Study on Simplified Model of Detonation Based on Wave Front Curvature

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1 Introduction

Although the detonation model constructed by Euler system contains almost all the necessary elements in real physical reality, the research work is still difficult due to high nonlinearity of the equations, etc. The simplified model proposed by Fickett[1,2] contains only one scalar conservation equation and one reaction rate equation, which simplifies the nonlinear problem of Euler reaction equations mathematically. Although this model omits many physical details, it can reflect the characteristics of one-dimensional detonation in the Euler equations well. This simplified model can consider the effects of shock wave and rarefaction wave, and can study many detonation dynamics from a qualitative perspective, such as the problems of stable propagation of detonation wave structures, initiation of explosion and boundary layer loss, etc. Fickett [1,2] 's simplified model of detonation was later developed by Majda et al.[3] and Faria et al.[4].They added an energy release term to the Burgers equation. If the source term of modified Burgers equation contains loss terms at the same time, the existence of a critical condition is one of the signature characteristics of detonation wave. Wood et al. [5] did numerical iterations on the reaction zone and found that there is a point of inflection in the iterative image. This inflection point can be defined as the critical condition for detonation failure. However, not all eigen curves have such a critical condition, and the occurrence of inflection point is closely related to detonation itself.

In this paper, a simplified model of analog system is considered for the dynamics of one-dimensional detonation with generic losses. The simplified model consists of a single partial differential equation which can describe many properties of detonation waves at a qualitative level. The critical characteristic of detonation wave propagation is captured by studying the influence of curvature on detonation dynamic using analytic method. Direct numerical simulation is used to observe the propagation of detonation wave and verify the analytic method. The simulation results show that the front curvature has decisive influence on the failure of detonation wave propagation.

2 Simplified model of detonation and theoretical analysis

Based on Fickett's simplified model, we can construct a one-dimensional Burgers equation with reaction term and loss term. The governing equation is as follows:

$$\frac{\partial u}{\partial t}+\frac{\partial}{\partial x^L}(\frac{1}{2}u^2)=Q\frac{\partial \lambda}{\partial t}-c(\frac{u}{u_{CJ}})^m \tag{1}$$

In the formula, u is a scalar; Q is chemical energy per unit mass; λ is reaction progress

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variable, $0 \le \lambda \le 1$, $\lambda = 0$ when there is no reaction, $\lambda = 1$ when the reaction is complete; Coefficient of loss term c can be used to simulate detonation wave front curvature; m is state correlation of loss rate; t is reaction time; x^L is location of detonation wave in the space coordinate system; u_{CJ} can be used to simulate detonation wave velocity in the CJ state.

Reaction rate equation uses a single-step Arrhenius expression [6,7]. That is

$$\frac{\partial \lambda}{\partial t} = k(1-\lambda)\exp(-\frac{u_0}{u}) \tag{2}$$

In the formula, u_0 can be used to simulate the activation energy in the Euler equation; The pre-exponential factor k is a parameter defining the spatial and temporal scales. In the equation, u is used to simulate some intrinsic properties in the compressible flow, such as density, velocity or specific energy. The value of pre-exponential factor k usually changes half reaction length $L_{1/2}$ of detonation wave in ZND model to unit length. The reaction is ideal detonation when curvature $c = 0$. Here taking $Q = 0.5$, steady state CJ detonation velocity is as follows(D_{CJ} is detonation velocity in the CJ state) :

$$u_{CJ} = D_{CJ} = 2Q = 1 \tag{3}$$

Since detonation velocity D is the main research object, for the sake of convenience, we can build the coordinate system on the detonation wave propagating at velocity D to transform equations (1) and (2) using the relationship $x = x^L - Dt$. We obtain

$$\frac{\partial u}{\partial t} + (u - D)\frac{\partial u}{\partial x} = Q(\frac{\partial \lambda}{\partial t} - D\frac{\partial \lambda}{\partial x}) - c(\frac{u}{u_{CJ}})^m \tag{4}$$

$$\frac{\partial \lambda}{\partial t} - D\frac{\partial \lambda}{\partial x} = k(1-\lambda)\exp(-\frac{u_0}{u}) \tag{5}$$

2.1 Stationary solution

For detonation waves that propagate stably at velocity D, let all time derivative terms in equations (4) and (5) be equal to 0.We obtain

$$(u-D)\frac{du}{dx} = Q(-D\frac{d\lambda}{dt}) - c(\frac{u}{u_{CJ}})^m \tag{6}$$

$$-D\frac{d\lambda}{dx} = k(1-\lambda)\exp(-\frac{u_0}{u}) \tag{7}$$

Combined with reaction rate equation, the equation for variation of u and λ in the reaction zone can be derived:

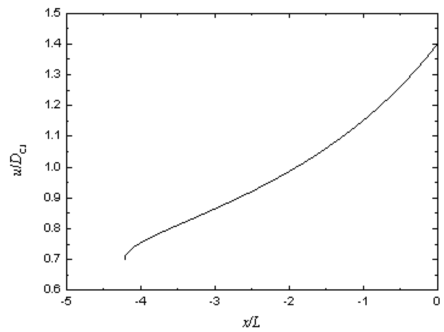
$$\frac{du}{dt} = \frac{Qk(1-\lambda)\exp(-\frac{u_0}{u}) - c(\frac{u}{u_{CJ}})^m}{u - D} \tag{8}$$

$$\frac{d\lambda}{dx} = \frac{k(1-\lambda)\exp(-\frac{u_0}{u})}{-D} \tag{9}$$

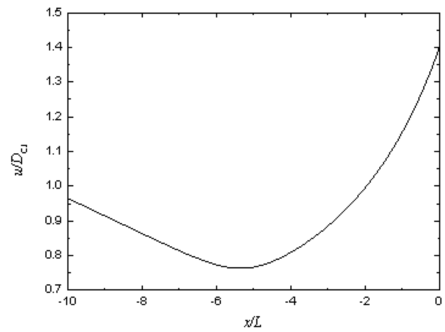
The detonation wave is led by leading shock wave with jump discontinuity, and no energy is released when passing through leading shock wave, but the density and pressure will have jump changes. With the shock wave acting as discontinuous line, we can apply the discontinuous condition of unreacted wave front (Rankine - Hugoniot condition) to obtain :

$$u(x = 0) = 2D, \lambda(x = 0) = 0 \tag{10}$$

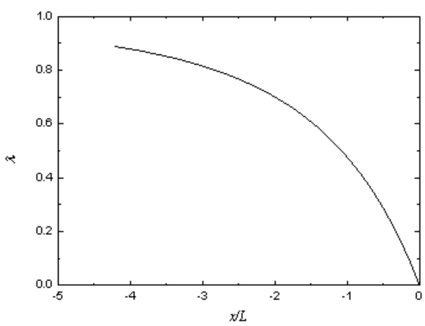
We arbitrarily select a shock wave velocity and integrate steady-state equations (8) and (9). If the numerator and denominator of the equation are not both 0, the sound singularity appears when $u - D \to 0$. Regular solution criterion requires that the numerator is also 0 when the sound velocity singularity occurs. That is generalized CJ criterion, and usual CJ criterion is that when $u - D \to 0$ gets balanced, the numerator follows denominator and becomes 0 at the same time [8]. Taking D =0.7, k =1, u_0 =1, m = 2, the result of the integration is shown in Fig 1. Left and right diagrams in Fig.1 are the cases that meet and do not meet the regular conditions respectively. Propagation distance x and analog quantity u are normalized by the reaction zone length L and steady-state detonation velocity D_{CJ} respectively.



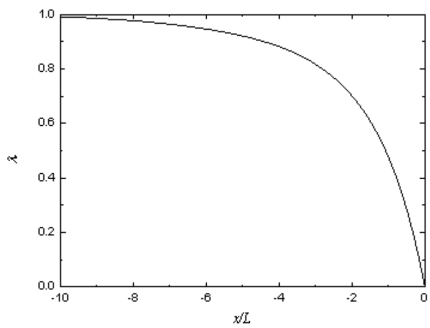
(a) Analog quantity as a function of propagation distance(c=0.015)



(b) Analog quantity as a function of propagation distance(c=0.016)



(c)Reaction process variable as a function of propagation distance(c=0.015)



(d)Reaction process variable as a function of propagation distance(c=0.016)

Fig.1 Integration results of analog quantity u and reaction process variable λ

2.2 Influence of curvature on detonation wave propagation

The curve of detonation velocity as a function of curvature can be obtained by solving the steady-state equations (8) and (9) with curvature structure, as shown in Fig.2. Detonation velocity loss increases when curvature c increases. In Fig.2, there is a turning point on all three curves, which corresponds to the maximum allowable curvature, beyond which there is no sound velocity surface. The physical explanation beyond this limit is that any disturbance after detonation wave can catch up with detonation wave and cause it to extinguish, so the existence of self-sustaining detonation is not allowed. For c < c*, there are multiple solutions to detonation velocity, resulting in a Z-shaped curve (the bottom branch has no physical meaning and is not drawn in Fig.2). The trend of detonation velocity decreasing with the increase of curvature is consistent with experimental results, which of course is consistent with actual situation. However, there may be no physical meaning when a curvature value corresponds to multiple detonation velocity solutions. The typical case is that lower branch of the curve is unstable, so only upper branch has a physical meaning.

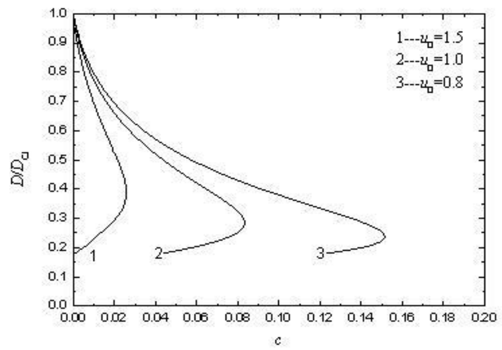
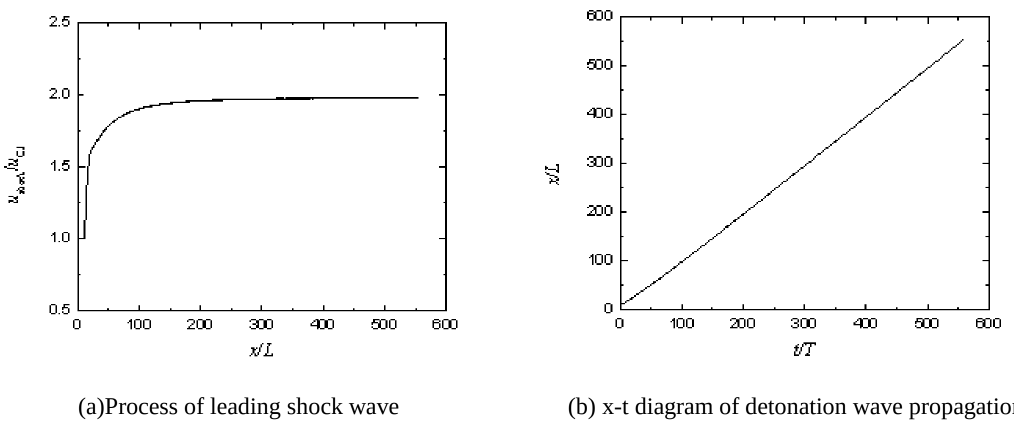


Fig.2 Steady detonation velocity as a function of curvature

3 Numerical simulation

Second-order Godunov method [9] with Riemann solver and two-step separation method is used to simulate equations (1) and (2). In the time direction, second-order Runge-Kutta formula is used for dispersion [10]. In all calculations, Courant–Friedrichs–Lewy (CFL) value is taken as 0.6. Propagation distance x and time t are normalized by length L of the reaction zone and time T respectively.

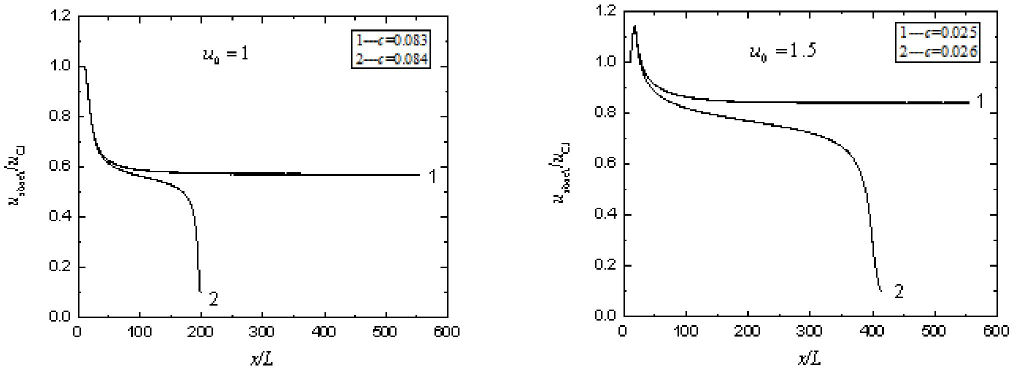
As shown in Fig.3(a), propagation of detonation wave approaches the steady state, and leading shock wave reaches von Neumann state value (u_s = 2) in the ideal state (c = 0) after the initial process. As can be seen from Fig.3(b), detonation velocity is in accordance with theoretical CJ value (D_{CJ} = 1).



(a)Process of leading shock wave (b) x-t diagram of detonation wave propagation

Fig.3 Process of leading shock wave and x-t diagram of detonation wave propagation

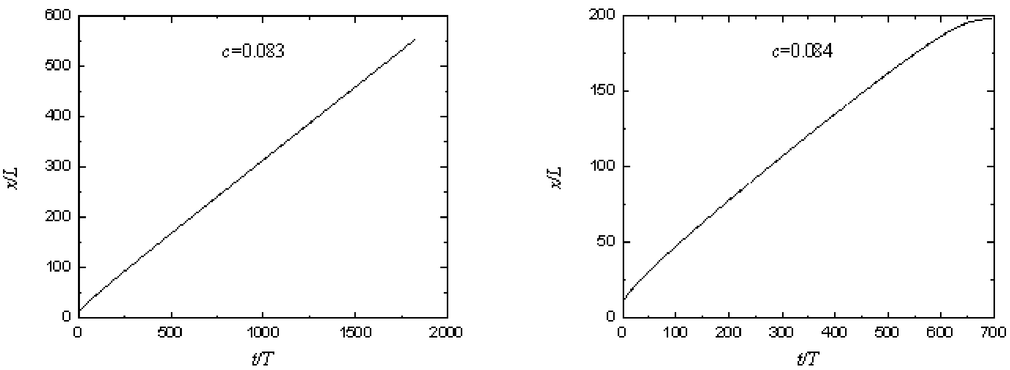
Fig.4 shows the curve of leading shock wave front pressure analog quantity u as a function of distance standard term. Figure 5 shows the x-t diagram of detonation wave propagation with different curvature values at $u_0 = 1$. When the reactants are detonated by initial high pressure region, detonation waves form and begin to propagate forward. Smaller value c in Fig.4 represents critical value of stable propagation of detonation wave. Exceeding this critical value will cause detonation to fail and detonation velocity to decrease rapidly (as shown in Fig.5(b), slope begins to decrease rapidly at t = 650). The steady-state velocity value obtained by numerical simulation (as shown in Fig. 5 (a)) is basically consistent with the steady-state velocity value corresponding to the critical curvature in the previous analytic method.



(a)Curve of leading shock wave front pressure at u_0=1

(b)Curve of leading shock wave front pressure at u_0=1.5

Fig.4 Curve of leading shock wave front pressure analog u as a function of distance standard term



(a)x-t diagram of detonation wave propagation at c=0.083

(b)x-t diagram of detonation wave propagation at c=0.084

Fig.5 x-t diagram of detonation wave propagation with different curvature values at $u_0 = 1$

4 Discussion

In this paper, a simplified model of detonation is established, and theoretical analysis and numerical simulation are carried out on this model. The following conclusions are obtained:

(1)Detonation wave propagation velocity is CJ detonation velocity under ideal conditions (as shown in Fig.3(b)); Detonation wave velocity is significantly smaller than CJ detonation velocity due to the influence of wave front curvature on detonation wave propagation. (as shown in Fig.2 and Fig.4); When curvature increases beyond the critical value, detonation wave is rapidly attenuated by steady-state propagation until it is extinguished (as shown in Fig.4 and Fig.5), and the solution of detonation wave does not exist; The characteristics of the detonation velocity decrease and detonation failure caused by curvature increase are consistent with experimental results [8].

(2)The results of numerical simulation show that there is only a stable propagation of detonation wave or detonation failure and no bifurcation or chaos, even if curvature is near the critical value c* (as shown in Fig.4). Therefore, the critical characteristics of detonation wave propagation with loss can be captured by simplified model of detonation based on the Burgers equation. Furthermore, we need to select a more complex chemical reaction model than Arrhenius reaction rate for the more complex characteristics such as pulsation instability and chaos.

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