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Analysis of Equivalent Concentration of Hydrogen Explosion in a Closed Cabin

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***Abstract*—In order to obtain the most intense concentration of hydrogen explosion in a confined space in the simulated environment, the methods of theoretical calculations and numerical simulations were used. Through comparison of multiple sets of data, it was concluded that the hydrogen explosion equivalent concentration of 26.9% is the most explosive concentration.**

***Keywords*—hydrogen explosion; equivalent concentration; analysis of accident consequences**

I. Introduction

In the background of reactor LOCA, the break causes the coolant to be lost, causing the core to be exposed, the zirconium shell to oxidize, the temperature of the fuel to rise, reaching the reaction temperature condition, and rapidly generating a large amount of hydrogen to be released into the closed cabin through the break of the pressure boundary of the main circuit[1].

After the hydrogen leaks, it gathers in a certain shape in the air. The experimental cost of the hydrogen explosion in the closed cabin is high and the sample is limited. With the maturity of the numerical simulation software, the analysis of the cabin explosion by theory combined with numerical simulation has become an important alternative. At present, research on the cloud explosion of flammable gas in the cabin is also underway. Guan Yifeng and Fang Shanyu have studied the impact response of the natural gas explosion in the CNG carrier on the ship structure[2]. Qian Xinming and Zhao Huanjuan conducted numerical simulations on the consequences of gas explosion damage in the thinnest shell structure[3].

II. Theoretical Analysis of Hydrogen Explosion Propagation

In the initial stage of hydrogen combustion, the flame surface expands outward in the direction of the ball. As the flame surface expands, the rate of hydrogen combustion increases and the rate of flame expansion increases. When subjected to turbulence, chemical reaction rate and wall surface, the flame surface cannot continue to expand in a spherical shape and begin to exhibit other forms.

During the deflagration process, the flame propagates at subsonic speed, and the pressure wave propagates at the speed of sound. Two waves with different propagation speeds form the two-wave and three-zone structure as shown in Fig. 1.

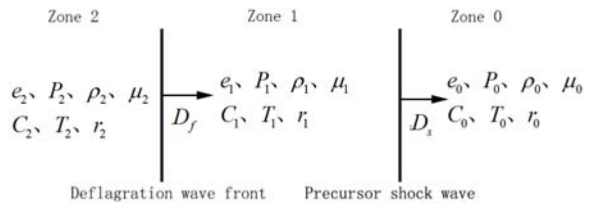

FIGURE I. TWO-WAVE AND THREE-ZONE STRUCTURE

For the states on both sides of the precursor shock wave front, the three conservation equations under the conditions of no viscosity and no heat conduction are as follows:

$$\rho_1(D_s-\mu_1)=\rho_0(D_s-\mu_0) \quad (1)$$

$$\rho_1(D_s-\mu_1)^2+P_1=\rho_0(D_s-\mu_0)^2+P_0 \quad (2)$$

$$e_1+\frac{P_1}{\rho_1}+\frac{1}{2}(D_s-\mu_1)^2=e_0+\frac{P_0}{\rho_0}+\frac{1}{2}(D_s-\mu_0)^2 \quad (3)$$

In the formula: e -Specific heat; P -Pressure; ρ -Density; μ -Particle velocity; D_s -Precursor shock wave velocity.

Under the condition of the shock wave wavefront state, with the equation of state: $e=e(P,\rho)$, four equations and five variables is formed, and the equations can be solved when one of the variables is determined.

III. Finite Element Model Establishment

A. Cabin Size

This paper is based on the hull structure and profile of a type of closed cabin. The length of the closed cabin is 12.0 meters, and the radius of the pressure shell is 4 meters. Regardless of the indoor facilities in the closed cabin, the finite element model of the air and hydrogen mixture in the cabin is shown in Figure 2.

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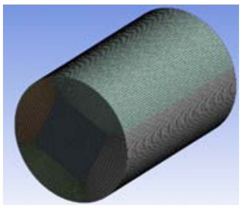


FIGURE II. FINITE ELEMENT MODEL OF GAS IN CLOSED CABIN

B. *Explosive Equivalent Concentration*

According to the chemical equation of hydrogen combustion, the most dangerous concentration of hydrogen explosion is calculated.

Assuming that the hydrogen volume fraction is 2X, the concentration relationship 2X+X/0.21=1 can be listed, and thus the relationship can obtain X=1/(2+1/0.21)=0.148=14.8%, thereby obtaining the most hydrogen gas that the violent volume concentration was 29.6%. The mass fraction of hydrogen obtained by conversion is 0.0283, which is the most intense concentration of hydrogen explosion in an ideal case, and called the explosive equivalent concentration.

C. *Ignition Condition*

According to the literature 1[3], when the fuel-coated zirconium alloy reacts violently with water, the core temperature rises rapidly, and the hottest component of the core reaches 3000K at a temperature of about 3000s, and then continues to rise slowly. In this paper, a 0.25 m radius spherical high temperature region with a temperature of 3000 K is set at the center of the closed cabin.

The gas pressure outside the ignition zone was set to 101,325 Pa and the temperature was set to 300 K; assuming that 10% of the fuel in the fuel center had been ignited, the ignition zone pressure was set to 10 MPa in order to better induce the chemical reaction to the right.

IV. CALCULATION RESULTS AND ANALYSIS

The three hydrogen concentration conditions are as shown in Table 1. At the same time, the gas center interface is selected as the monitoring section, and the center point of the boundary circular surface is the monitoring point-Point 1.

TABLE I. THREE INITIAL HYDROGEN CONCENTRATIONS

Hydrogen concentration	Hydrogen mass fraction
Equivalent concentration	0.0283
Low concentration	0.0183
High concentration	0.0383

A. *Temperature Cloud Diagram at Equivalent Concentration*

As can be concluded from Fig. 3, in the hydrogen combustion process, the flame is initially diffused outward in a spherical shape, and the combustion rate of hydrogen in all directions is substantially uniform. The flame still presents a relatively regular sphere at 6ms. At 20ms, the flames on the upper and lower sides are restricted by the wall surface, the rate of hydrogen reaction along the wall surface decreases, the flame diffusion rate decreases, and the flame propagates along the axial direction of the flame above the flame along the wall. As the flame spreads, it is affected by turbulence and wall effects, presenting the shape of the tulip flame, which points to the center of the cabin. At 0.443 s, the temperature in the entire cabin tends to be uniform and the combustion process has almost ended.

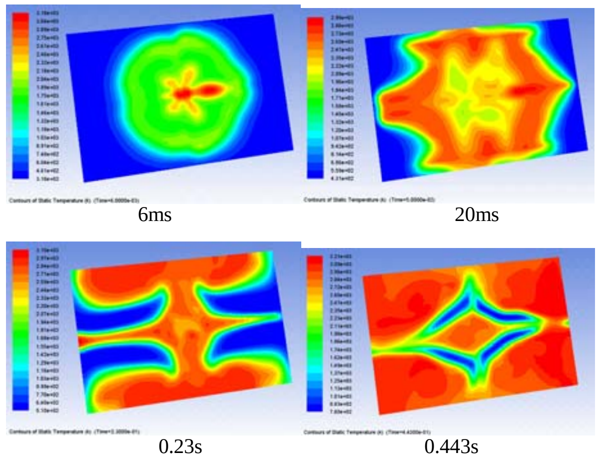


FIGURE III. MONITORING SURFACE TEMPERATURE CLOUD IMAGE AT EQUIVALENT CONCENTRATION

B. *Pressure Cloud Diagram at Equivalent Concentration*

It can be concluded from Fig. 4 that the pressure in the closed cabin is changed stepwise from the highest pressure of 10 MPa in the center of the ignition zone. As the high temperature and gas expansion generated by the explosion process, the pressure begins to rise rapidly, and the shock wave front begins to be spherical. At 3ms, the wavefront contact with the wall .By comparison, the wave velocity of the shock wave front is much larger than that of the flame front, which constitutes a two-wave three-zone structure under blast conditions. The pressure in the 0.614s chamber reached the highest value of 1.6MPa and did not exceed 2MPa, which was in line with the theoretical expectation. The pressure is finally maintained at a stable level without venting and adiabatic wall conditions.

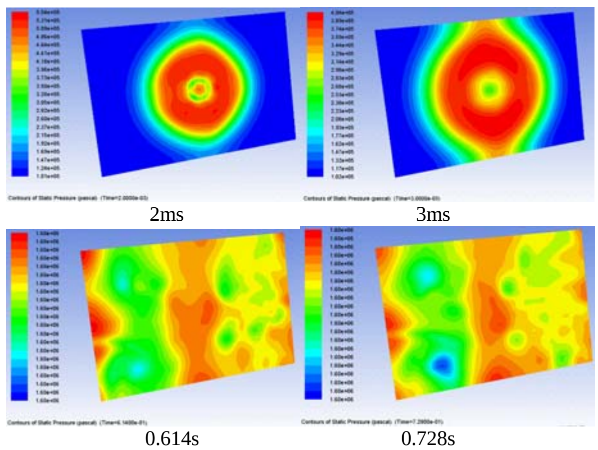
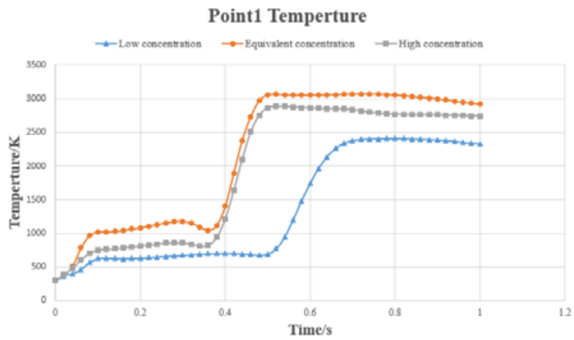


FIGURE IV. MONITORING SURFACE PRESSURE CLOUD IMAGE AT EQUIVALENT CONCENTRATION

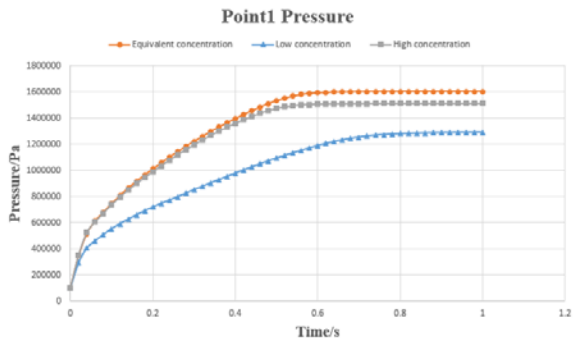
C. *Time History Curve of Monitoring Points*

It can be concluded from Fig. 5 that the temperature of Point1 at the equivalent concentration is always at the highest level among the three, and the temperature at the high concentration is always higher than the temperature at the low concentration. The rate of temperature rise at the equivalent concentration is the fastest among the three, and there is little difference in the case of high concentration. It can be considered that at the most violent concentration of the theoretical explosion, the wall temperature rise rate is the fastest and the temperature is the highest.

The pressure curves of Point 1 at the three concentrations in the initial stage coincide with each other. With the combustion diffusion, the pressure at the monitoring point is the largest at the equivalent concentration. The pressure curve at high concentration has a higher degree of coincidence with the pressure curve at the equivalent concentration.



(a) Temperature curve of Point 1



(b) Pressure curve of Point 1

FIGURE V. TEMPERATURE AND PRESSURE CURVE OF POINT 1

It can be seen from Fig. 6 that at the explosive equivalent concentration, hydrogen and oxygen react exactly and at the same time consume completely. At low concentrations, due to the low hydrogen concentration under the initial conditions, the hydrogen has completely reacted at the end of the reaction, but a large amount of oxygen remains. Since the concentration of hydrogen at a high concentration is too high, a large amount of hydrogen remains after the reaction is completed, and the oxygen reaction is complete. Comparing the changes of the composition of the three working conditions, the utilization of hydrogen and oxygen is the highest under the equivalent concentration, and the remaining two working conditions have a large residual of hydrogen or oxygen. And the amount of hydrogen involved in combustion at a high concentration is close to the equivalent concentration, and the equivalent concentration is almost the same as the consumption rate of hydrogen and oxygen at a high concentration.

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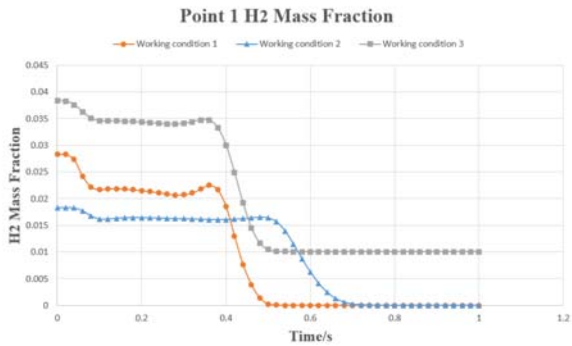
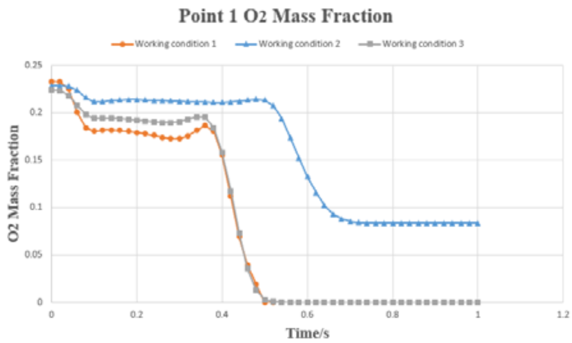


(a) H_2 mass fraction of Point 1



(b) O_2 mass fraction of Point1

FIGURE VI. CURVE OF THE MASS FRACTION OF EACH COMPONENT OF POINT 1

V. CONCLUSIONS

(a) Comparing the simulation results under the three hydrogen concentrations, the hydrogen explosion equivalent concentration is the most explosive concentration of 29.6%. Among the three concentrations, the explosion of hydrogen at the equivalent concentration has the greatest impact on the temperature and pressure of the wall of the closed cabin.

(b) At low concentrations, the hydrogen explosion is relatively violent, and the hydrogen explosion is relatively high under high concentration conditions. Therefore, reducing the hydrogen concentration is more obvious than reducing the hydrogen concentration to reduce the explosion shock.

(c) The simulation results are in agreement with the theoretical expectation, and the pressure is within 2MPa. The reaction rate and explosion pressure at the explosive equivalent concentration are the highest among the three. The side verifies the reliability of the FLUENT fluid simulation software in simulating the hydrogen explosion impact inside the closed chamber. When studying the consequences of a hydrogen explosion accident in a closed compartment, the explosive equivalent concentration of 29.6% can be directly used as the most dangerous condition for hydrogen explosion.

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