27 - August 1, 2003
- [5] Z.M. Hu *et al.*: Numerical simulation of gaseous detonation reflection over wedges with a detailed chemical reaction model, ACTA Mechanica Sinica, 20(4):385-391, 2004
- [6] Z. Jiang, K.Takayama, Y.S.Chen: Dispersion conditions for non-oscillatory shock capturing schemes and its applications. Comp Fluid Dynamics J, 4:137-150, 1995