Estimation of the specific heat capacity ratio of gasoline vapor based on the relationship between the maximum pressure rise rate and initial pressure of gas explosion

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Abstract: Gasoline is volatile and can form a flammable gas mixture with air easily. Researches on the gas explosions still need to be developed so that more effective explosion prevention techniques and measures can be proposed. The maximum overpressure rise rate and deflagration index are two important parameters for measuring gas explosion damage power. The relationship between these two parameters and the initial pressure is controversial. Razus et al. insisted that it was a linear relationship, however, Faghih et al. declared that it was an exponential relationship. In this paper, the relationship between the maximum pressure rise rate (the deflagration index) and the initial pressure is deduced and discussed. The results show that the relationship is still linear. On this basis, the deduced relationship formula is used to estimate the specific heat capacity of gasoline vapor. Results show that the estimated value is reasonable and acceptable.

1. Introduction
Gasoline, one of the most extensively used fuels, is volatile and can form a flammable gas mixture with air easily. Fire and explosions are still common safety accidents in industrial production and social life. Researches on the gasoline-air explosions still need to be developed so that more effective gasoline-air explosion prevention techniques and measures can be proposed. Overpressure caused by flammable gas explosion is the direct cause of all kinds of damage. In overpressure characteristic parameters, the maximum overpressure rise rate and deflagration index are two important parameters for measuring gas explosion damage power, and widely used in engineering design and risk assessment of pressure vessel involving gas explosion [1,2]. Therefore, lots of literatures were focused on these parameters [3-9].

Among these literatures, Faghiih et al. [3] studied the explosion process of hydrogen and methane in a spherical vessel by numerical simulation, and reported the values of the maximum pressure rise rate and deflagration index of methane, hydrogen and their mixtures. After analyzing the maximum pressure rise rate and explosion index data for methane, they had derived the following formula for \(\frac{dp}{dt}\)max:

\[
\left(\frac{dp}{dt}\right)_{\text{max}} = \frac{3S_{v,e}}{R_w} p_0 \left(\frac{p_{\text{max}}}{p_0} - 1\right) \left(\frac{p_{\text{max}}}{p_0}\right)^{1/\gamma_u}
\]

(1)

where \(R_w\) is the radius of the spherical vessel, \(p_0\) and \(p_{\text{max}}\) are, respectively, the initial pressure and the maximum pressure, \(S_{v,e}\) is the burning velocity at peak explosion pressure, \(\gamma_u\) is the specific heat capacity ratio of unburned gas. Combined with a laminar burning velocity formula obtained by Stone et al. [10]:

...
\[ s_u = 0.366 \left( \frac{T_u}{T_{u,0}} \right)^{1.42} \left( \frac{p}{p_0} \right)^{-0.297} \]  \hspace{1cm} (2)

where \( T_u \) is the temperature, \( T_{u,0} \) is the temperature at initial conditions.

By substituting Eq. (2) into Eq. (1), they finally obtained the following equations for \((dp/dt)_{\text{max}}\) and \(K_G\):

\[ (dp/dt)_{\text{max}} = C_2 \cdot p_0^{0.703} \]  \hspace{1cm} (3)

\[ K_G = C_3 \cdot p_0^{0.703} \]  \hspace{1cm} (4)

where \( C_2 = \frac{1.098}{R_w} \left( \frac{p_e}{p_0} - 1 \right) \left( \frac{p_e}{p_0} \right)^{(1.123y_u-0.42)/y_u} \), \( C_3 = 1.770 \left( \frac{p_e}{p_0} - 1 \right) \left( \frac{p_e}{p_0} \right)^{(1.123y_u-0.42)/y_u} \).

Based on formulas above, they concluded that “for methane, the deflagration index (or maximum pressure rise rate) is proportional to the initial pressure to the power of 0.7; Therefore, the linear relationship between deflagration index and initial pressure proposed in previous studies [3, 8-9] is not correct.”.

However, in fact, some mistakes may exist in their derivation process from Eq. (1) to Eq. (4). So, in this paper, the relationship between the maximum pressure rise rate (or deflagration index) and initial pressure will be discussed, and expression for the right relationship will be deduced as well. This may be useful to the gas explosion intensity calculation or assessment in confined vessel explosions.

### 2. Derivation and discussion of the relationship between the maximum pressure rise rate and initial pressure in confined vessel

Assuming the explosion process is isentropic, the temperature and pressure of unburned gas can be related by means of the adiabatic compression equation:

\[ T = T_0 \left( \frac{p}{p_0} \right)^{1-1/y_u} \]  \hspace{1cm} (5)

Applying Eq. (5), we have

\[ \left( \frac{T}{T_0} \right)^{1.42} = \left( \frac{p}{p_0} \right)^{(1.42y_u-1.42)/y_u} \]  \hspace{1cm} (6)

By substituting Eq. (6) into Eq. (2), we can obtain

\[ s_u = 0.366 \left( \frac{p}{p_0} \right)^{(1.42y_u-1.42)/y_u} \left( \frac{p}{p_0} \right)^{-0.297} = 0.366 \left( \frac{p}{p_0} \right)^{(1.123y_u-0.42)/y_u} \]  \hspace{1cm} (7)

By substituting Eq. (7) into Eq. (1), we finally have

\[ (dp/dt)_{\text{max}} = \frac{1.098}{R_w} p_0 \left( \frac{p_e}{p_0} - 1 \right) \left( \frac{p_e}{p_0} \right)^{(1.123y_u-0.42)/y_u} \]  \hspace{1cm} (8)

For a common combustible gas explosion, the relative change in \( p_e/p_0 \) is always within 1.5% as \( p_0 \) changes from 1 to 10 bar. Such conclusion can be drawn from many research paper easily, for example, Mitu et al. on ethanol/air mixture and methane-air mixture [6-7], Movileanu et al. on ethylene–air mixtures [8], Oppong et al. on 2-methylfuran/air mixture [11], etc. Fig. 1, Fig. 2 and Fig. 3 are the results of their experiments.
Therefore the pressure ratio \( p_e/p_0 \) can be nearly viewed as independent of the initial pressure [3]. Therefore, \((dp/dt)\text{max}\) yields the following correlation:

\[
\left( \frac{dp}{dt} \right)_{\text{max}} = C_2 p_0 \tag{9}
\]

where

\[
C_2 = \frac{1.098}{R_w} \left( \frac{p_e}{p_0} - 1 \right) \left( \frac{p_e}{p_0} \right)^{(1.123\gamma_u - 0.42)/\gamma_u}
\]

By substituting Eq. (1) into definition equation of the deflagration index \( K_G \), we have following correlation for deflagration index:

\[
K_G = C_3 p_0 \tag{10}
\]

where

\[
C_3 = 1.770 \left( \frac{p_e}{p_0} - 1 \right) \left( \frac{p_e}{p_0} \right)^{(1.123\gamma_u - 0.42)/\gamma_u}
\]

From Eq. (9) and Eq. (10), it can be seen that the relationship between the maximum pressure rise rate \((dp/dt)\text{max}\) (or deflagration index \( K_G \)) and initial pressure \( p_0 \) is still linear, not proportional to the initial pressure to the power of 0.7 that the authors derived. Obviously, the author maybe made mistakes in the derivation process, and the previous studies [2, 7, 9] are still correct.

In fact, since the pressure ratio \( p_e/p_0 \) is independent of the initial pressure [3], the flame burning
velocity at the peak pressure $S_{\text{ac}}$ is also independent of the initial pressure, according to Eq. (2). As a consequence, even if substituting Eq. (2) into Eq. (1), the relationship between $(dp/dt)_{\text{max}}$ and $p_0$ is still linear. This conclusion has been confirmed not only by the hydrogen and methane explosion studies, but also by studies on other gaseous explosion, such as methanol [12], ethanol [6], ethylene [8-9], propane [2], propylene [13], liquefied petroleum gas [14] etc..

3. Estimation of the specific heat capacity ratio of gasoline vapor

Eq. (9) and Eq. (10) can be used to estimate the specific heat capacity of gasoline vapor during gasoline vapor/air mixture explosion. Qi et al. [15] conducted reliable gasoline vapor explosion experiments in a 20L spherical container ($R_W=0.168m$). The specific heat capacity of gasoline vapor in the gasoline vapor explosion process is estimated as follows based on the data in literature [15].

According to literature [15], the experimental data under the initial condition of temperature 300 K, pressure $p_0=101325$ Pa and gasoline vapor volume concentration 1.65% were selected. Under this initial condition, the maximum pressure is 0.791MPa, and the maximum pressure rise rate $(dp/dt)_{\text{max}}$ is 32.892 MPa/s.

By substituting these data into Eq. (9), we can obtain

$$32.892 = \frac{1.098}{0.068} \left( \frac{0.791}{0.101} - 1 \right) \left( \frac{0.791}{0.101} \right)^{(1.123\gamma_u-0.42)/\gamma_u} \times 0.101$$

therefore $\gamma_u = 1.535$.

Under normal temperature and pressure condition, the specific heat capacity of air is about 1.42, and that of propane (volume fraction 2.8%) is about 1.377. Therefore, the specific heat capacity of gasoline vapor estimated in this work is reasonable and acceptable.

4. Conclusions

In this paper, the relationship between the maximum pressure rise rate (or deflagration index) and initial pressure is deduced and discussed, and the main conclusions can be drawn as follows:

(1) The relative change in $p_e/p_0$ of a common combustible gas explosion is always within 1.5% as $p_0$ changes from 1 to 10 bar, therefore, the pressure ratio $p_e/p_0$ are nearly viewed as independent of the initial pressure.

(2) The relationship between the maximum pressure rise rate $(dp/dt)_{\text{max}}$ and deflagration index $K_G$ and initial pressure $p_0$ are still linear, and yield the following correlations:

$$\frac{(dp)}{(dt)}_{\text{max}} = C_2 p_0$$

$$K_G = C_3 p_0$$

where $C_2 = \frac{1.098}{R_w} \left( \frac{p_e}{p_0} - 1 \right) \left( \frac{p_e}{p_0} \right)^{(1.123\gamma_u-0.42)/\gamma_u}$, $C_3 = 1.770 \left( \frac{p_e}{p_0} - 1 \right) \left( \frac{p_e}{p_0} \right)^{(1.123\gamma_u-0.42)/\gamma_u}$.

(3) Eq. (9) and Eq. (10) can be used to estimate the specific heat capacity of gasoline vapor during gasoline vapor/air mixture explosion. Under normal temperature and pressure condition, the specific heat capacity of gasoline vapor is about 1.535.

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