

# Numerical simulation of premixed Hydrogen/air combustion pressure in a spherical vessel

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**Abstract.** In order to study the development process of hydrogen combustion in a closed vessel, an on-line chemical equilibrium calculator and a numerical simulation method would be used to analysis the combustion pressure and flame front of mixed gas, which based on 20L H<sub>2</sub>/air explosion experiments in spherical vessel(Crowl and Jo,2009). The results showed that, the turbulent model could reflect the process of combustion, and the error of combustion pressure by simulation is smaller than the Chemical Equilibrium Calculation. The heat loss and incomplete combustion are the main reason to cause the error.

## 1 Introduction

Gas explosion in the closed vessel is a typical accident in the process of industrial production. A small ignition can cause explosions once combustible gases mixed with air when it leakage and diffusion in the process of production, transport, storage and use, and the gas mixture components are located on the combustible gas explosion limit of range. According to the statistics, there are more than 300 combustible gas explosion accidents which death toll more than 3 in our country in 2010~2015 [1], in particular of Dong Huang Qingdao Sinopec oil pipeline leakage and explosion accidents, which left 62 dead, 136 wounded and a direct economic loss of up to 751.72 million yuan, had extremely serious consequences [2]. The similar accident would cause a large number of casualties and economic loss and affect the stability of social development directly.

With the fossil fuel exploitation and use and the earth's environmental problems challenging, new energy will be used more and more widely. The fossil fuel does not meet the long-term needs of modern industrial development because of their inherent scarcity. And it also has a large number of CO, CO<sub>2</sub> and SO<sub>2</sub> are produced in the use of fossil fuel, which can cause global warming and a lot of secondary disasters. As a new energy, hydrogen have a high calorific value, low pollution, renewable and advantages of rich, which makes it can be widely applied to chemical production, automobile manufacturing, aerospace and food industries. But hydrogen also may cause heavy casualties and losses because of the flammable and explosive properties, which is a problem that people use the hydrogen in the future.

There have lots of research on combustion process of hydrogen we can achieve. Crowl and Young-do Jo measurement of different concentrations of flammable gases such as hydrogen, methane explosion limits in air by experiment, comparison of traditional fuels and hydrogen in industrial production process, and calculated explosion limits of combustible gases by second derivation method [3,4]. Hansen and Crowl estimate the explosive limit by thermodynamic calculations and empirical formula method, and the results showed that explosion limits of gases and oxygen concentration exists linear relationship at fixed initial conditions [5]. Liu studied the ignition temperature and ignition delay time by changed the initial pressure, and explained the reasons for the formation of the third explosive limit form the perspective of chemical kinetic [6]. Young-do Jo predict the hydrogen-air premixed combustion characteristics of explosion parameters in different concentration of hydrogen, and the results showed that the maximum explosion pressure and  $K_G$  does not appear in stoichiometric concentration [7]. Tao calculated the fixed nitrogen concentration of hydrogen/oxygen/nitrogen explosion characteristics of premixed gas by Chemical Equilibrium Calculation, and get the general equations of the maximum explosion pressure and  $K_G$  in the fixed nitrogen concentration [8, 9]. Molkov have simulated the Hydrogen-air combustion in open space by the Large Eddy Simulation, and the results show that the turbulence is the main cause of flame instability [10]. Xiao study on the combustion of hydrogen-air premixed gases in the pipe by experiment, and make a simulation by using laminar flow thickness of flame model to analyze the causes of formation the Tulip flame [11]. Bao study on the characteristics of the maximum explosion pressure in

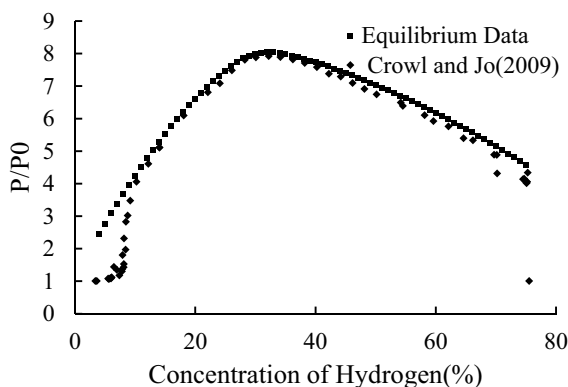
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different initial conditions by using constant volume combustion bomb experiment [12].

This paper focused on the hydrogen-air premixed gas explosion pressure variations by using Chemical Equilibrium Calculation and numerical simulation for a 20L spherical vessel, to study of premixed gases explosion in the vessel by comparing the calculated data and experimental data.

## 2 Chemical Equilibrium Calculation

The full combustion of premixed gas combustion parameters could be calculated by using the initial status parameter based on the thermodynamic theory. According to a known set of initial conditions, an online calculation of chemical equilibrium, which based on the iterative computation of STANJAN, can be used to calculate the explosion pressure. According to initial condition in the experiment of Crowl, which the initial pressure is 1atm and the initial temperature of 300K, the parameters can be calculated. Considered the formation of  $\text{NO}_x$ , the products include H,  $\text{H}_2$ ,  $\text{H}_2\text{O}(\text{g})$ , OH, N,  $\text{N}_2$ ,  $\text{N}_2\text{O}$ ,  $\text{NH}_3$ ,  $\text{NH}_2$ , NH, O,  $\text{O}_2$ ,  $\text{NO}_2$ , NO and  $\text{H}_2\text{O}(\text{l})$  [8]. The hydrogen-air premixed gases explosion pressure in different concentration by calculation as shown in Fig.1 [13]. From chart show, there are a small differences in middle of hydrogen content, but the calculated results with experimental chemical equilibrium value larger than the difference in the hydrogen concentration near the explosion limits. The actual burning condition and heat dissipation is the main cause of the difference. In the premixed gas combustion process, content of active substances is so less that could not enough to support a smooth chain reaction when the oxygen or hydrogen content at low levels. But it would be calculated in accordance with the combustible gases react at all in the Chemical Equilibrium Calculation, which is the main reason to cause the calculation results bigger than the experimental results. Meanwhile, a small amount of heat loss in the process of experiment, which due to slow chemical reaction near the explosion limits, also is a reason lead to lower combustion temperature and pressure at the terminal state.



**Figure 1.** Maximum Pressure in equilibrium and experimental Data vs. Concentration of Hydrogen

## 2 Numerical methods

**The governing equations.** Because of the complexity of the combustion process, laminar flame propagation model only to explain the simplified characterization of flame propagation. In fact, flame propagation folds due to the instability of the flame in the actual combustion process, therefore turbulent propagation model can explain the flame propagation process better than laminar model. Numerical simulation select spherical vessel as the physical model based on the experiment of Crowl and Jo, meanwhile, for ease of calculation, the model is reduced to 2D. Mass equation, momentum equation and energy are as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0 \quad (1)$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ji}}{\partial x_j} \quad (2)$$

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial}{\partial x_j}(u_j(\rho E + p)) = \frac{\partial}{\partial x_i}\left(k_{\text{eff}} \frac{\partial T}{\partial x_i} - \sum_j h_j J_j + \tau_{i, \text{eff}} u_j\right) + S_h \quad (3)$$

Where  $t$  is the time,  $\rho$  is the density,  $E$  is the total energy of micro-turbulence,  $p$  is the pressure,  $k_{\text{eff}}$  is the heat conductivity,  $J_j$  is the diffusion flux of component  $J$ ,  $S_h$  is the chemical reaction heat source and other volume heat source.

$k$ - $\epsilon$  equations would be selected as the turbulent model, and the equations are as follows:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\left(\mu + \frac{\mu_t}{\sigma_k}\right) \frac{\partial k}{\partial x_j}\right) + G - \rho \epsilon \quad (4)$$

$$\frac{\partial(\rho \epsilon)}{\partial t} + \frac{\partial(\rho \epsilon u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\left(\mu + \frac{\mu_t}{\sigma_k}\right) \frac{\partial \epsilon}{\partial x_j}\right) + C_1 G \frac{\epsilon}{k} - C_2 \rho \frac{\epsilon^2}{k} \quad (5)$$

Where  $G$  is the turbulent kinetic energy caused by velocity gradient,  $C_1$ ,  $C_2$  are the empirical constant.

Composition PDF transport, which based on the chemical reactions, would be selected as the combustion model, calculation method is SIMPLE. And the 19-step reaction mechanism of hydrogen would be used in the simulation. The initial pressure is 1atm, and the initial temperature of 300K. The ignition location at the central of vessel, and ignition temperature for 2000K. monitor point would be selected on the wall, to detect the change of pressure in the combustion process.

## 3 Results and discussion

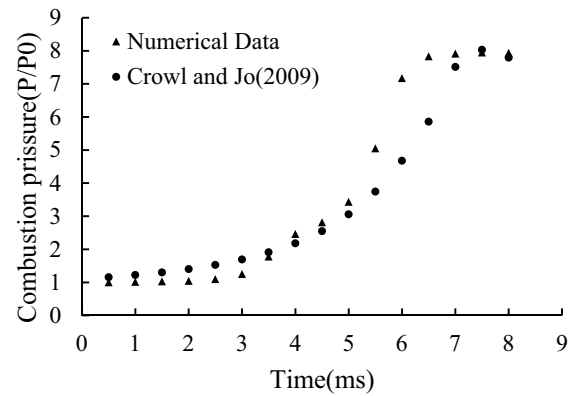
According with the model based on the above numerical methods, the simulation results of CFD are shown in the Table 1. And the relative error  $\delta$ , which is the result of combustion pressure between the Chemical Equilibrium Calculation, simulation and experimental at the selected concentration of hydrogen, are also shown in the Table 1.

Near the stoichiometric concentration, the relative error of Chemical Equilibrium Calculation are less than 4%, and the relative error of Numerical simulation are less than 3%. But both errors are higher in the areas near the explosion limits. In general, the result of simulation is better than Chemical Equilibrium Calculation. And the reason of error as mentioned above.

**Table 1.** The Combustion Pressure in different Concentration of Hydrogen by Calculated and Numerical

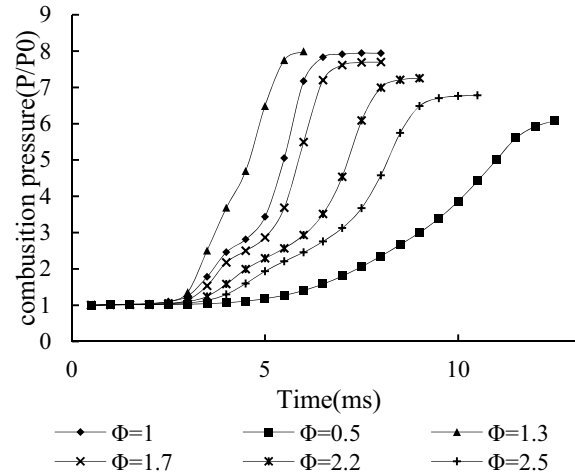
Concentration of Hydrogen	Calculated Data		Numerical Data	
	$P_{max}(P/P_0)$	$\delta$	$P_{max}(P/P_0)$	$\delta$
17.75%	6.19	1.48%	6.16	0.98%
22.73%	7.13	4.85%	7.16	5.29%
29.59%	7.95	1.92%	7.82	0.26%
35.33%	7.96	2.05%	7.89	1.15%
41.67%	7.63	3.11%	7.58	2.43%
45.67%	7.36	3.66%	7.27	2.39%
51.23%	6.91	3.13%	6.79	1.34%

Different from the Chemical Equilibrium Calculation, numerical simulation of premixed gases could simulate the combustion process, and chemical equilibrium calculation can only get the final result. So the premixed combustion process can be analyzed based on simulation results. The pressure curve of stoichiometric concentration is shown in the Fig.2. Compared with the experimental data, the time of maximum explosion pressure in experiment is longer than the simulation required. In the simulation process, the pressure would rise at 2.5ms, and reached the maximum value at 6.8ms, but in the experiment process, the pressure rise is more gentle, it would be 5.5ms to reach the maximum totally. In the actual combustion process, the shape of the flame will change because of different flame burning speed in the different directions, which due to the influence of gravity, would delay the combustion process. However, the effects of buoyancy on flame kernel would not be considered in the simulation, which lead to flame propagation speeds in different directions almost identical in flame. After the acceleration of turbulence, the time of the combustion process would be reduced.



**Figure 2.** Comparison of combustion-explosion pressure between experiment and Simulation

With the change of hydrogen concentration, combustion pressure and combustion process would vary, the curve of combustion pressure at different hydrogen concentration as shown in Fig.3. The fastest burning is not at stoichiometric concentration. From the figure, we can find the rate of pressure rise at equivalence ratio  $\Phi=1.3$  was higher than stoichiometric concentration, and this conclusion is consistent with experimental results [7]. As the  $\Phi$  increases (or decreases), combustion pressure gradually reduces, and the time to the maximum combustion pressure are gradually increases.



**Figure 3.** Combustion pressure vs. Time in different equivalence ratio

#### 4 Conclusions

An online Chemical Equilibrium Calculation was used to calculate the combustion pressure of hydrogen-air premixed gas, and the calculation results agree well with experimental results in the area of near stoichiometric concentration, but the error was big at explosion limits. And the main reason causing the error is the heat loss in the actual explosion and incomplete combustion.

The composition PDF transport model can be used to simulated the combustion process of hydrogen-air premixed gas in the spherical vessel. Compared the simulation and experiment, the results show that the turbulent combustion model can well simulate the combustion process, but the area near the explosion limits is still need to study.

By comparing different stoichiometric ratio of combustion process, the results show that the maximum explosion pressure and the rate of pressure rise is not occur at stoichiometric concentration and it is consistent with experimental results. it indicates that the most dangerous concentrations of premixed gases are not the stoichiometric concentration in the actual explosion.

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