

Theoretical Study on the Deflagration to Detonation Transition Process

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Detonation is a fast and efficient form of energy transfer. The energy density of detonation wave could reach $10^{10}\text{W}/\text{cm}^2$, which is quite destructive. Thus, detonation has great application potential in hypersonic propulsion. Under different ignition conditions, detonation wave initiation can be divided into direct initiation and deflagration-to-detonation transition(DDT). DDT process is a research hotspot in the field of detonation at present. To clarify the physical mechanism of DDT process and predict the critical condition of DDT accurately is of great significance to understand detonation phenomena and to prevent production accidents.

DDT process is a complex non-linear physical process, which involves shock wave mechanics, thermodynamics and chemical reaction kinetics. To describe and predict DDT process completely, the coupling of shock wave interaction, combustion and turbulence should be considered. In this paper, a one-dimensional model of DDT process is proposed. The theoretical criterion of DDT is given and a series of experimental results are compared. The theory is supported by numerical calculation.

1 DDT Criterion

The study of detonation physics shows that there exists a critical state in the process of DDT. When the state of experimental gas reaches this critical state, deflagration is converted into detonation. Under this condition, which is called quasi-detonation (or CJ deflagration), the detonation wave can propagate steadily for a long distance. The transition from quasi-detonation to detonation is abrupt. Namely, there is no intermediate state between them. The experimental results show that the flow field structure of quasi-detonation wave is quite different from that of detonation wave. The quasi-detonation wave has a long wave-front, and the distance between the shock surface and the flame surface is much larger than that under the detonation condition, showing a remarkable double discontinuous structure. The results of Zhu Yujian^[5] show that the area between shock wave and flame surface (zone 2 in figure 1) in quasi-detonation wave is affected by both leading shock wave and flame surface. This phenomenon cannot be described by ZND model.

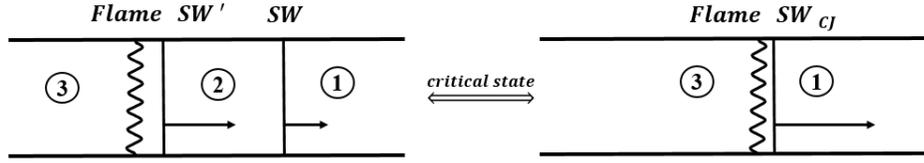


Figure 1. Critical Condition for DDT Process

In order to determine the gas parameters in the critical state, a one-dimensional model (figure 1) is proposed. In the critical state, there exists another moving shock SW' between the leading shock and the flame surface. SW' is accelerated by the flame surface. The velocity of SW' in the laboratory reference system is higher than that of the leading shock wave. Consequently, SW' catches up with SW during a short time and DDT occurs. The combination of the two produces a C-J detonation wave SW_{CJ} . Meanwhile, the detonation wave is coupled with the flame surface and enters a stable self-propagating detonation state.

At critical state, the gas parameters in zone 1 and 3 are the same as those in detonation state, while the gas parameters in zone 2 satisfy the compatibility relationship, which is determined by the gas parameters in zone 1 and 3. The relationship between critical state and stable detonation state can be established using the theory of shock mechanics and thermodynamics.

The temperature and gas velocity in zone 2 satisfy the moving direct shock equation

$$\frac{T_2}{T_1} = \frac{[2\gamma M_1^2 - (\gamma - 1)][(\gamma - 1)M_1^2 + 2]}{(\gamma + 1)^2 M_1^2} \quad (1.1)$$

$$\frac{V_2}{c_1} = \frac{2}{\gamma + 1} \left(M_1 - \frac{1}{M_1} \right) \quad (1.2)$$

When the gas passes through the second intersection, if the characteristic time of the chemical reaction is much less than that of the flow ($Da = \tau_r/\tau_f \ll 1$), the combustion process will be constant-volume combustion

$$\frac{p_3}{p_2} = \frac{T_0}{T_2} \quad (1.3)$$

The change of pressure is caused by the second shock wave

$$\frac{p_3}{p_2} = \frac{2\gamma M_2^2 - (\gamma - 1)}{\gamma + 1} \quad (1.4)$$

At critical state

$$D_{CJ} = D_2 + V_2 \quad (1.5)$$

Under the approximation that $\gamma \approx 1.4$, $\frac{a_1^2}{D_1^2} \ll 1$, $\frac{T_2}{6T_0} \ll 1$, The critical criterion takes the simple form

$$D_c = 1.2(D_{CJ} - \sqrt{1.2RT_0}) \quad (1.6)$$

Temperature T_0 can be measured in experiments and D_{CJ} can be calculated by CJ theory. The DDT process occurs when the velocity of the leading shock reaches D_c . When the two shock waves are decoupled, the detonation transfers to deflagration and the velocity decreases to D_c .

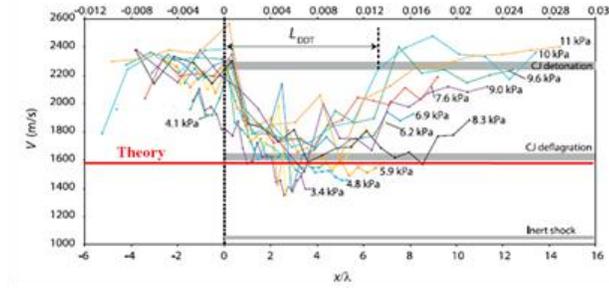


Figure 2. Comparison of Critical Criterion and Experimental Results^[6].

The comparison between the above theoretical criteria and experimental results is given in figure 2. Under the experimental condition, critical wave velocity $D_c \approx 0.635D_{CJ}$, as shown by the red line in the figure. The theoretical prediction is in good agreement with the experimental measurement. By this criterion, the ratio D_c/D_{CJ} is about 60% when different fuel is selected for experiments^{[7]-[10]}.

2 Mechanism of quasi-detonation

In numerical calculation, it is difficult to simulate quasi-detonation directly. To study the propagation mechanism of quasi-detonation, a simplified three-dimensional model is proposed in this paper.

In Cartesian coordinates, the inviscid governing equation of the one-step overall reaction model is

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0 \quad (2.1)$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} = 0 \quad (2.2)$$

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho vu)}{\partial x} + \frac{\partial(\rho v^2 + p)}{\partial y} + \frac{\partial(\rho vw)}{\partial z} = 0 \quad (2.3)$$

$$\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho wu)}{\partial x} + \frac{\partial(\rho wv)}{\partial y} + \frac{\partial(\rho w^2 + p)}{\partial z} = 0 \quad (2.4)$$

$$\frac{\partial(\rho e)}{\partial t} + \frac{\partial(\rho e + p)u}{\partial x} + \frac{\partial(\rho e + p)v}{\partial y} + \frac{\partial(\rho e + p)w}{\partial z} = 0 \quad (2.5)$$

$$\frac{\partial(\rho Z)}{\partial t} + \frac{\partial(\rho uZ)}{\partial x} + \frac{\partial(\rho vZ)}{\partial y} + \frac{\partial(\rho wZ)}{\partial z} = \dot{w} \quad (2.6)$$

$$e = \frac{RT}{\gamma - 1} + \frac{1}{2}(u^2 + v^2 + w^2) + Zq \quad (2.7)$$

$$\dot{w} = -K\rho Z \exp\left(-\frac{E_a}{RT}\right) \quad (2.8)$$

Where ρ is gas density, u, v, w the velocity of X, Y, Z direction, e the energy density, Z the mass fraction of reactants, q the density of heat release, γ the specific heat ratio, \dot{w} the mass formation rate of combustion products, K the pre-exponential coefficient, E_a the activation energy, T the temperature, R the gas constant, respectively.

Suppose there is a main direction X. The above equation can be simplified on condition that partial derivatives along the Y and Z directions are ignored

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0 \quad (2.9)$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} = 0 \quad (2.10)$$

$$\frac{\partial(\rho e)}{\partial t} + \frac{\partial(\rho e + p)u}{\partial x} = 0 \quad (2.11)$$

$$\frac{\partial(\rho Z)}{\partial t} + \frac{\partial(\rho u Z)}{\partial x} = \dot{w} \quad (2.12)$$

$$e = \frac{RT}{\gamma - 1} + \frac{1}{2}(u^2 + v^2 + w^2) + Zq \quad (2.13)$$

$$\dot{w} = -K\rho Z \exp\left(-\frac{E_a}{RT}\right) \quad (2.14)$$

The equations are similar to one-dimensional inviscid governing equations. The only difference is that the kinetic energy term contains the velocity in the Y and Z directions. Consider the velocity of main direction then total kinetic energy can be expressed as:

$$\frac{1}{2}(u^2 + v^2 + w^2) = \frac{1}{2}Cu^2 \quad (2.15)$$

$C < 0$ does not correspond to the real physical process, so $C \geq 0$. The simplified governing equation is used to simulate the behavior of quasi-detonation wave and the DDT process, as shown in figure 3. It is shown that $C=2.8$ corresponds to a critical state in which the wave velocity is about 50%~60% of the detonation wave velocity, which is similar to the quasi-detonation wave velocity observed experimentally. As C continues to decrease, DDT occurs and the velocity rises to CJ detonation velocity. There is no intermediate state between the two states.

Studies show that the quasi-detonation wave is thermally choked. In this example, the chemical energy released by the complete combustion of fuel is not fully converted to the kinetic energy corresponding to the main direction velocity. Therefore, the simplified one-dimensional governing equation manages to simulate the quasi-detonation state and DDT process.

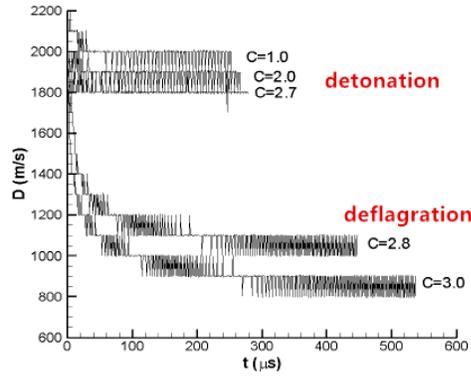


Figure 3. The variation of combustion velocity with time under different values of proportional coefficient C

3 Numerical simulation of flow field

In the above one-dimensional example, when the ratio coefficient C is between 1.0 and 2.7, detonation could occur. In this paper, the following two-dimensional numerical examples are used to explain the physical meaning of C . The computational domain is a rectangular region in a two-dimensional pipeline. The left and right sides of the pipeline are free boundaries, and the upper and lower sides are fixed walls. A $1\mu\text{m}$ grid is used. After initiation, the maximum pressure at each point is recorded and the cell pattern is shown in figure 4. The variation of detonation velocity with time at section 1 is also given in the figure. Detonation velocity becomes highest near the triple point and the lowest at a certain location inside the cell. Detonation velocity changes periodically due to the stable cell structure.

The distribution of velocity u and v in the X and Y directions in the cell diagram is also shown in figure 4. V is perpendicular to the propagation direction of detonation wave. Thus it has no direct contribution to the propagation of detonation wave. At a certain time, u varies at different sections. Then the velocity perpendicular to the propagation direction is needed to adjust the flow field structure. Therefore, v relates to the energy loss to adjust the flow field. The kinetic energy corresponding to the velocity u in the main direction occupies a certain proportion C of total kinetic energy. It can be seen from the figure that v/u is about 0.5-0.6 on the cell boundary, and the corresponding C value is about 1.3.

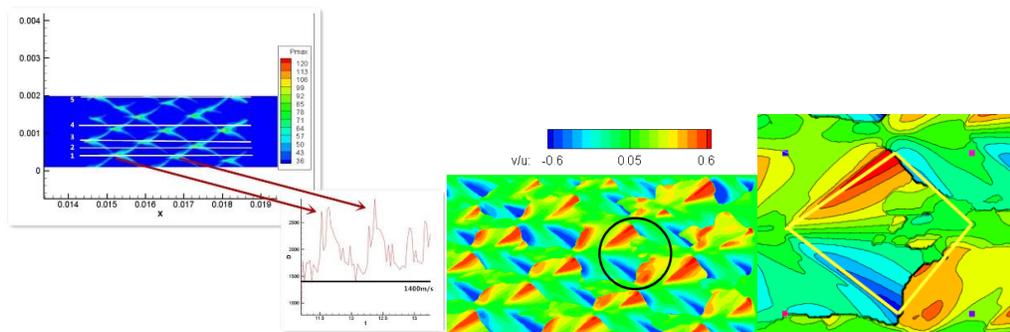


Figure 4. Left: variation of detonation wave velocity in cells; right: the distribution of v/u in two-dimensional cells

4 Conclusion

A one-dimensional model describing DDT process is proposed. The critical criterion of DDT is obtained by theoretical analysis, which is in good agreement with the experimental results. The propagation state of quasi-detonation wave and the critical state of DDT are obtained by numerical simulation with simplified three-dimensional equation. The physical meaning of the proportional coefficient C in the simplified model is explained by a numerical example of two-dimensional detonation.

Acknowledgments

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