

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}W/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. It is a complex non-linear physical process which involves shock wave mechanics, thermodynamics, chemical reaction kinetics, etc. 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. In this paper, the quantitative criteria of DDT is given and a series of experimental results are compared.

Detonation phenomenon was observed by Berthelot, Vieille and Le Chatelier in the study of flame propagation in 1881. The theoretical study of DDT started soon after the discovery of detonation phenomenon in experiments. In 1883, Mallard and Le Chatelier published the first photographic observations of detonation. Their figure indicated that the flame fluctuates intensely as detonation initiates. Due to the limit of experimental equipment, researchers cannot reveal more details of DDT process. In 1928, Payman and his associates observed the shock wave interaction in the DDT process directly with rotating mirror camera. In 1935, Bone, Fraser and Wheeler founded that shock waves propagate ahead of flame surface in the unburned mixture. They postulated that the combustion of shock-compressed medium at some point in front of the flame initiates the detonation wave. In 1951, Schmidt, Steinicke and Neubert published a series of high frequency stroboscopic schlieren photographs, revealing more details of the interaction between shock waves and flame surface during DDT process. In 1966, Urtiew and Oppenheim adopted soot imprint technique and stroboscopic schlieren photographs with intense light source to study DDT process. They proposed that the transition takes place in various modes depending on the wave interaction processes which occur ahead of the accelerating flame^[1]. The DDT process occurs in such short time that one can get little inspiration from experimental observations.

The application of CFD greatly promoted the theoretical study of DDT. Numerical simulations for obstacle-laden channels with a one-step Arrhenius chemical model has become a common approach to study DDT. Zel'dovich proposed a gradient mechanism to explain DDT process. The compression wave formed at the initial ignition is coupled with the heat release of reaction along the temperature gradient of the mixture.

The process is intensified to form detonation. Lee and his associates conducted more accurate numerical simulation using detailed chemical reaction model and proposed SWACER(Shock Wave Amplification by Coherent Energy Release) theory to explain DDT^[12]. The formation of detonation wave is due to the coupling and amplification of shock wave and chemical energy release. The theory is supported by some experimental and numerical results. But the detailed mechanisms of the amplification of shock wave and chemical reaction remain unknown.

The study of detonation shows that there exists a critical state in the process of DDT. When the state of experimental gas reaches the 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 theories mentioned above cannot explain quasi-detonation state and the abrupt transition. In this paper, a new model of DDT process is proposed. The main idea of the model is that in the laboratory coordinate system, the detonation wave surface and the flame surface are transonic. The supersonic and subsonic flow region of the flame surface will produce different flow behavior, which directly affects the DDT process of the detonation wave. The idea comes from the fact that detonation wave decouples under expansion caused by obstacles. The model is supported by numerical calculation of one dimensional Euler equation with an expansion term. Furthermore, it is verified that detailed chemical reaction model produces the same conclusion.

1 Quantitative Criteria of DDT

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.

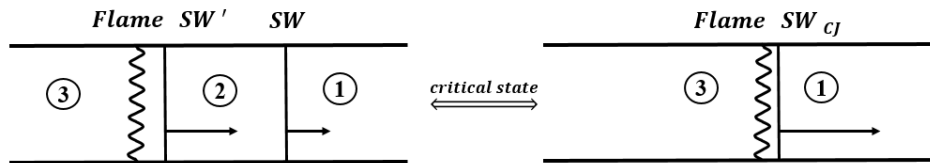


Figure 1. Critical Condition for DDT Process

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 .

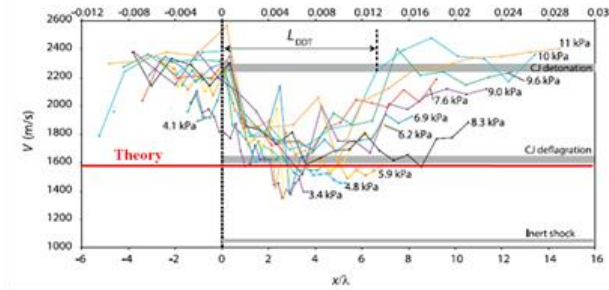


Figure 2. Comparison of Critical Criterion and Experimental Results^[6].

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 Physical Model of DDT

2.1 Inspiration from flow field of 2d detonation

The idea of the model comes from two-dimensional numerical simulation of Euler equation with detailed chemical reaction model. Figure 3 shows the distribution of pressure and Mach number along pipeline direction of detonation. The unburned gas is stoichiometric hydrogen-air mixture. From the distribution of Mach number in the flow field, one can find that most area of flame surface is supersonic. When the detonation wave passes through obstacles in closed pipe, temperature and pressure of supersonic gas decrease after expansion. As a result, detonation wave decouples into deflagration wave. This phenomenon inspires us to simulate the critical state of DDT through expansion effect.

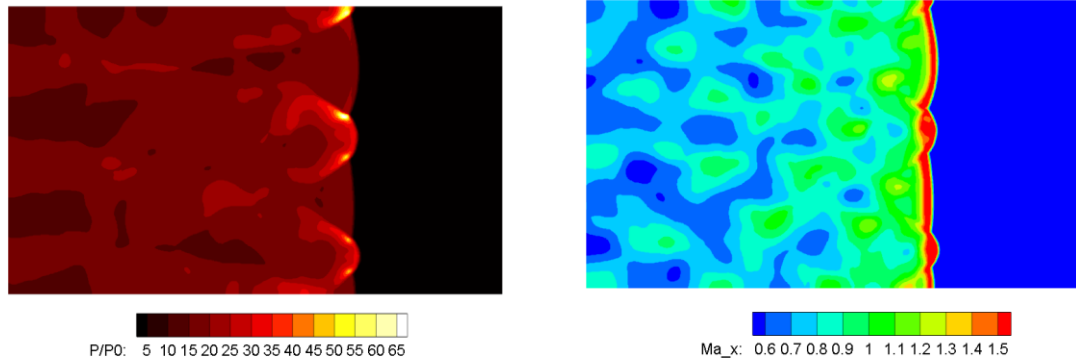


Figure 3. Left: distribution of pressure in CJ detonation; right: distribution of Mach number in the same position

2.2 Numerical simulation of 1D Euler equation with an expansion term

In numerical calculation, it is difficult to simulate the critical state of DDT directly. To study the mechanism of DDT, an expansion term is introduced to simulate quasi-detonation state, which is also the critical state of DDT.

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

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

Suppose there is a main direction X. The 3d equation can be simplified on condition that partial derivatives along the Y and Z directions are ignored.

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

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

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

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

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

Where ρ is gas density, u the velocity, 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.

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:

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

$C > 1$ is an expansion coefficient, which represents the expansion from one dimension to higher dimensions. The introduction of the expansion term is a special technique to simulate quasi-detonation^[13]. Figure 4 shows the velocity of combustion wave under different expansion coefficient. When $C > 2.8$, the detonation wave decouples and propagates at the speed of nearly $0.5D_{CJ}$.

The results can be explained by the DDT model in the paper. In the laboratory coordinate, most areas of flame surface are supersonic. According to the principle of gas dynamics, the heat release from combustion in the subsonic region of the flame surface cannot affect the leading shock wave. The expansion term in Euler equation makes the pressure and temperature of the gas in the supersonic area of flame surface decrease. Then the intensity of the leading shock wave decreases and the velocity of the wave decreases. The slowing down of the leading shock wave further leads to the decrease of gas velocity, pressure and temperature behind the wave, and the further weakening of the leading shock wave intensity, which forms a positive feedback. Eventually, the positive feedback leads to the decoupling of the detonation wave and the formation of a quasi-detonation wave. Since the supersonic region cannot be completely converted to subsonic velocity by the expansion effect alone, the quasi-detonation state can be simulated by this special technique.

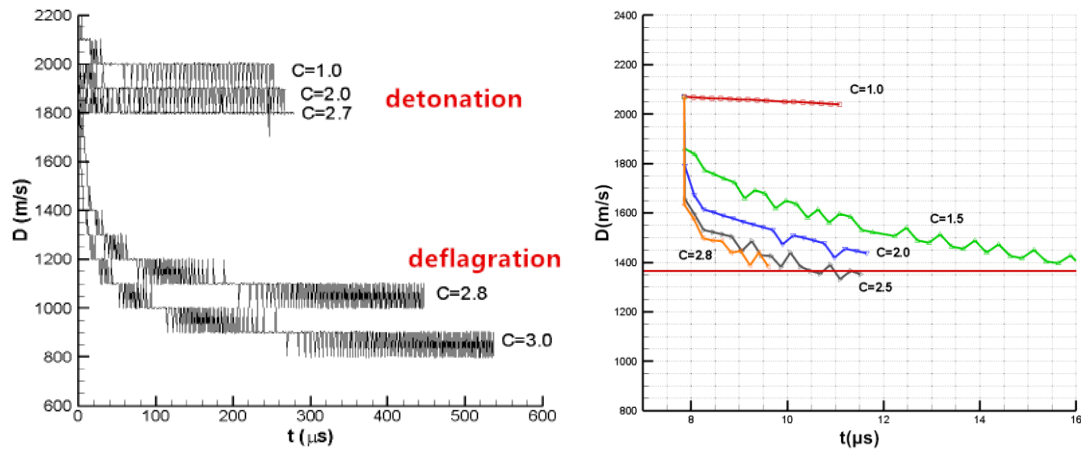


Figure 4. The variation of combustion velocity with time under different values of expansion coefficient C . Left: one-step model; right: detailed chemical reaction model

2.3 Numerical simulation with detailed chemical reaction model

The model is further verified by the numerical simulation with detailed chemical reaction model. The velocity of combustion wave under different expansion coefficient is also shown in figure 4. The detonation wave also decouples under certain expansion effect. But the critical value of expansion coefficient C is smaller than that calculated by one-step model. Since the heat release in detailed model is slower, the

supersonic region in the flame surface is large. Consequently a weak expansion could trigger the aforesaid positive feedback and make the detonation wave decouple.

3 Conclusion

A quantitative criteria of DDT is obtained by theoretical analysis, which is in good agreement with experimental results. By introducing an expansion term in Euler equation, the quasi-detonation state is simulated successfully with one-step overall model or detailed chemical reaction model. A physical model of DDT is proposed. In this model, the detonation wave surface and the flame surface are transonic in the laboratory coordinate. The supersonic and subsonic flow region of the flame surface will produce different flow behavior, which directly affects the DDT process of the detonation wave. This model can explain the physical mechanism of DDT process and decoupling process of detonation explicitly.

Acknowledgments

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