Simulation Study on the Explosion Characteristics of Premixed Hydrogen-air Mixtures

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Abstract: In order to study the explosion characteristics of hydrogen in the air and the influence of concentration on the explosion characteristics of hydrogen, the fire and explosion of small-scale hydrogen cloud with different concentration are simulated. The distribution of explosion characteristic parameters, such as overpressure, temperature and velocity, as well as the change rule with time, are obtained. The explosion characteristic parameters in horizontal and vertical directions are discussed. The results show that under the influence of the ground and gravity, oblate elliptical fireballs with horizontal direction larger than vertical direction are formed in the early stage of ignition development. With the continuous combustion, they develop into hemispherical fireballs with the diameter of the ground and spread around. The influence of concentration on the law of fire and explosion is studied, and the maximum overpressure under different concentration is obtained, which provides support for building the fire field model of liquid hydrogen leakage. It is also of great significance for the evaluation of explosion hazards and the design of corresponding protection system.

1. Introduction
Since the success of hydrogen liquefaction, liquid hydrogen has been widely used in aerospace fields such as launch space station, manned lunar landing and Mars landing [1-2]. Once liquid hydrogen leaks, it will quickly evaporate and diffuse. The diffusion speed is inversely proportional to the square root of the molecular weight of the gas. It is generally considered that the diffusion speed of hydrogen is the largest in almost all gases. Hydrogen is combustible within the range of 4% - 75% volume concentration under air conditions, 48.3% - 59% of them are likely to explode, which poses a huge threat to the safety of personnel, equipment and launch vehicles on site [3]. Therefore, scholars at home and abroad have carried out many simulation and experimental researches on combustible premixed gases such as hydrogen. Bragin has simulated the transition process from spontaneous combustion to continuous combustion [4], and believes that the transition process is related to the process of vortex entrainment of combustion mixture to the reflux zone. Kim has studied the combustion and flow process of hydrogen, focusing on the ignition surface and the development of shock wave [5]. Zhao xiang Huang solved the unsteady ignition problem of premixed gas ignited by a small fireball, treated the relationship between the critical ignition diameter and the reaction rate dimensionless [6]; Yan Huo et al. Carried out the experimental study of premixed gas deflagration flame propagation in a large diameter pipeline, deduced the deflagration flame propagation model and obtained the coefficient value of the flame propagation distance and time relationship [7]. In this paper, the numerical simulation of fire and explosion of hydrogen air premixed gas with different
concentrations is carried out by using the fluid simulation software, and the distribution of explosion characteristic parameters such as overpressure, temperature and velocity and the change rule with time are obtained when the hydrogen cloud is in fire and explosion. The differences of explosion characteristic parameters in the horizontal and vertical directions are discussed, not the law of concentration on fire and explosion. It is also of great significance to evaluate the explosion hazards and the corresponding protection system design.

2. Physical model
The flow field of hydrogen air premixed gas fire and explosion belongs to the turbulent flow field with high temperature, high speed and high pressure gradient, which follows the laws of mass conservation, momentum conservation and energy conservation.

Conservation of mass equation:
\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0 \]  
(1)

Conservation equation of momentum:
\[ \frac{\partial}{\partial t} (\rho u_j) + \frac{\partial}{\partial x_i} (\rho u_j u_i) = \rho f_i - \frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ji}}{\partial x_j} \]  
(2)

Energy conservation equation:
\[ \frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x_j} (\rho u_j E) = \rho f_{ij} u_j - \frac{\partial}{\partial x_j} (\rho u_j u_i) + \frac{\partial}{\partial x_j} (k \frac{\partial T}{\partial x_j}) + S \]  
(3)

Equation of state:
\[ P = P(\rho, T) \]  
(4)

It is very difficult to directly solve the partial differential equations of (1) - (4). In general, the finite volume method is used to discretize the control equations and the numerical solution is used to approximate the analytical solution. The deformation of the governing equation is as follows:
\[ \frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho \phi V) = \nabla \cdot (\Gamma_{\phi} \nabla \phi) + S_{\phi} \]  
(5)

Integral in the control body to obtain:
\[ \iiint_{CV} \nabla \cdot (\rho \phi V) d\tau = \iiint_{CV} \nabla \cdot (\Gamma_{\phi} \nabla \phi) d\tau + \iiint_{SV} S_{\phi} d\tau \]  
(6)

Where, \( \phi \) represents general variable; \( \Gamma_{\phi} \) represents diffusion coefficient; \( V \) represents control volume; \( S_{\phi} \) represents source term.

In the solution of reaction flow of fire and explosion, in addition to the above four control equations, in order to close the control equations and supplement the component control equation, in which all components involved in the chemical reaction meet the conservation of mass, the component equation is as follows:
\[ \frac{\partial (\rho Y_s)}{\partial t} + \nabla \cdot (\rho Y_s V_s) = \nabla \cdot (\rho D_s Y_s) + R_s \quad (s = CH_4, O_2, CO, CO_2, H_2, O) \]  
(7)

Where \( Y_s \) a is the mass fraction of component \( s \); \( D_s \) is the diffusion coefficient of component \( s \); \( R_s \) is the mass generation rate of component \( s \).

\( k - \varepsilon \) model is generally used in the turbulent model of hydrogen air premixed gas explosion.
\[ K = \frac{1}{2} \overline{u'w'} = \frac{1}{2} \left( \overline{u'v'} + \overline{w'w'} \right) \]  
(8)
\[ \varepsilon = \frac{\mu \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_i}}{\rho} \]  

(9)

Among them, the \( K \) equation represents the turbulent kinetic energy equation, the \( \varepsilon \) equation represents the turbulent dissipation rate equation, and the \( u'_i \) represents the turbulent pulsation velocity component in the rectangular coordinate system; the turbulent dynamic viscosity coefficient \( \mu_t \) can be expressed as:

\[ \mu_t = C_{\mu} \rho \frac{K^2}{\varepsilon} \]  

(10)

3. Simulation model

Establish small-scale fire and explosion model of hydrogen air premixed gas, diameter 0.5m. The premixed cloud cluster of 10 m × 10 m × 10 m exploded, and the ignition position was located at the distance from the ground 0.25m. See Table 1 for relevant initial parameters of height, fire and explosion calculation.

| Air pressure | Air temperature | Cloud diameter | Ignition energy | Ignition area diameter | Ignition duration |
|--------------|-----------------|----------------|-----------------|------------------------|------------------|
| 101325Pa     | 300K            | 0.5m           | 0.01J           | 0.001m                 | 0.001s           |

3.1. Selection of calculation conditions

It is generally considered that the minimum ignition energy of hydrogen 0.019mj. It can only ignite the stoichiometric hydrogen with volume fraction of concentration 29.5%. The ignition energy of hydrogen air mixture is much higher than that of other concentrations, especially at the lower and upper flammability limits. Ryono et al. [8] research results show that when the volume fraction of hydrogen is less than 10%, the ignition can jump rapidly, that is, when the hydrogen content is lower than this value, the hydrogen ignition is strongly inhibited. Similarly, when the volume fraction is greater than 70%, the hydrogen ignition is also strongly inhibited. The results are shown in Figure 1.

![Figure 1. Determination results of minimum ignition energy of hydrogen air bath mixed gases with different volume fractions](image-url)

It can be seen from the relevant literature that after the leakage of liquid hydrogen, the volume fraction of hydrogen cloud generated is generally lower than 52%, and the higher volume fraction is concentrated near the leakage source or the surface of liquid hydrogen pool, where the temperature is extremely low and it is not easy to ignite. Therefore, this paper selects the hydrogen volume fraction of 10%, 29% and 45% for calculation.
3.2. Assumptions
During the simulation, the following assumptions are made: a) the premixed gas is considered as an ideal gas; b) the hydrogen combustion reaction uses one-step lump sum reaction without considering the detailed reaction mechanism of hydrogen combustion; c) the specific heat of the gas is constant; d) the physical viscosity coefficient of the gas conforms to Sutherland's law.

4. Calculation results and analysis

4.1. Analysis of explosion characteristics when volume fraction is 29%
The calculation result of hydrogen volume fraction of 29% is shown in the figure below, and Figure 2 is $t=0.0002s$, $t=0.0006s$, $t=0.002s$ And $t=0.0006s$ Cloud chart of flow field at four times.

| Time  | Pressure | Temperature | Velocity |
|-------|----------|-------------|----------|
| 0.2ms | ![Pressure](image1) | ![Temperature](image2) | ![Velocity](image3) |
| 0.6ms | ![Pressure](image4) | ![Temperature](image5) | ![Velocity](image6) |
| 2ms  | ![Pressure](image7) | ![Temperature](image8) | ![Velocity](image9) |
| 6ms  | ![Pressure](image10) | ![Temperature](image11) | ![Velocity](image12) |

Figure 2. Distribution of flow field at different times

As shown in Figure 2, the pressure distribution diagram at different times after ignition of hydrogen air premixed gas can see the whole propagation process of pressure wave, including the reflection wave formed when the pressure wave moves to the ground, and the superposition of reflection wave and pressure wave. The superposition area of pressure wave and reflection wave near the ground is the peak area of overpressure. At $t=0.2ms$ Hour diameter is 0.1m the pressure is greater than 0.1Mpa The pressure decreases from the center ignition area to the outside. At $t=0.6ms$ When the pressure wave moves to the ground and is reflected, the maximum pressure appears on the ground. Due to the superposition of reflection waves, the pressure near the ground is greater than 0.18Mpa The pressure...
in the ignition center appears hollow with the movement of the pressure wave, the center pressure decreases, and the peak surface of the pressure wave has a diameter of 0.58m. Area of. t=1ms shows that in the vertical direction, the reflected pressure wave is about to catch up with the original pressure wave, and the superimposed pressure of the pressure wave is the largest at a diameter of 1m close to the ground. t=6ms shows that the pressure wave has moved to the area with a diameter greater than 5m, and the pressure in the whole 5m area tends to average gradually, and the maximum pressure is also getting smaller and smaller.

The temperature shows the spread of flame. At the same time, compared with the pressure, the high temperature region is far less than the high pressure region, indicating that the flame propagation speed is far less than the pressure wave propagation speed. The velocity shows that the maximum temperature increases with the development of fire, which is opposite to the attenuation of pressure wave with time. In addition, the ignition center temperature changes continuously with the flame spread, sometimes higher than the surrounding temperature and sometimes lower than the surrounding temperature, which depends on the flame development and spread. t=1ms shows that after the flame spreads to the ground, a high temperature area will be formed near the ground. Because the ground is set as an insulated wall in the simulation process, which is inconsistent with the actual situation, the actual fire will transmit heat to the ground after it spreads to the ground, and the ground temperature will be less than this value. t=6ms shows that the ground flame and the ignition center flame have been completely fused.

The velocity shows the velocity of the gas after the pressure wave. The larger the pressure wave, the greater the gas velocity. Better observe the change rule of pressure, temperature and speed at the ignition center position, i.e. from the ground 0.25m. Take the central axis horizontally on the height, and get the pressure, temperature and temperature curves of different positions at different times as shown in the figure below.

Figure 3 (a) shows the continuous attenuation of the maximum pressure wave over time on the horizontal central axis. The high-pressure area continues to move outward, and the high-pressure area changes greatly at different times. At the initial stage of ignition, the high-pressure area is in the center. When the reflected pressure wave moves to the height of the central axis, the pressure wave in the center area rises again, and at other times, the high-pressure area moves in front of the pressure wave.

Figure 3 (b) the change curve of the speed temperature along the central axis with the position at different times shows that the high temperature area is small in the early stage of explosion, the temperature of the whole explosion area is not particularly high, and the ignition center temperature is lower than the temperature of the surrounding high temperature area. 0.2ms The difference between the explosion center and the maximum temperature is about 100k, reaching 600k in 1ms. With the explosion going on, the temperature of the explosion area continues to rise, the high temperature area continues to expand, and the ignition center temperature continues to rise. After 2ms, the ignition center temperature is the highest, and with the temperature away from the explosion center decreases.
Figure 4 shows the pressure wave transmission and attenuation process of five measuring points in different positions of the central axis. Maximum overpressure occurs at ignition center $X=0$, at 0.26ms. When the overpressure reaches the maximum value 0.205Mpa, as the $X$ direction becomes larger, at $X=0.4m$, 0.8m, 1.0m, 2.0m. The maximum overpressure decreases continuously and appears later. Figure 4(a) can predict that the maximum overpressure is less than 20KPa in the area 2m away.

Figure 4(b) shows the process of temperature rise in the real explosion area after ignition. The ignition center will have instantaneous high temperature, and then the temperature will rise to about 2400k after a slight drop. In the whole process, the center temperature is always at the highest temperature.

Figure 5 shows that when $t=5$ms, $X=0.6m$. The temperature at the measuring point began to rise, i.e. the explosion flame developed to this area, while at $Y=0.6m$. The vertical temperature can reach the horizontal temperature in a short time, that is, the vertical temperature gradient is larger. It is the same at $X=1m$ and $Y=1m$. The difference is that the temperature gradient is less than 0.6m. This is because under the joint influence of the ground and gravity, the high temperature area of the explosion is not completely circular, but a flat elliptical fireball with the horizontal direction greater than the vertical direction. The obvious ellipse can be seen in the 1ms temperature cloud figure in Figure 2. After 30ms, the horizontal and vertical temperatures are basically the same. At 30ms, the temperature cloud chart is as shown in Figure 6. The high temperature area is a hemisphere with the diameter of the ground. The highest temperature is the same at 2400k and 1ms.
Figure 6. Cloud chart of temperature distribution when $t = 30$ms

4.2. Comparison of different volume fraction results

Figure 7(a) shows that when the volume fraction is 10%, 29% and 45% hydrogen air premixed gas is ignited, the overpressure attenuation curve at the ignition center is basically the same, and when the volume fraction is 10%, the maximum overpressure is 0.103Mpa. When the volume fraction is 29%, the maximum overpressure is 0.21Mpa. When the volume fraction is 45%, the maximum overpressure is 0.045Mpa. It can be seen that the maximum overpressure after ignition of different concentrations of hydrogen air premixed gas just starts with the concentration (a large number of studies show that the maximum overpressure decreases with the increase of concentration. This law is consistent with the law of minimum ignition energy required at different concentrations.

Figure 7(b) shows that the temperature change rule is the same under the concentration of 10% and 29%, and the 29% concentration of ignition center temperature is far greater than the center temperature under the concentration of 10%; the temperature change curve is not the same under the higher concentration, but the highest temperature basis of ignition center is the same. That is to say, when the concentration is increased to a certain extent, the ignition center temperature will not continue to increase when it is increased to about 2400K.

The variation trend of explosion temperature and overpressure under the above 10%, 29% and 45% hydrogen volume fraction increases with the increase of hydrogen volume fraction, and the peak value of explosion temperature and overpressure also increases, but when the hydrogen volume fraction reaches a certain critical value, the explosion power decreases. The maximum overpressure and maximum temperature of ignition center under three concentrations are summarized in the table below, which provides a reference for the design of protection system.

5. Conclusion

Through the above simulation calculation and analysis, we can get the following conclusions:

1. In the initial stage of hydrogen air, under the combined influence of the ground and gravity, a flat elliptical fireball with horizontal direction larger than vertical direction is formed. With the continuous
combustion, a hemispherical high temperature area with the diameter of the ground is formed after 30ms at 29% hydrogen concentration, and it spreads around.

2. With the increase of hydrogen concentration, the maximum overpressure and explosion power increase. When the volume concentration of hydrogen reaches 29%, the overpressure reaches 0.21Mpa. With the increase of hydrogen, the maximum overpressure will decrease and the explosion power will decrease.

3. With the increase of hydrogen concentration, the temperature in the explosion zone increases continuously at the initial stage of ignition, and it will not increase after it reaches 2450k.

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