Study on Non-ideal Detonation Behaviour Based on Analog System

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1 Introduction

The original Euler system which simulates behavior of detonation contains too much physical details, these will cause mathematical difficulties because of the nonlinearity of the equations. To simplify the reactive Euler equation in the theory of detonation, the analog system of detonation as a simple model to study detonation behavior, can capture a rich set of detonation phenomenon.

Non-ideal detonation is affected by loss and its steady-state velocity is less than ideal CJ velocity. The detonation velocity decreases as the diameter of the explosives decreases, and if the diameter of the explosives decreases to a certain threshold, detonation speed will gradually decay until the final explosion. When the detonation wave front area expands, the curvature of the detonation surface must be considered. On the curved detonation surface, when the airflow passes through the shock surface, it will be affected by the lateral expansion, which will lead to the slowdown of subsonic flow and the decrease of heat release. The curvature increases, detonation velocity loss increases[1].

2 Analog System of Detonation

On the basis of the Fickett[2,3] model, consider the effect of the loss term[4], and establish a new analog system of detonation as follows:

$$\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}(\frac{1}{2}u^2)=q\frac{\partial \lambda}{\partial t}-\kappa\left(\frac{u}{u_{CJ}}\right)^m \tag{1}$$

Analog quantities u can represent such as speed, pressure, temperature. The reaction term is used to simulate the reaction rate in the Euler equation, where the form of the simplified combustion model[5] is chosen. In the reaction term, q is the exothermic coefficient of the reaction, that unit of chemical reaction to release energy, and λ is the reaction progress variable that records the completion of the reaction. In the loss term, κ is the loss parameter, which represents the curvature of the detonation wave front. The loss index m represents the sensitivity of the loss term to the local thermal state, and u_{CJ} is a constant based on

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the CJ state. The chemical reaction is a two-step induction-reaction model[6] with independently controlled induction and reaction stages in the form:

$$\begin{aligned} \frac{\partial \lambda_i}{\partial t} &= -H\left(\lambda_i\right) e^{\alpha\left[\left(u/2u_{CJ}\right)-1\right]} \\ \frac{\partial \lambda_r}{\partial t} &= \left[1-H\left(\lambda_i\right)\right] H\left(1-\lambda_r\right)(1-\lambda_r)^{\upsilon}\left(u/u_{CJ}\right)^n \end{aligned} \tag{2}$$

In the chemical reaction, λ_i is the process variable of the induction zone, λ_r is the process variable of the reaction zone, v is the reaction order, H ( ) is the Heaviside function, α is the reaction rate induction parameter, and the reaction rate index n is the sensitivity of the reaction rate to the local thermal state. The analog system of detonation is obtained by integrating the specific forms of all equations. The coordinate system is rewritten to follow the wave coordinate system:

$$\begin{aligned} &\frac{\partial u}{\partial t} + \left(u-D\right)\frac{\partial u}{\partial x} = q\left(\frac{\partial \lambda}{\partial t} - D\frac{\partial \lambda}{\partial x}\right) - \kappa\left(\frac{u}{u_{CJ}}\right)^m \\ &-D\frac{\partial \lambda_i}{\partial x} + \frac{\partial \lambda_i}{\partial t} = -H\left(\lambda_i\right) e^{\alpha\left[\left(u/2u_{CJ}\right)-1\right]} \\ &-D\frac{\partial \lambda_r}{\partial x} + \frac{\partial \lambda_r}{\partial t} = \left[1-H\left(\lambda_i\right)\right] H\left(1-\lambda_r\right)(1-\lambda_r)^{\upsilon}\left(u/u_{CJ}\right)^n \end{aligned} \tag{3}$$

Assuming that the detonation wave is already in a stable propagation state, the partial derivative with respect to time t is zero, then the equation of the change of the u is deduced:

$$\begin{aligned} \frac{\partial u}{\partial x} &= \frac{-qD\dfrac{\partial \lambda}{\partial x} - \kappa\left(\dfrac{u}{u_{CJ}}\right)^m}{\left(u-D\right)} \\ \frac{\partial \lambda_i}{\partial x} &= \frac{1}{D} H\left(\lambda_i\right) e^{\alpha\left[\left(u/2u_{CJ}\right)-1\right]} \\ \frac{\partial \lambda_r}{\partial x} &= -\frac{1}{D}\left[1-H\left(\lambda_i\right)\right] H\left(1-\lambda_r\right)(1-\lambda_r)^{\upsilon}\left(u/u_{CJ}\right)^n \end{aligned} \tag{4}$$

The initial conditions of the equation are obtained according to the Rankine-Hugoniot condition:

$$u(x=0) = 2D, \lambda_i(x=0) = 1, \lambda_r(x=0) = 0 \tag{5}$$

The ideal state CJ speed[7] is:

$$u_{CJ} = D_{CJ} = 2q \tag{6}$$

A shock wave velocity is arbitrarily selected, and the steady-state equation is numerically integrated. If the numerator and denominator of the governing equation are not zero at the same time, the singularity of the velocity of sound occurs when u-D→0. The criterion solution requires that when the speed of sound is singular, the numerator is 0, which is the generalized CJ criterion.

2.1 Criticality of detonation

Based on the generalized CJ criterion, the relationship between detonation velocity and curvature is drawn(Fig.1). With the increase of the curvature, the steady-state detonation velocity decreases gradually. The turning point that appears on the curve corresponds to the maximum permissible curvature above which the detonation fails. Since the value of n is small, the reaction term can not compensate for the increase in curvature, so the curvature increases monotonically without turning points. As the value of n increases, the steady-state detonation curve is shifted to the left.

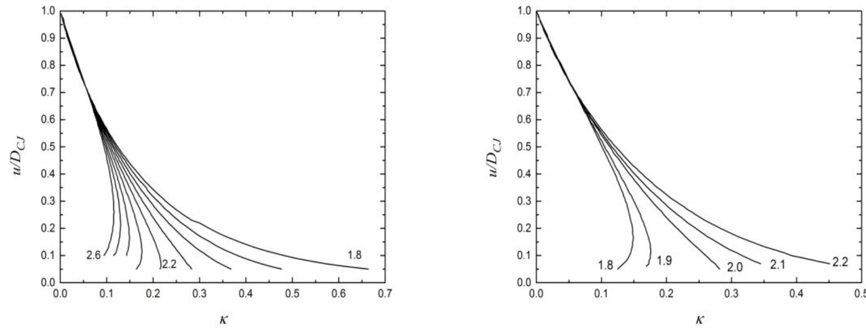


Figure 1. Left: detonation velocity and curvature curve with n different values; right: m different values.

Each different response rate index n corresponds to a different maximum loss coefficient κ, so a linear boundary of detonation propagation and failure can be made(Fig.2, left). The detonation below the boundary can always be stably propagated, and the detonation above the boundary can not be stably propagated because the loss exceeds the limit value. The inflection point required for the relationship between n and m. Where the reaction rate of the local thermal state of the sensitivity of n than the loss rate of the local thermal state of the sensitive m degree of 0.2 and above the case will appear inflection point.

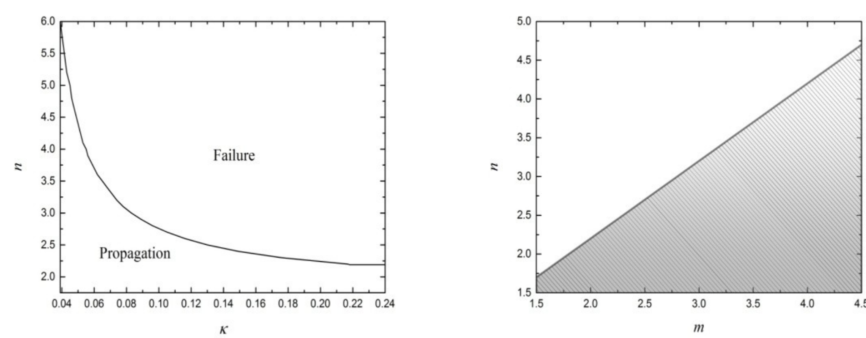


Figure 2. Left: linear boundary of detonation propagation and failure; right: the diagram of m and n when the inflection point.

2.2 Linear model analysis

The linear stability problem is observed by applying the unsteady small perturbations in the steady-state ZND solution to observe the perturbation growth or decay process. Assuming that the perturbation is very small, the basic equation can be linearized near the steady one-dimensional ZND solution. The steady-state solution with one-dimensional small perturbation is:

$$D = D_0 + \varepsilon\sigma \exp(\sigma t), u = u_0 + \varepsilon u_1(x)\exp(\sigma t), \lambda = \lambda_0 + \varepsilon\lambda_1(x)\exp(\sigma t) \tag{7}$$

By introducing the disturbance into the steady-state equation, the higher order term and the steady state solution are obtained, and the binomial theorem[8] is used：

$$\begin{aligned} &\sigma u_1 + (u_0 - D_0)u_1' + u_0' u_1 - \sigma u_0' = q\left(\sigma\lambda_1 - D_0\lambda_1' - \sigma\lambda_0'\right) - \kappa m \frac{u_1}{u_{CJ}}\left(\frac{u_0}{u_{CJ}}\right)^m \\ &\sigma\lambda_1 - D_0\lambda_1' - \sigma\lambda_0' = \frac{n u_1 (1-\lambda_0)^\nu}{u_{CJ}}\left(\frac{u_0}{u_{CJ}}\right)^{n-1} - \nu\lambda_1(1-\lambda_0)^{\nu-1}\left(\frac{u_0}{u_{CJ}}\right)^n \end{aligned} \tag{8}$$

The initial boundary conditions of the equation variables are obtained by bringing the steady-state solution with small perturbations into the initial shock condition:

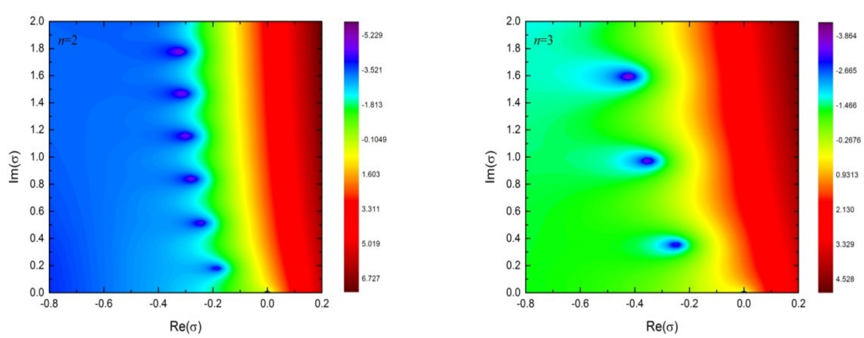
$$u_1(x=0) = 2\sigma, \lambda_1(x=0) = 0 \tag{9}$$

In order to determine the eigenvalues of the frequency eigenvalue σ, we can get the following result by suppressing the perturbation on the front-finger characteristic line of the steady-state wave.

$$\frac{u_1}{\omega_1(u_0 - D_0)i + a} + \frac{\lambda_1}{\omega_2(u_0 - D_0)i + a} = 0 \tag{10}$$

In order to determine the frequency eigenvalue σ in the stability equation, we first need to satisfy the dispersion condition. The absolute value of the dispersion relation Y(σ) is calculated by setting the frequency eigenvalues of different real and imaginary parts, and the dispersion condition is satisfied only when its value is equal to zero, and then the logarithm of the absolute value is made in the complex plane high-line chart.

The local minimum value (purple point) in the contour plot represents the frequency eigenvalue satisfying the dispersion condition. If the frequency eigenvalues satisfying the condition are present only in the negative region of the real part of the eigenvalue, the perturbation of the steady-state solution will not increase with time and the anaolg system is stable. The region of the detonation steady-state solution will decrease gradually, but it still does not appear in the positive region of the real part of the eigenvalue. The steady-state solution of the anaolg system of detonation is stable for one-dimensional linear perturbations. When the value of the reaction rate index n is equal to or greater than 5.8, no matching frequency characteristic value can be found in the contour map of the existing area.



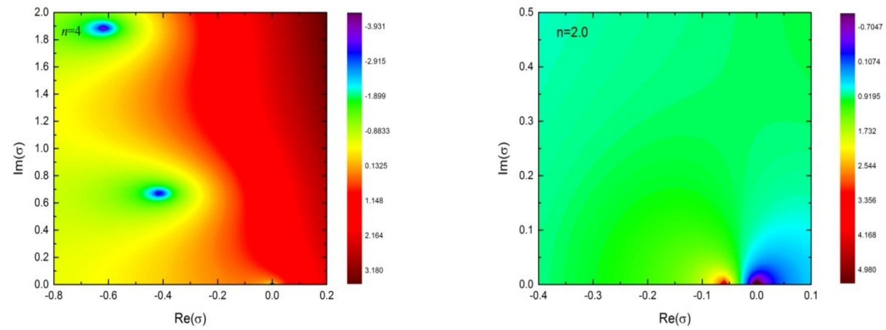


Figure 3. Stability results under ideal conditions and non-ideal conditions.

Under the non-ideal condition, let the loss item parameter is equal to 0.05, the other parameters remain unchanged, to make the response rate index contour chart as shown. The frequency characteristic value satisfying the dispersion condition does not appear in the contour plot. Therefore, the steady-state solution of the anaolg system of detonation is always unstable for one-dimensional linear perturbations due to the existence of the loss term.

3 Numerical simulation results

The second-order Godunov method and the two-step separation method with Riemann solver[9] are used to numerically solve this problem. In order to measure the change of detonation intensity, the change of shock amplitude with shock location is captured. For q=0.5, m=2.0, v=0.75, when detonated by the initial high-pressure region, the detonation wave begins to propagate forward. When n is equal to 2.0, the detonation wave does not extinguish. When n is equal to 2.2, the smaller value of κ in the figure represents the critical value of the detonation wave's stable propagation. If the critical value is exceeded, the detonation failure will occur and the detonation velocity will decrease rapidly.

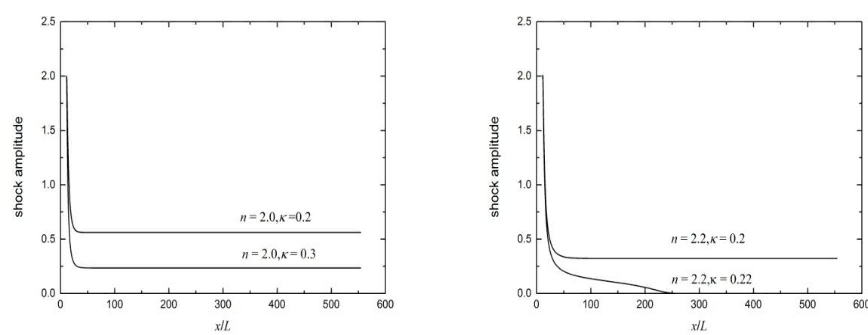


Figure 4: The change of shock amplitude with shock location.

The steady-state velocity obtained by numerical simulation is consistent with the steady-state velocity corresponding to the critical curvature in the previous analytical method.

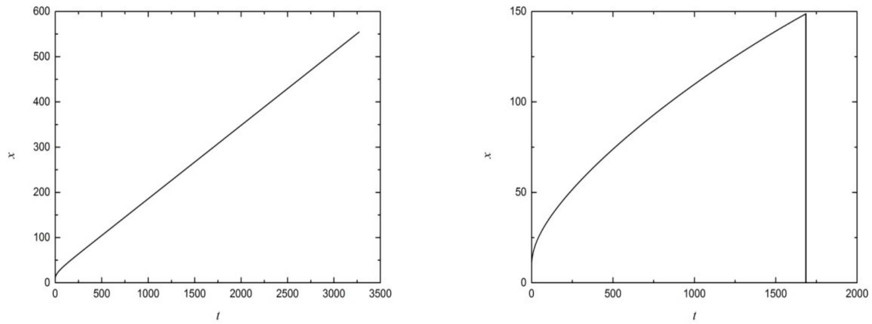


Figure 5: The *x*-*t* diagram for a detonation wave(n=2.2), and left: κ=0.2; right: κ=0.22.

Many different behaviours of detonation can be presented by analog system, such as critical property, chaos and cell phenomenon. There are indications that a reasonable reduction in reaction Euler equation can still maintain its basic physical components, so the analog system of detonation is simple and practical.

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