

Transition between detonation and deflagration in a tube with a cavity

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Abstract. In this paper, the transition of a detonation from deflagration was investigated numerically while a detonation wave propagates in a tube with a sudden change in cross section, referred to as the expansion cavity. The dispersion-controlled scheme was adopted to solve Euler equations of axis-symmetric flows implemented with detailed chemical reaction kinetics of hydrogen-oxygen (or hydrogen-air) mixture. The fractional step method was applied to treat the stiff problems of chemical reaction flow. It is observed that phenomena of detonation quenching and reigniting appear when the planar detonation front diffracts at the vertex of the expansion cavity entrance. Numerical results show that detonation front in mixture of higher sensitivity keeps its substantial coupled structure when it propagates into the expansion cavity. However, the leading shock wave decouples with the combustion zone if mixture of lower sensitivity was set as the initial gas.

1 Introduction

Transition of a detonation from deflagration has been a fundamental topic in the detonation research for many years and received more attention recently due to the increasing interest in detonation-based propulsion systems. Many relevant experimental and numerical works [1–5] can be found. In [1,2] the interaction of detonation wave with structures such as wedges and bends was studied experimentally with the technique called smoked-foil recording. Experimental results of decoupling and re-coupling of detonation in tubes with sudden change in cross section can be found in [3,4]. Such problems was also simulated numerically with a simple chemical reaction model called two-step model in [5]. The present study is concerned with the transition of a detonation from deflagration when a detonation wave propagates in a tube with a sudden change in cross section, referred to as the expansion cavity. In addition, the detailed chemical reaction model was used to describe hydrogen-oxygen reaction mechanisms. When a detonation front moves into a cavity from a detonation tube, the leading shock wave and the combustion zone may decouple as a result of wave diffraction at the 90° bent corner. After the leading shock wave reflects from the sidewall of the cavity, the generated Mach stem will elevate the flow pressure of the compressed gas, which may lead to re-coupling of the leading shock wave and the combustion zone. Moreover, complex wave interactions in the cavity may induce an overdriven detonation front, which is an important phenomenon in detonation-driven shock tunnels and PDEs.

In this paper, the transition of a detonation from deflagration was investigated numerically. The dispersion-controlled scheme was adopted to solve Euler equations of axis-symmetric flows implemented with detailed chemical reaction kinetics of hydrogen-oxygen/air mixture. The fractional step method was applied to treat the stiff problem. Considering differences in the scales between the shocked flow and chemical reaction, multi-time steps were used to integrate the species continuity equations.

In order to examine influences of the sensitivity of the detonable gas on the detonation wave process, the gas mixtures of different composition at different pressure were used as initial conditions for the calculation.

2 Problem description

The problem can be simplified as the sketch in Fig. 1. The tube which is 40mm in length 20mm in diameter is connected with a cavity ring which is 100mm in length 60mm in diameter. In the beginning, the tube and cavity were charged with combustible gas mixture. Ignition zone with high pressure and temperature was set at the left end of the tube to obtain a planar detonation wave directly, So DDT process was not taken into consideration. The detonation wave travels into the cavity ring. Then complex wave interactions occur in the cavity due to the sudden change in the section area.

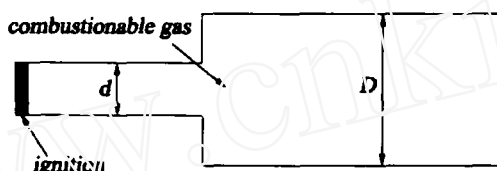


Fig. 1. Sketch of computational domain

3 Numerical methods

In this numerical study, Euler equations of axis-symmetric flows implemented with detailed chemical reaction kinetics of hydrogen-oxygen (or hydrogen-air) mixture was applied. For the reaction model 11 species ($H_2, O_2, O, H, OH, HO_2, H_2O_2, H_2O, N_2, N, NO$) and 23 detailed reactions were considered. The heat capacity at constant pressure of each species was obtained by the fitting formula given by B.J. McBride et al [6], which is function of gas temperature. The finite chemical reaction rate of each detailed reaction assumed to follow the Arrhenius laws. The dispersion-controlled scheme [7] was adopted to solve Euler equations. The fractional step method was applied to treat the stiff problems of chemical reaction flow.

Four kinds of combustible gas of different composition, pressure and temperature were set as the initial condition as following: (1) $2H_2 + O_2, P_0 = 60kPa, T_0 = 298K$ (2) $2H_2 + O_2 + 4N_2, P_0 = 60kPa, T_0 = 298K$; (3) $2H_2 + O_2 + 4N_2, P_0 = 50kPa, T_0 = 298K$ (4) $2H_2 + O_2 + 4N_2, P_0 = 40kPa, T_0 = 298K$. The temperature and pressure of the ignition zone were evaluated as $10T_0$ and $30P_0$ respectively. Non-catalyze and slip boundary condition was given for all walls and symmetric condition for the center line.

4 Solution verification

Fig. 2 shows the one dimensional detonation wave front structure at different time sequences. In this case, mixture (1) $2H_2 + O_2, P_0 = 60kPa, T_0 = 298K$ was set as the initial gas. The detonation wave velocity $D=2827$ is very close to the value of 2813.7 given in the report [8].

As to the tow dimensional cases, after the planar detonation wave discharges into the cavity ring form the detonation tube, the leading front becomes into a fan-shaped wave front step by step due to the diffraction process. As a result, the marginal part of the curved front gets attenuated instantly. If the combustible gas mixture is of low sensitivity, the attenuation can induce decoupling of the leading shock wave and the combustion zone.

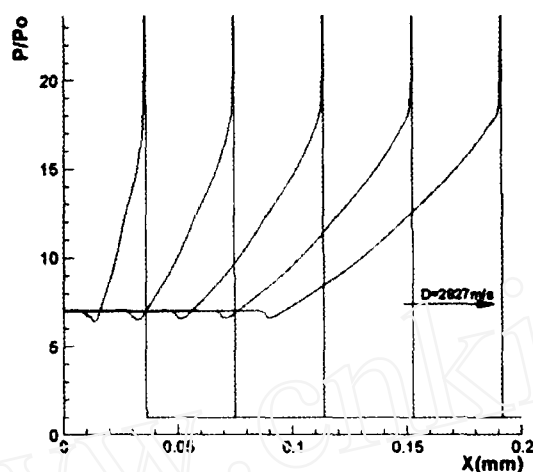


Fig. 2. One-dimensional detonation wave

5 Results and discussion

5.1 Case 1: $2H_2 + O_2$, $P_0 = 60kPa$, $T_0 = 298K$

In this case the initial gas mixture was set as $2H_2 + O_2$, $P_0 = 60kPa$, $T_0 = 298K$, which is of high detonation sensitivity. The numerical results showing the detonation wave propagation in the detonation tube and the cavity was shown in Fig. 3 in a time sequence. Isobars are plotted in the upper half of each sub-figure and isopycnics of H_2 in the lower half. These figures show that the leading shock wave and the combustion zone keep their couple structure after the detonation wave moves into the cavity. Planar detonation wave front as shown in Fig. 3a gets into a fan-shaped front (Fig. 3b), and reflects from the side wall of the cavity (Fig. 3c). The reflection develops from regular reflection into Mach reflection, which increases the wave strength near the side wall and push the spherical front into a new approximate planar shape (Fig. 3d). From distributions of density of H_2 in these figures, none decoupling process of detonation structure can be found. In this case, the combustible gas mixture is sensitive enough to keep the couple structure of the leading shock wave and the reacting zone.

5.2 Case 2: $2H_2 + O_2 + 4N_2$, $P_0 = 60kPa$, $T_0 = 298K$

To decrease the sensitivity of the combustible gas mixture, N_2 was added into the mixture as the diluent in case 2 while keeping the initial pressure and temperature unchanged. The sequential distribution of pressure and density of H_2 was given in Fig. 4. As shown from Figs. 4a-b, shortly after the detonation front moves into the cavity, the diffraction induces decoupling of the leading wave and the reacting zone at edge of the spherical detonation front. However, the center part of the detonation front still keeps its couple structure. In the decoupled zone as shown in Fig. 4b, the gas mixture is compressed and heated by the leading shock wave. While the detonation wave reaches the side wall and reflect back, the high pressure and temperature reignites the compressed combustible gas in the decoupled zone (Fig. 4c). Consequently, a more strong annular detonation wave comes into being and moves upstream. This annular detonation wave reflects over the end wall of the cavity and interacts with the vortex near the vertex at the

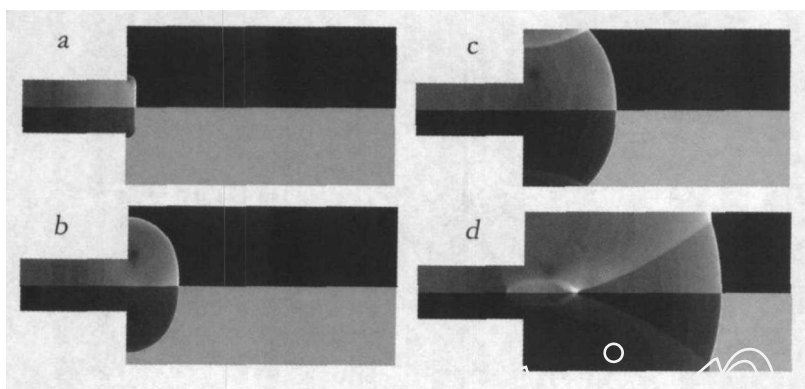


Fig. 3. Sequential numerical isobars(upper half) and isopycnics of H_2 (lower half), $a : 15.2\mu s$, $b : 20.7\mu s$, $c : 26.4\mu s$, $d : 40.6\mu s$ (case1: $2H_2 + O_2$, $P_0 = 60kPa$, $T_0 = 298K$)

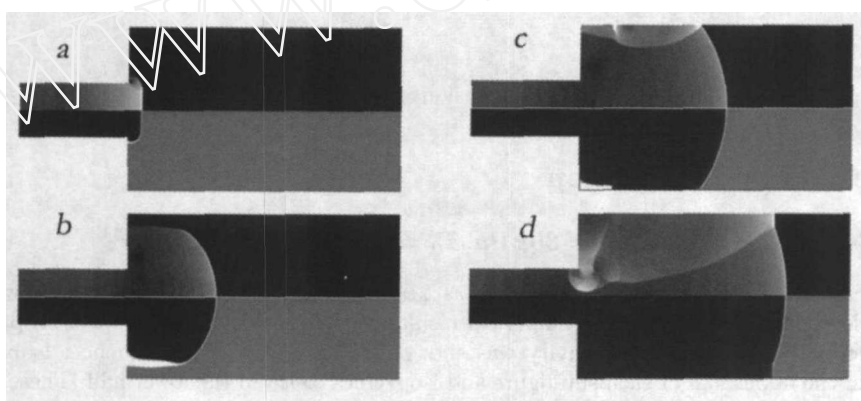


Fig. 4. Sequential numerical isobars(upper half) and isopycnics of H_2 (lower half), $a : 23.8\mu s$, $b : 39.1\mu s$, $c : 51.9\mu s$, $d : 64.6\mu s$ (case2: $2H_2 + O_2 + 4N_2$, $P_0 = 60kPa$, $T_0 = 298K$)

exit of the detonation tube. As a result, a spherical and strong shock comes into being(Fig. 4d) near the exit of the tube. The Mach stem developed over side wall drives the spherical leading shock front and will overtake the latter, which is as seem as the process in case 1.

5.3 Case 3: $2H_2 + O_2 + 4N_2$, $P_0 = 50kPa$, $T_0 = 298K$

In case 3, the composition of the gas mixture is set as same as that of case 2, while the initial pressure is reduced to $50kPa$. The results were plotted in Fig. 5 in a time sequence. As shown in Figs. 5a-b, a larger part of the detonation front gets decoupled. The center part of the detonation moves on and keeps the coupled structure all the way. Before reaching the side wall the leading shock wave slacks, and the reflection is so weak that none upstream detonation wave can be generated as in case 2(Figs. 5c-d).

5.4 Case 4: $2H_2 + O_2 + 4N_2$, $P_0 = 40kPa$, $T_0 = 298K$

In this case the initial pressure P_0 is reduced to $40kPa$. Isobars and isopycnics of H_2 were drawn in Fig. 6. From Figs. 6a-c, we can see that the decoupled zone extends to the center line from

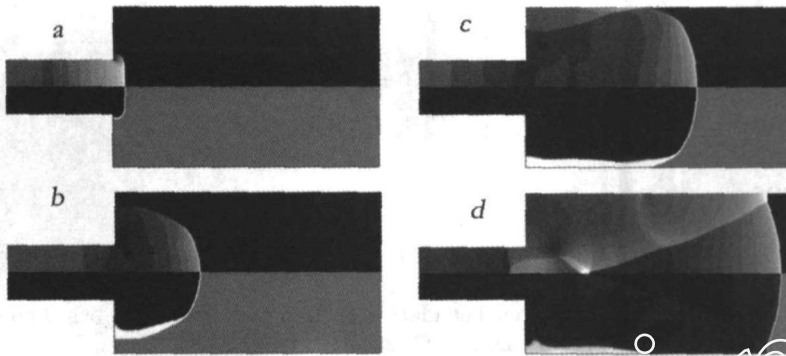


Fig. 5. Sequential numerical isobars(upper half) and isopycnics of H_2 (lower half), $a : 24.5\mu s$, $b : 40.3\mu s$, $c : 60.5\mu s$, $d : 79.6\mu s$ (case3: $2H_2 + C_2 + 4N_2$, $P_0 = 50kPa$, $T_0 = 298K$)

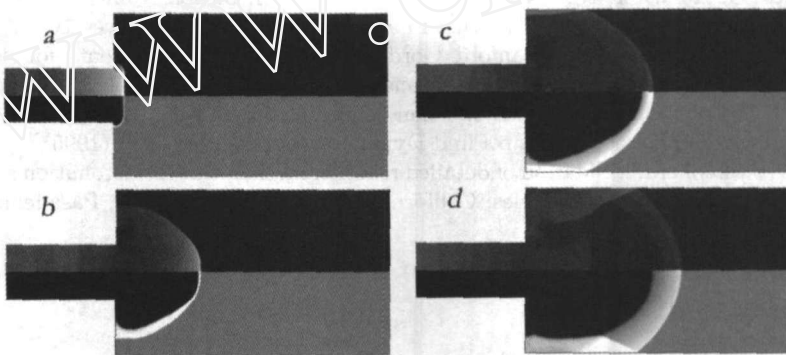


Fig. 6. Sequential numerical isobars(upper half) and isopycnics of H_2 (lower half), $a : 22.6\mu s$, $b : 40.6\mu s$, $c : 54.6\mu s$, $d : 68.8\mu s$ (case3: $2H_2 + O_2 + 4N_2$, $P_0 = 40kPa$, $T_0 = 298K$)

the edge of the fan-shaped detonation front. Finally, the entire combustion zone detach from the leading shock(Figs. 6c-d). The shock gets attenuated and the reflected shock over the side wall isn't strong enough to reignite the gas mixture. Then the detonation wave quenches and degenerates into deflagration completely.

6 Conclusions

In this paper detonation propagation in a tube with a cavity was simulated with detailed chemical reaction model. Four kinds of $H_2 + O_2/H_2 + O_2 + N_2$ gas mixture of different sensitivities were considered as the the initial combustible reactants. From these numerical results, it is observed that the planar detonation front changes its shape into spherical one after it diffracts at the vertex of the cavity entry. However, the leading shock wave decouples with the combustion zone can be found in the gas mixture of low sensitivity but not in that of high sensitivity such as in case 1. Complex wave interactions due to the process of reflection, focus and reigniting in the cavity can induce an overdriven detonation front. Finally, this work extended firstly the DCS scheme proposed by Jiang et al [7] to the Euler system considering multi-species and detailed reaction model. This scheme is robust and capable of simulating the detonation wave well without local grid refinement.

7 Acknowledgement

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