Wave Dynamic Process in Detonation Reflection from Wedges

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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 detonation 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 acetylene-air 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 $n_s$ continuity equations for a perfect gas in Cartesian coordinates:

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

where,

$$U = \begin{bmatrix} \rho C_1 \\ \rho C_2 \\ \vdots \\ \rho C_m \\ m \\ n \\ E \end{bmatrix} \quad S_g = \begin{bmatrix} nC_1 \\ nC_2 \\ \vdots \\ nC_m \\ mn/\rho \\ n^2/\rho \\ (E + p)n/\rho \end{bmatrix} \quad S = \begin{bmatrix} \dot{w}_1 \\ \dot{w}_2 \\ \vdots \\ \dot{w}_m \\ 0 \\ 0 \end{bmatrix} \quad F = \begin{bmatrix} mC_1 \\ mC_2 \\ \vdots \\ mC_m \\ m^2/\rho + p \\ mn/\rho \end{bmatrix} \quad G = \begin{bmatrix} nC_1 \\ nC_2 \\ \vdots \\ nC_m \\ mn/\rho \\ n^2/\rho + p \end{bmatrix}$$

where $U$ is unknown variable, $F$ and $G$ numerical flux, $S_g$ and $S$ source and chemical reaction terms. $C_i (i = 1, \cdots n_s)$ are mass concentration, $m = \rho u$, $n = \rho v$, $u$ and $v$ are velocity component in x- and y-direction, $\rho = \sum_{i=1}^{n} \rho_i$, the density of each species is
denoted by \( \rho_i \) \((i = 1, \ldots, ns)\), the total energy per specific volume \( E \) is defined as
\[ E = \rho h - p + \rho v^2 / 2 \]  
(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.
\[ p = \sum_{i=1}^{n} \rho_i R_i T \]  
(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 \( c_{pi} \) could be computed as following:
\[ \frac{c_{pi}}{R_i} = a_{i_1} \frac{1}{T^2} + a_{2i} \frac{1}{T} + a_{3i} + a_{4i} T + a_{5i} T^2 + a_{6i} T^3 + a_{7i} T^4. \]  
(4)

The enthalpies \( h_i \) per unit mass for each species are written as
\[ \frac{h_i}{R_i T} = -a_{i_1} \frac{1}{T^2} + a_{2i} \frac{1}{T} \ln T + a_{3i} + \frac{a_{4i}}{2} T + \frac{a_{5i}}{3} T^2 + \frac{a_{6i}}{4} T^3 + \frac{a_{7i}}{5} T^4 + \frac{b_{ii}}{T}. \]  
(5)

The constants \( a_{ii}, \ldots, a_{7i} \) and \( b_{ii} \) can be found in Ref.[3]. As to the enthalpy of the gaseous mixture \( h \), the following relation holds
\[ h = \sum_{i=1}^{ns} Y_i h_i, \quad Y_i = \rho_i / \rho \]  
(6)

The chemical production rates \( \dot{w}_i \), derived from a reaction mechanism that consists of \( NR \) chemical reactions, can be calculated by
\[ \dot{w}_i = W_i \sum_{k=1}^{NR} (\nu^{*}_{ik} - \nu^{'}_{ik}) \left( K_{f,k} \prod_{j=1}^{n} (M_j)^{\nu^{*}_{ik}} - K_{b,k} \prod_{j=1}^{n} (M_j)^{\nu^{*}_{ik}} \right) \]  
(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 \( W_i \); \( \nu^{'}_{ik} \) and \( \nu^{*}_{ik} \) 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 hydrogen-oxygen 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 \etal 1995 for shock wave capturing can be given as follows:
\[ U_{j,k}^{n+1} = U_{j,k}^{n} - \frac{\Delta t}{\Delta x} \left( F_{j+1/2,k}^{n} - F_{j-1/2,k}^{n} \right) - \frac{\Delta t}{\Delta y} \left( G_{j,k+1/2}^{n} - G_{j,k-1/2}^{n} \right) - \frac{\Delta t}{y} S_{g,j,k}^{n} - \Delta t S_{j,k}^{n} \]  
(9)
where
\[
\begin{align*}
F_{j+1/2}^k &= F_{j+1/2L,k} + F_{j+1/2R,k} \\
G_{j,k+1/2}^- &= G_{j,k+1/2L}^+ + G_{j,k+1/2R}^-
\end{align*}
\]
\[
\begin{align*}
F_{j+1/2L,k}^+ &= F_{j+1,k}^+ + \frac{1}{2} \Phi_a^- \min \left( \Delta F_{j+1/2,k}^+, \Delta F_{j+1/2,k}^- \right) \\
F_{j+1/2R,k}^- &= F_{j+1,k}^- - \frac{1}{2} \Phi_a^+ \min \left( \Delta F_{j+1/2,k}^-, \Delta F_{j+1/2,k}^+ \right) \\
G_{j,k+1/2L}^+ &= G_{j,k+1}^+ + \frac{1}{2} \Phi_a^- \min \left( \Delta G_{j,k+1/2}^+, \Delta G_{j,k+1/2}^- \right) \\
G_{j,k+1/2R}^- &= G_{j,k+1}^- - \frac{1}{2} \Phi_a^+ \min \left( \Delta G_{j,k+1/2}^-, \Delta G_{j,k+1/2}^+ \right)
\end{align*}
\]

where
\[
\begin{align*}
\Delta F_{j+1/2,k}^+ &= F_{j+1,k+1}^+ - F_{j+1,k}^+ \\
\Delta G_{j,k+1/2}^+ &= G_{j,k+1}^+ - G_{j,k}^+
\end{align*}
\]

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 \(U\) for 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**

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.

![Fig.1 CFD code verification](image)

Fig.1 CFD code verification

By setting a wedge of \(\alpha=19.3^\circ\) and selecting a mixture of \(2\text{H}_2+\text{O}_2+\text{Ar}\) at initial state conditions of \(P_0=16\text{kPa}\) and \(T_0=298\text{K}\), 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.

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 reflection leads to higher pressure rise behind the Mach stem and the transition from 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.

References