Criterions for the stability of flame propagation and deflagration detonation transition of carbon monoxide-oxygen mixture

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1 Introduction

The criterion for the shift of lamellar flame to turbulent flame is very important in engineering. So far, the research works of these fields are not perfect. In this paper, the Lyapunov stability theory is used to obtain a criterion for the stability of flame propagation. It is known that, under the certain condition, deflagration can be transformed into detonation. The detonation of the combustible gas is the most devastating gas explosion. In the early stage of the combustion accident, it needs to avoid the destruction of effect of the shift of the deflagration to the detonation. So, the research on DDT has been widespread concerned. It is shown experimentally [l-4] that detonation waves can originate in the vicinity of the flame zone. Some authors [5-8] modeled the onset of detonation numerically considering one-dimensional models and simplified one-stage reactions. Eder A [9] derived the mechanism of deflagration, detonation state and deflagration detonation transition. Although, the study about the deflagration detonation transition involved theoretical studies, numerical studies and experimental studies, until now, the theoretical research on criterion for the transition from deflagration to detonation study are also lacking. In this paper, we specifically conduct a study for the combustible gas of carbon monoxide, use linear stability analysis methods to propose the criterion of the deflagration to detonation for carbon monoxide.

2. Criterion for the stability of flame propagation

For unsteady combustion, the heat conduction, the gravity and thermal diffusion effect are neglected. Take a straight pipe, the right side of the pipe is opening, the left is closed. Discuss a single reaction channel and a single reaction medium in case of A→B. Then the unsteady flow of the combustion flame meets N-S equations [10]：

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$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \dfrac{\partial(\rho u)}{\partial x} = 0 \\ \dfrac{\partial(\rho u)}{\partial t} + \dfrac{\partial(\rho u^2 + P)}{\partial x} - \dfrac{\partial}{\partial x}\left(\eta \dfrac{\partial u}{\partial x}\right) = 0 \\ \dfrac{\partial(\rho h - P)}{\partial t} + \dfrac{\partial}{\partial x}\left[(\rho u h) - \left(\dfrac{\lambda}{c_p}\right)\dfrac{\partial h}{\partial x}\right] = 0 \\ \dfrac{\partial \rho_0}{\partial t} + \dfrac{\partial(\rho_0 u)}{\partial x} = -\omega \end{cases} \qquad (1)$$

Where, $\omega = \omega_0 \rho_0 e^{-E_a/(RT)}$, E_a is the reaction activation energy, ω_0 is the constant greater than zero, ρ_0 is the density of the reactants. ρ、u、p、T、γ、λ、η、h、ρ_0、ω respectively signify density, velocity, pressure, temperature, specific heat ratio, unit reaction degree, the density of the fluid viscosity coefficient, reaction medium, chemical reaction rate, gas enthalpy of the reaction medium density and chemical reaction rate.

Reynolds number is a dimensionless number, which can be used to characterize fluid flow situation. According to the definition of Reynolds number and the relationship between Reynolds number and the N-S equation, we can know that local Reynolds number (Re) is defined as: $\mathrm{Re} = \rho u D / \eta$, D is the characteristic length. Take the critical Reynolds number for steady spread of flame is Re^l, stability analysis is carried out on the Reynolds number. If adding a small disturbance to the system, after a long enough time, flame propagation is still spreading in the form of laminar flow. In other words, any point on the surface of the flame array at any time, the Reynolds number is not more than the critical Reynolds number Re^l, the stability is proved. Take any point on the surface of the flame array as the research object, the Reynolds number after total differential and transformation can be obtained that:

$$\frac{d\,\mathrm{Re}}{dt} = \frac{D}{\eta^2}\left[\eta\left(\frac{\partial(\rho u)}{\partial t} + \frac{u\partial(\rho u)}{\partial x}\right) - \rho u\left(\frac{\partial \eta}{\partial t} + \frac{u\partial \eta}{\partial x}\right)\right] \qquad (2)$$

Suppose δ is incremental, the perturbation equations of the unsteady combustion flame one-dimensional unsteady navier-stokes equations are:

$$\begin{cases} \dfrac{\partial \delta\rho}{\partial t} + \dfrac{\partial \delta(\rho u)}{\partial x} = 0 \\ \dfrac{\partial \delta(\rho u)}{\partial t} + \dfrac{\partial \delta(\rho u^2 + P)}{\partial x} - \dfrac{\partial \delta}{\partial x}\left(\eta \dfrac{\partial u}{\partial x}\right) = 0 \\ \dfrac{\partial \delta(\rho h - P)}{\partial t} + \dfrac{\partial \delta}{\partial x}\left[(\rho u h) - \left(\dfrac{\lambda}{c_p}\right)\dfrac{\partial h}{\partial x}\right] = 0 \\ \dfrac{\partial \delta\rho_0}{\partial t} + \dfrac{\partial \delta(\rho_0 u)}{\partial x} = -\delta\omega \end{cases} \qquad (3)$$

Reynolds number on the time derivative adds perturbation incremental can be obtained:

$$\frac{d\delta\,\mathrm{Re}}{dt} = \frac{D}{(\delta\eta)^2}\left[\delta\eta\left(\frac{\partial(\delta\rho\delta u)}{\partial t} + \frac{\delta u\partial(\delta\rho\delta u)}{\partial x}\right) - \delta\rho\delta u\left(\frac{\partial \delta\eta}{\partial t} + \frac{\delta u\partial \delta\eta}{\partial x}\right)\right] \qquad (4)$$

In order to guarantee the stability of flame propagation, according to Lyapunov stability theory, we get:

$$\int \frac{D}{(\delta\eta)^2}\left[\delta\eta\left(\frac{\partial(\delta\rho\delta u)}{\partial t} + \frac{\delta u\partial(\delta\rho\delta u)}{\partial x}\right) - \delta\rho\delta u\left(\frac{\partial \delta\eta}{\partial t} + \frac{\delta u\partial \delta\eta}{\partial x}\right)\right]dt \le \mathrm{Re}^l - \rho u D / \eta \qquad (5)$$

In this case, the lamellar flame is stable. Eq. (5) is the theoretical criterion of the stability of flame propagation under the critical Reynolds number.

When $\delta \mathrm{Re} > \mathrm{Re}^l - \rho u D / \eta$, the flame fronts will be unstable, front instability speed up the flame. Further instability of the flame forms turbulent flame.

3.The criterion of deflagration detonation transition

The following specific works is to analyze the chemical kinetics of carbon monoxide and oxygen and obtain the stability condition for the spread of flame. Consider a closed pipeline enclosed a mixed gas of carbon monoxide and oxygen. Igniting at one end of the pipeline, then the deflagration detonation transition (Fig.1).

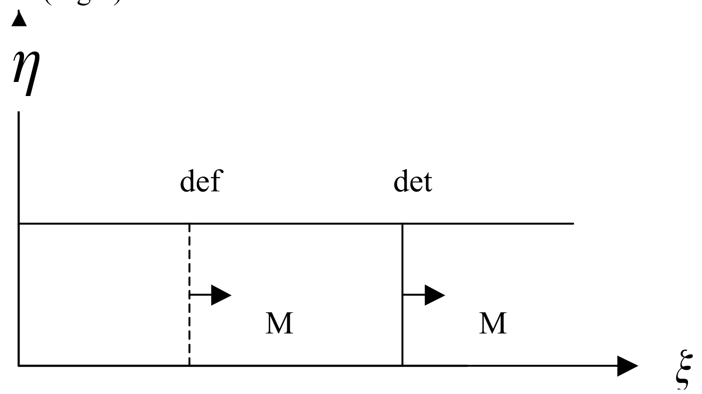

Fig.1 Deflagration detonation transition

In the system of $2CO + O_2$, complete chemical reaction is extremely complex, the reaction mechanism is generally considered 7-step reaction[15]:

(1) $CO + O_2 \xrightarrow{k_1} CO_2 + O$

(2) $CO + O \xrightarrow{k_2} CO_2^\bullet$

(3) $CO_2^\bullet + O_2 \xrightarrow{k_3} CO_2 + 2O$

(4) $O + O_2 + M \xrightarrow{k_4} O_3 + M$

(5) $CO + O_3 \xrightarrow{k_5} CO_2 + 2O$

(6) $CO + O + M \xrightarrow{k_6} CO_2 + M$

(7) $CO_2^\bullet + M \xrightarrow{k_7} CO_2 + M$

Where, k_i ($i = 1,2,3,\ldots.7$) represents the i -step reaction rate constant. M represents the third body of the three-molecule reactions, which only play a role of energy transfer.

If, $A = [CO]$, $B = [O_2]$, $X_1 = [O]$, $X_2 = [O_3]$, $X_3 = [CO_2^\bullet]$, $m = [M]$, then the kinetic equations are as follows:

$$\begin{cases} \dfrac{\partial X_1}{\partial t} = k_1 AB - (k_2 A + k_4 Bm + k_6 Am) X_1 + 2k_5 AX_2 + 2k_3 BX_3 + D_1 \Delta X_1 \\ \dfrac{\partial X_2}{\partial t} = k_4 BmX_1 - k_5 AX_2 + D_2 \Delta X_2 \\ \dfrac{\partial X_3}{\partial t} = k_2 AX_2 - (k_3 B + k_7 m) X_3 + D_3 \Delta X_3 \end{cases} \quad (6)$$

Where, $D_i (i = 1,2,3)$ represents the diffusion coefficient of O, O_3 and $CO_2^\bullet$ in the system, Δ represents the Laplace operator.

If, $\frac{\partial X_i}{\partial t} = 0, (i = 1,2,3)$, then the kinetic equations (6) become:

$$\begin{cases} k_1 AB - (k_2 A + k_4 Bm + k_6 Am)X_1 + 2k_5 AX_2 + 2k_3 BX_3 = 0 \\ k_4 BmX_1 - k_5 AX_2 = 0 \\ k_2 AX_2 - (k_3 B + k_7 m)X_3 = 0 \end{cases} \tag{7}$$

So the steady-state solution of eq. (7) as follows:

$$\begin{cases} X_{1s} = \dfrac{k_3 k_5 AB(k_3 B + k_7 m)}{k_5 (k_2 A + Amk_6 - k_4 Bm)(k_3 B + k_7 m) - 2mk_2 k_3 k_4 B} \\ X_{2s} = \dfrac{k_3 k_4 B^2 m(k_3 B + k_7 m)}{k_5 (k_2 A + Amk_6 - k_4 Bm)(k_3 B + k_7 m) - 2mk_2 k_3 k_4 B} \\ X_{3s} = \dfrac{k_3 k_2 k_4 AB^2 m}{k_5 (k_2 A + Amk_6 - k_4 Bm)(k_3 B + k_7 m) - 2mk_2 k_3 k_4 B} \end{cases} \tag{8}$$

We assume that in the steady-state solution (X_{1s}, X_{2s}, X_{3s}), there is a small perturbation (x_1, x_2, x_3) .Make $X_1 = X_{1s} + x_1$, $X_2 = X_{2s} + x_2$, $X_3 = X_{3s} + x_3$ $(where,\ x_i << X_{is}, i = 1,2,3)$.

We introduce the above formulas into the corresponding kinetic equation combined with the steady-state solution of the equations, we can get that:

$$\begin{cases} \dfrac{\partial x_1}{\partial t} = -(k_2 A + k_4 Bm + k_6 Am)x_1 + 2k_5 Ax_2 + 2k_3 Bx_3 + D_1 \Delta x_1 \\ \dfrac{\partial x_2}{\partial t} = k_4 Bmx_1 - k_5 Ax_2 + D_2 \Delta x_2 \\ \dfrac{\partial x_3}{\partial t} = k_2 Ax_2 - (k_3 B + k_7 m)x_3 + D_3 \Delta x_3 \end{cases} \tag{9}$$

That is:

$$\frac{\partial}{\partial t}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -(k_2 A + k_4 Bm + k_6 Am) + D_1 \Delta & 2k_5 A & 2k_3 B \\ k_4 Bm & -k_5 A + D_2 \Delta & 0 \\ 0 & k_2 A & -(k_3 B + k_7 m) + D_3 \Delta \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \tag{10}$$

The Fourier components of the perturbed solution is:

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} e^{\varpi t + ik\eta} (k \geq 0) \tag{11}$$

Introducing eq. (9) into eq. (8), we can get that:

$$\varpi \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} -k_2 A - k_4 Bm - k_6 Am - D_1 k^2 - \varpi & 2k_5 A & 2k_3 B \\ k_4 Bm & -k_5 A - D_2 k^2 - \varpi & 0 \\ 0 & k_2 A & -k_3 B - k_7 m - D_3 k^2 - \varpi \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} \tag{12}$$

The necessary and sufficient condition of non-zero solution of the above equation is:

$$\begin{vmatrix} -k_2 A - k_4 Bm - k_6 Am - D_1 k^2 - \varpi & 2k_5 A & 2k_3 B \\ k_4 Bm & -k_5 A - D_2 k^2 - \varpi & 0 \\ 0 & k_2 A & -k_3 B - k_7 m - D_3 k^2 - \varpi \end{vmatrix} = 0 \tag{13}$$

That is:

$$\left(k_2A + k_4Bm + k_6Am + D_1k^2 + \varpi\right)\left(k_5A + D_2k^2 + \varpi\right)\left(k_3B + k_7m + D_3k^2 + \varpi\right)$$
$$- k_4Bm\left[2k_5A\left(k_3B + k_7m + D_3k^2 + \varpi\right) + 2k_3Bk_2A\right] = 0 \tag{14}$$

Then we get the following equation:

$$\varpi^3 + a\varpi^2 + b\varpi + c = 0 \tag{15}$$

Of where:

$$\begin{cases} a = k_2A + k_4Bm + k_6Am + D_1k^2 + k_5A + D_2k^2 + k_3B + k_7m + D_3k^2 \\ b = \left(k_2A + k_4Bm + k_6Am + D_1k^2\right)\left(k_5A + D_2k^2\right) + \\ \left(k_3B + k_7m + D_3k^2\right)\left(k_2A + k_4Bm + k_6Am + D_1k^2\right) + \\ \left(k_5A + D_2k^2\right)\left(k_3B + k_7m + D_3k^2\right) - 2k_5Ak_4Bm \\ c = \left(k_2A + k_4Bm + k_6Am + D_1k^2\right)\left(k_3B + k_7m + D_3k^2\right)\left(k_5A + D_2k^2\right) \\ - k_4Bm\left[2k_5A\left(k_3B + k_7m + D_3k^2\right) + 2k_3Bk_2A\right] \end{cases} \tag{16}$$

According to the linear stability theory [11], if all of the three roots $\left(where, \varpi_i, i = 1.2.3\right)$ of the above characteristic equation are zero-negative (or have negative real parts), then disturbance $\left(x_1, x_2, x_3\right)$ will decay over time index, thus the equations of the steady-state solution is linearly stable; if there is a zero solution and the rest of the solution is negative, the steady solution is marginally stable.

According to the theory of a cubic equation, the necessary and sufficient condition of eq. (15) has three negative roots (or has negative real parts) is as follows:

$$\begin{cases} a > 0 \\ ab - c > 0 \\ c. > 0 \end{cases} \tag{17}$$

The value of a, b, c determined by eq. (16) shows that $a > 0, ab - c > 0$, thus the necessary and sufficient condition for the eq. (15) has a zero root and the rest of the root is negative is $c = 0$.

By $c = 0$, we can get:

$$\left(k_2A + k_4Bm + k_6Am + D_1k^2\right)\left(k_3B + k_7m + D_3k^2\right)\left(k_5A + D_2k^2\right)$$
$$- k_4Bm\left[2k_5A\left(k_3B + k_7m + D_3k^2\right) + 2k_3Bk_2A\right] = 0 \tag{18}$$

That is:

$$D_1D_2D_3k^6 + \left[\left(k_2A + k_4Bm + k_6Am\right)D_2D_3 + \left(k_3B + k_7m\right)D_1D_2 + k_5AD_1D_3\right]k^4$$
$$+ \begin{bmatrix} \left(k_2A + k_4Bm + k_6Am\right)\left(k_3B + k_7m\right)D_2 + \left(k_3B + k_7m\right)k_5AD_1 + \\ k_5A\left(k_2A + k_4Bm + k_6Am\right)D_3 - 2k_5Ak_4BmD_3 \end{bmatrix} k^2 +$$
$$k_5A\left(k_2A + k_4Bm + k_6Am\right)\left(k_3B + k_7m\right) - k_4Bm\left[2k_5A\left(k_3B + k_7m\right) + 2k_3Bk_2A\right] = 0 \tag{19}$$

Now the steady solution （X_{1s}, X_{2s}, X_{3s}）is in the state of marginally stable.

We know that, $k \geq 0$, so, $k^6, k^4, k^2 \geq 0$, the above equation can be expressed as a cubic equation which the k is the unknown, according to eq.(17):

$$k_5\left(k_2A + k_4Bm + k_6Am\right)\left(k_3B + k_7m\right) - k_4Bm\left[2k_5\left(k_3B + k_7m\right) + 2k_3Bk_2\right] = 0 \tag{20}$$

Thus, when

$$k_5\left(k_2A + k_4Bm + k_6Am\right)\left(k_3B + k_7m\right) - k_4Bm\left[2k_5\left(k_3B + k_7m\right) + 2k_3Bk_2\right] \geq 0 \tag{21}$$

the system is stable. Thus, the deflagration detonation transition inevitable condition is:

$$k_5\left(k_2A + k_4Bm + k_6Am\right)\left(k_3B + k_7m\right) - k_4Bm\left[2k_5\left(k_3B + k_7m\right) + 2k_3Bk_2\right] < 0 \tag{22}$$

That is :
$$A > \frac{k_4 k_5 Bm(k_2 k_5 + k_5 k_6 m) - k_4 Bm[2k_5(k_3 B + k_7 m) + 2k_3 Bk_2]}{(k_3 B + k_7 m)(k_2 k_5 + k_5 k_6 m)} \tag{23}$$

So, only when the carbon monoxide concentration meets the above (eq.25) conditions the system becomes unstable.

Through experiment and calculation [12, 13] we know that DDT needs the methane concentration is more than 12.5%. By the calculation of eq. (23), only when A reach a critical value (the right side of eq.12), the DDT happen. Thus, the validity of eq. (23) is proved to some extent.

4. Conclusions

By above analyses, the criterion for the stability of flame propagation is obtained by using the Lyapunov stability theory; the criterion of the deflagration detonation transition for carbon monoxide is proposed by using the linear stability theory. The criterions can be used as a theoretical support for the prevention and control of gas explosion.

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