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Instability Criterion of One-Dimensional Detonation Wave with Three-Step Chain Branching Reaction Model *

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One-dimensional detonation waves are simulated with the three-step chain branching reaction model, and the instability criterion is studied. The ratio of the induction zone length and the reaction zone length may be used to decide the instability, and the detonation becomes unstable with the high ratio. However, the ratio is not invariable with different heat release values. The critical ratio, corresponding to the transition from the stable detonation to the unstable detonation, has a negative correlation with the heat release. An empirical relation of the Chapman–Jouguet Mach number and the length ratio is proposed as the instability criterion.

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Detonation waves are supersonic combustion waves, which are induced by a strong shock and sustained by post-shock rapid heat release. In recent years, potential applications of the detonation wave in hypersonic propulsion systems have been explored.[1] However, the coupling of the shock and the combustion makes the detonation unstable, so studies of its initiation and propagation have encountered some problems. Erpenbeck[2,3] has carried out a hydrodynamic stability analysis using an initial value Laplace transform method. Lee *et al.*[4] have studied the detonation instability with the normal-mode approach. Short *et al.*[5] studied the dynamics of the low-frequency instability with the asymptotic method. However, theoretical analysis can only be used to study the linear or weakly nonlinear instability. In recent years, the time-dependent reactive Euler equations have been solved to study the detonation instability. Numerical results may provide the full nonlinearity of the detonation waves, which is difficult to covered in theoretical models. He *et al.*[6] studied the influence of activation energy, and the detonation quench is observed with a high activation energy. Gamezo *et al.*[7] simulated two-dimensional cellular detonations and found out that the activation energy in the chemical models would influence the detonation structures. Han *et al.*[8] studied the cylindrical detonation propagation, and the mechanism of transverse wave formation with the influence of the curvature is discussed. Generally, the high activation energy makes the detonation unstable, but there are some other factors that have affect the instability, and the instability criterion needs to be clarified. Ng *et al.*[9] proposed a combination parameter to decide the neutral boundary. The activation energy and the length ratio of the induction zone and the reaction zone are used to study the detonation instability. However, the activation energy is still a chemical parameter, not the gas dynamics parameter. In this letter, another parameter with a clear physical meaning is proposed as the instability criterion for different heat release values.

The governing equations are one-dimensional Euler equations, and the gas is assumed to be a perfect gas with a constant specific heat ratio γ. The chemical kinetic model used for the present study is a generalized three-step chain branching reaction model, which is proposed by Short *et al.*[10] Generally, this model is composed of three parallel steps,

(i) chain initiation $F \to Y, k_I = \exp\Big[E_I\Big(\dfrac{1}{T_I}-\dfrac{1}{T}\Big)\Big]$,

(ii) chain branching $F+Y \to 2Y$,

$$k_B = \exp\Big[E_B\Big(\frac{1}{T_B}-\frac{1}{T}\Big)\Big],$$

(iii) chain termination $Y \to P$, $k_c = 1$,

where F, Y and P denote the fuel, the intermediate radical and the product, respectively. The chain initiation and branching reactions are sensitive to temperature, but the chain termination reaction is independent of temperature, which has a fixed rate constant. Denoting the variables f and y to be the mass fraction of the fuel F and radical Y, the consumption equations for the fuel and radical can be written as

$$\frac{\partial \rho f}{\partial t}+\frac{\partial(\rho u f)}{\partial x} = -\rho(w_I+w_B),$$
$$\frac{\partial \rho y}{\partial t}+\frac{\partial(\rho u y)}{\partial x} = -\rho(w_I+w_B-w_C),$$

where

$$w_I = f\exp\Big[E_I\Big(\frac{1}{T_I}-\frac{1}{T}\Big)\Big],$$
$$w_B = \rho f y\exp\Big[E_B\Big(\frac{1}{T_B}-\frac{1}{T}\Big)\Big], w_C = y,$$

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and the heat release is given by $q = Q - fQ - yQ$.

In this chain-branching model, four new chemical parameters are introduced, which are the activation energies E_I and E_B, and the cross-over temperatures T_I and T_B. Referring to previous calculations,[10,11] the default constants are E_I=37.5, $E_B = 10$, $T_I = 3T_S$ and $\gamma = 1.2$, and T_S is the post-shock temperature. There are two bifurcation parameters of the detonation instability in this study. One is the ratio of T_B to T_S due to its effect on the chain branching reaction. The other is the heat release Q, which may change T_S, and then the two cross-over temperature values. The governing equations are solved with the MUSCL-Hancock scheme.[12]

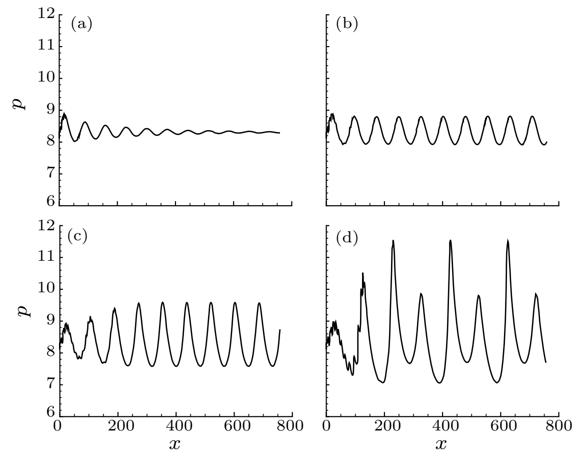

Fig. 1. The post-shock pressure when the detonation propagates with the ratio of T_B to T_S: 0.88 (a), 0.89 (b), 0.90 (c) and 0.92 (d).

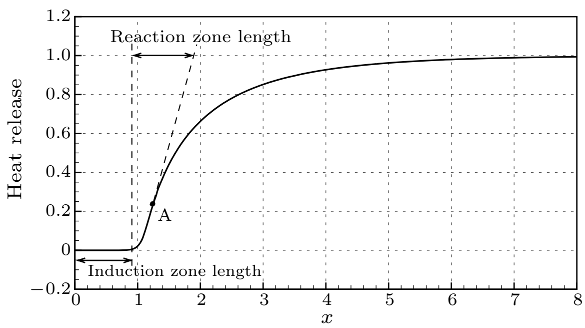

Fig. 2. The definition of the induction and reaction zone with the three-step chain branching reaction model.

First, the detonation waves with the heat release $Q = 8.33$ are simulated. The ratio of T_B to T_S is the bifurcation parameter and it varies from 0.88 to 0.92, as shown in Fig. 1. Initially the Chapman–Jouguet (CJ) detonation is located behind the $x = 0$ point and it will propagate forward. The post-shock pressure is recorded with its position, which shows the detonation pulse propagation. Although the early stage of the detonation propagation is influenced by numerical errors, the pressure fluctuation will be decided by its own instability. It can be observed that the fluctuation will decay and finally the CJ detonation forms with the ratio 0.88, as shown in Fig. 1(a). However, the fluctuation will not decay but keep the same amplitude with the ratio 0.89, as shown in Fig. 1(b). Because the amplitude is decided by the detonation itself after the early stage, it can be concluded that the detonation becomes unstable. With the ratio 0.90, the amplitude becomes larger and reaches a constant after the early stage, as shown in Fig. 1(c). Increasing the ratio to 0.92, two-mode oscillation can be observed, as shown in Fig. 1(d). This demonstrates that the detonation instability becomes stronger when the ratio of T_B to T_S rises, and the ratio 0.88 corresponds to the critical stable detonation wave with the given parameters.

Although the ratio of T_B to T_S can be used to decide the detonation instability, its physical mechanism needs to be clarified. Ng *et al.*[11] proposed the ratio of the induction zone length and the reaction zone length could be used as the criterion of the instability. The definition of the induction and reaction zones is shown in Fig. 2. The reaction zone length is defined by the inflexion point A on the heat release curve. The tangent from the point to the end of the heat release will give the end of the reaction zone length. Actually, the heat release is assumed to keep the same after the inflexion point in this definition, so the uncertainty in the long heat release process is avoided. The ratio of the induction zone length and the reaction zone length is

$$\delta = \Delta_i/\Delta_r,$$

where δ is the ration, Δ_i and Δ_r are the induction zone length and the reaction zone length, respectively. The zone lengths and their ratio are listed in Table 1 with the different ratio of T_B to T_S. Generally, when the temperature ratio rises, meanwhile both the zone lengths rise. However the induction zone length rises faster than that of the reaction zone length, which raises the length ratio eventually. With a temperature ratio of 0.88, the detonation is stable, while with a ratio of 0.89, the detonation is unstable. Therefore the ratio δ has a critical value between 0.92 and 0.95, which is the neutral boundary of the one-dimensional detonation instability.

Table 1. The induction/reaction zone length ratios with different ratios of T_B to T_S.

T_B/Ts	Δ_i	Δ_r	δ
0.88	0.86	0.94	0.92
0.89	0.92	0.97	0.95
0.90	0.99	1.00	0.99
0.91	1.07	1.02	1.05
0.92	1.15	1.05	‘1.09

The detonation instability derives from the coupling of the shock and the combustion, which can be characterized by the length ratio. That is why the length ratio can be used as the instability criterion. Traditionally, the activation energy in a one-step reaction mechanism is used as the instability criterion. With the high activation energy, the detonation becomes unstable. It is impossible to separate the induction zone and the reaction zone in a one-step reaction mechanism, but definitely the high activation energy means the weak coupling of the shock and the combustion. This length ratio provides a parameter for the coupling relation, which is more physically meaningful than the activation energy in the one-step reaction mechanism. However, whether or not the length ratio δ is quantitatively a universal criterion needs to be studied further, especially for the detonation with different CJ Mach numbers. Then the detonation with the heat release $Q = 20.0$ is simulated. The numerical results show that the detonation is stable when the temperature ratio is less than or equal to 0.98, and the corresponding length ratio is about 0.68. Therefore the length ratio of the induction zone and the reaction zone, δ, cannot be used simply.

Table 2. The critical temperature ratio and the length ratio with different heat release values.

Q	Critical T_B/T_s	δ
8.33	0.88	0.92
10.0	0.89	0.87
15.0	0.93	0.77
20.0	0.98	0.68

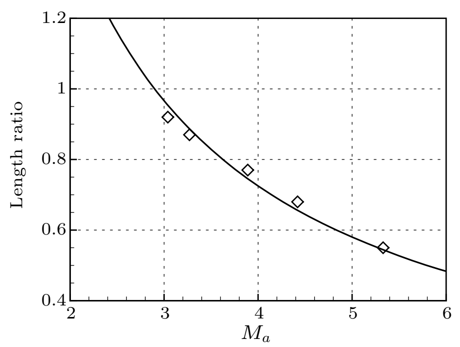

Fig. 3. The induction/reaction zone length ratios and the corresponding CJ Mach numbers in the critical stable cases.

To determine the relationship between the heat release and the length ratio, the detonation waves with two other heat release values $Q = 10.0$ and $Q = 15.0$ are further simulated and all the critical results are listed in Table 2. It can be observed that the critical temperature ratio increases when the heat release rises, but the corresponding length ratio decreases meanwhile. Although the length ratio decreases as the heat release increases, they do not have a simple reciprocal relationship. To establish the quantitative relation of the heat release and the length ratio, various functions have been tried. The best choice adopted now is shown in Fig. 3, which demonstrates a fitted curve $\delta M_a = 2.90$. The point with the heat release $Q = 30.0$ is calculated further and it also locates on the curve. Therefore the parameter δM_a may be used as the instability criterion from the present numerical results.

For the critical stable detonation, it is reasonable that the high heat release induces the length ratio decrease. The high heat release will induce the high CJ Mach number and the high critical temperature ratio, which is shown in Table 2. For the induction zone, the high heat release will make the induction zone length short due to the high CJ Mach number, but the high temperature ratio makes the induction zone length greater. Therefore the induction zone length changes little. For the reaction zone, both the high heat release and the high temperature ratio make the reaction zone length greater, so the reaction zone length increases obviously. Therefore the length ratio decreases in the case of high heat release. Here, δM_a remains constant with acceptable error, but it is not exclusive. We can conclude that the length ratio has a negative correlation with the heat release. The final precise function expression needs to be decided on the basis of more results, especially data from other chemical reaction models.

In summary, one-dimensional detonation waves have been simulated with the three-step chain branching reaction model and the instability criterion is studied. When the ratio of the induction zone length and the reaction zone length increases, the instability will be triggered and the critical length ratio has been decided from the numerical results. However, with different heat release values, the critical length ratio is not the same. In the case of the critical stable detonation, the length ratio has a negative correlation with the heat release. An empirical relation of the instability criterion is proposed, which shows the reciprocal relationship of the CJ Mach number and the length ratio. The precise instability criterion based on the length ratio and the heat release needs more work.

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