Numerical Analysis of Hydrogen Transport Behavior Driven by Cold-Heat Sources in Containment

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Abstract - When a breach occurs in a reactor and causes a severe accident, the high-temperature hydrogen gas inside the primary loop piping will be released into the large space of the containment, which will possibly seriously endanger the integrity of the containment. In order to study the gas transport behavior inside the containment after a severe accident, this paper adopts numerical simulation to establish a full-scale two-dimensional model of the containment, and comprehensively analyses the effects of different factors on the gas transport inside the containment driven by high-temperature gas from the breach and heat exchangers. The results show that factors such as breach size and direction, hydrogen concentration, and condensation on the heat exchanger surface affect the gas transport. When the gas injection velocity of the breach is large, the momentum factor plays a dominant role in hydrogen transportation; when the gas flow rate of the breach is small, the buoyancy factor has a more significant effect on hydrogen distribution. The settling effect caused by steam condensation on the surface of heat exchangers in the containment will affect the direction of flow of surrounding gas to some extent. In addition, increasing the opening of the compartment where the breach is located allows for a more even distribution of hydrogen.

Keywords: Hydrogen transport; Steam condensation; Jet injection; Numerical simulation

1. Introduction

The analysis of hydrogen transport behavior is an important part of the safety risk assessment of nuclear power plants. When a nuclear reactor suffers a loss of cooling accident (LOCA) or a main steam line break (MSLB), a large amount of hydrogen will be released into the large space of the containment along with steam. When the hydrogen concentration increases, hydrogen flaring may occur, seriously jeopardizing the integrity of the containment. With the deepening of the understanding of hydrogen diffusion and transport mechanism, as well as the optimization of numerical analysis software development, people have also carried out relevant research on the hydrogen transport behavior in the containment.

Yang et al.^[1] studied the changes of hydrogen concentration and hydrogen stratification phenomenon in different locations of the containment, and found that hydrogen would form vortex in the steam generator compartment and the dome, and the concentration of hydrogen near the mainstream area would fluctuate greatly under the influence of turbulent diffusion. Xue et al.^[2,3] utilized an experimental setup with a scaling ratio of 1:10, and carried out a mixed-gas emission experiment by using helium as an alternative working medium to hydrogen. The volumetric concentration measured in the experiment was converted into the dimensionless buoyancy force, and the equation of the dimensionless buoyancy force with respect to the altitude and time was fitted.

In the existing studies on hydrogen transport behavior, the main research object basically adopts the experimental device or numerical model after the height direction scaling, which seldom involves the full-size containment large space area, and the influence of steam condensation on hydrogen diffusion and transport in containment is seldom considered in the study. Therefore, based on the multi-component gas diffusion model, this paper investigates the hydrogen transport behavior in the full-scale containment space, obtains the laws of the hydrogen circulation mode driven by cold and heat sources, and obtains a reasonable improvement scheme to avoid the problem of hydrogen accumulation and combustion explosion.

2 Numerical model

2.1 Conservation equations

The conservation equations for mass, momentum and energy need to be followed in calculating the motion of multicomponent gases including air, steam and hydrogen as shown below.

$$\frac{\partial \rho}{\partial t} + \nabla(\rho w) = S_m \tag{1}$$

$$\frac{\partial(\rho w)}{\partial t} + \nabla(\rho w w) = \nabla \cdot P + \rho f + S_{\rho \nu}$$
(2)

$$\frac{\partial(\rho E)}{\partial t} + \nabla(\rho w E) = \nabla(Pw) + \rho f w + \nabla(k_{eff} \nabla T) + S_h$$
(3)

where ρ is the density, kg/m³; *t* is the time, s; *w* is the velocity, m/s; S_m is the mass source term, kg/(m³ ·s); *P* is the surface force, N/m²; *f* is the volume force, N/m³; $S_{\rho\nu}$ is the momentum source term, N/m³; *E* is the energy, J; k_{eff} is the equivalent thermal conductivity, W/(m·K); S_h is the energy source term, J/(m³ ·s).

2.2 Turbulence modeling

The turbulence model is Realizable k- ε model with the following transport equations:

$$\frac{\partial(\rho k_{ui})}{\partial x_i} = \frac{\partial}{\partial x_j} \left[(\mu + \frac{\mu_t}{\sigma_k}) \frac{\partial k}{\partial x_j} \right] + G_k - \rho \varepsilon$$
(4)

$$\frac{\partial(\rho\varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left[(\mu + \frac{\mu_t}{\sigma_{\varepsilon}}) \frac{\partial\varepsilon}{\partial x_j} \right] + \rho C_1 E\varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu\varepsilon}}$$
(5)

Where: *i*, *j* are tensor subscripts; *k* is the turbulent kinetic energy, m^2/s^3 ; ε is the turbulent dissipation rate, J/kg; G_k is the turbulent kinetic energy generated by the mean velocity gradient; σ_k , σ_{ε} are the turbulent Planck numbers for *k*, ε ; C_l , C_2 are constants; μ_t is the turbulent viscosity.

2.3 Multi-component gas diffusion modeling

The multi-component gas diffusion model used in this paper is based on the Stefan-Maxwell model, and the binary diffusion coefficients between different components are expressed as follows^[4]:

$$D_{AB} = \frac{CT^{b} (1/M_{A} + 1/M_{B})^{1/2}}{p[\sum_{A} v_{i}^{\alpha 1} + \sum_{B} v_{i}^{\alpha 2}]^{\alpha 3}}$$
(6)

where C is a constant; T is the temperature, K; p is the pressure, atm; M_A and M_B are the molar mass, g/mol; the rest of the parameters are obtained by the least squares method.

3 Influencing factors for hydrogen transportation

3.1 Geometric Model

In order to save the computational cost, this study adopts a two-dimensional model and a polyhedral mesh for the mechanism study and analysis. Two key physical phenomena are involved in the research, namely the diffusion and transport of hydrogen in large space, and the influence of steam condensation on gas transport. Therefore, the model verification of these two key factors is carried out according to LSGMF experiment^[5] and COAST experiment^[6] respectively, as shown in Fig. 1. The error between the calculation result and the experiment is basically within 15%.

The geometric model of this study is shown in Fig. 2. The containment is 64m high and 40m in diameter, the breach for studying the compartment influencing factors is located 4.5m from the bottom in the steam generator compartment close to the side of the pressure vessel, whereas the baseline breach for studying the other factors is located in the median axis 25m

from the bottom. The heat exchangers are arranged symmetrically in the upper space of the containment with a length of 5 m, 2.4 m from the wall and 40 m from the bottom. Negative component source terms equal to the steam flow rate of the breach are set on their side, with a surface temperature of 390 K. Four detecting points are arranged in the middle position at 37 m, 42 m, 47 m, and 52 m from the bottom, and the change of concentration of the points is observed.



3.2 Baseline conditions

Under the baseline condition, the initial temperature inside the containment is 420 K, the pressure is 0.25 MPa, and the mass fraction of air and steam is 0.5 each. The two-dimensional converted gas flow rate at the breach is 0.1 kg/s, and the diameter of the breach is 0.0168 m. The gas temperature is 590 K, the ratio of the mass fractions of steam to hydrogen is 9:1, and the duration of the accident is 1000 s. The hydrogen concentration and the motion trajectory at different moments are obtained, as shown in Fig. 3.







Under the baseline condition, the gas from the breach is ejected upward and subject to the joint action of buoyancy and momentum. It spreads to both sides after reaching the top of the containment, flows downward along the sidewalls of the containment and the surface of the heat exchanger, and forms a more symmetrical gas cycle along the central axis in the area above the breach. In the whole accident process, the hydrogen concentration in the upper space is increasing. Driven by the concentration difference, hydrogen is easy to gather in the higher position, along the direction of the height of the containment there will be hydrogen concentration stratification phenomenon. At 1000s the hydrogen concentration in the whole upper space has reached 4% and above, as shown in Figure 4.

3.3 Effect of injection direction

In breach accidents, pipe breaks in different directions produces different flows, so it is necessary to consider the effect of injection direction on hydrogen transportation.





Fig. 6 Hydrogen concentration at different altitudes

As can be seen from Fig. 5, after changing the injection direction from vertical upward to horizontal leftward, the gas flow under the influence of momentum is biased toward the left space of the containment, and spreads to both sides after reaching the top. As a result, a larger gas circulation has been formed on the right side at 400s and keeps crowding out the area on the left side until the gas circulation on the left side is completely swallowed by the large circulation on the right side, eventually forming a complete gas circulation. Under the influence of centrifugal force, the hydrogen concentration is larger in the region with large velocity on the outer side of the cycle and smaller in the region with small velocity on the inner side, so that the concentration at the detection point in the middle position is lower than the baseline condition.

3.4 Effect of breach size

In the baseline condition, the breach diameter of 0.0168m is about 9cm in 3D condition. When the breach size is smaller, the injection velocity at the same flow rate will be larger, so the diameter is changed to 1/2 of the baseline, and the injection velocity is two times of the original one, to analyze the effect of the breach size on the behavior of hydrogen transport.



Fig. 7 Hydrogen concentration and flow diagrams at different times

Fig. 8 Hydrogen concentration at different altitudes

Figure 7 illustrates the hydrogen concentration and streamlines at high flow rates through the small breach. Although the injection direction is vertically upward, by the disturbance of the gas in the upper space of the containment, the direction of the gas will be shifted to a certain extent after it flows out of the breach. Due to the larger injection velocity, the momentum

is more obvious to the breach area, and the flow shift near the breach has a more significant effect on the whole area, so that although lagging behind the condition of horizontal injection, a large circulation will still be formed in the upper space, and the concentration of the detection point will also be lower than the baseline condition.

3.5 Effect of hydrogen concentration

In order to examine the effect of the concentration at the breach on hydrogen transport, the 9:1 concentration ratio of steam to hydrogen in the baseline condition was changed to 7:3 with reference to the gas share of the AP1000 in a loss of coolant accident^[7,8].



Fig. 9 Hydrogen concentration and flow diagrams at different times

As can be seen from Fig. 9, when the hydrogen concentration is larger, the jet velocity is larger at the same flow rate due to the lower density of hydrogen, and the effect of momentum is more obvious. The gas in the breach region is shifted in direction by the perturbation of the surrounding gases, and a complete gas cycle is formed in the upper space at 700s. The velocity of the formation of the large cycle is in between that of the horizontal jet condition and that of the small breach condition.

3.6 Effect of breach flow rate

In the baseline condition, the breach flow rate of 0.1 kg/s is equivalent to 3 kg/s in the three-dimensional condition. In order to analyze the effect of the breach flow rate on hydrogen transport, the breach flow rate of the horizontal leftward condition is changed to 0.01 kg/s, and the results obtained are shown in Fig. 10. Compared with the high flow rate condition of horizontal to left injection, the gas under the small flow rate condition shows a different flow trajectory. Under the dominance of buoyancy, the gas still flows upward after being ejected from the left breach, forming a more symmetric gas circulation on both sides similar to that of the baseline condition.



Fig. 10 Hydrogen concentration and flow diagrams at different times

3.7 Effect of heat exchangers

When steam condenses on the heat exchanger surface, it will have a certain effect on the surrounding gas. Taking the working condition in 3.2 as an example, due to the sedimentation effect brought about by condensation, the gas on the surface will have a tendency to flow downward, which to a certain extent curtails the circulation pattern of the gas flowing out of the breach on the left side of the containment, as shown in Fig. 11(a). On the other hand, when the gas flows through the corner between the horizontal and vertical surfaces of the heat exchanger, the flow direction will also be shifted to a certain extent. However, as the accident continues, the gas circulation formed on the right side of the containment expands and eventually still overcomes the effect of vapor condensation, allowing the gas on the left side of the containment to flow upward and merge into the circulation in the larger space, as shown in Figure 11(b).



Tig. TT velocity vectors at anterent moment

4 Analysis of hydrogen transport behavior in compartments

4.1 Impact of compartments

In order to simulate the hydrogen transport behavior in a real environment, reference is made to the arrangement of the main compartments such as the steam generator compartment, pressure vessel compartment, pressurizer compartment, and relief tank compartment in a nuclear power plant, and calculations are carried out after the breach location is set in the area between the steam generator and the pressure vessel.





When the gas is ejected from the breach, it is obstructed by the compartment and will form a circulation in the compartment, and the rest of the gas flows through the opening in the upper part of the compartment to the large space of the containment. Because the opening is located to the left side of the containment, the gas in the upper space can easily form a complete circulation, as shown in Figure 12. Due to the lack of hydrogen abatement measures, the hydrogen concentration in the compartment and the upper space became higher and higher, and the area with hydrogen concentration higher than 4% in the containment accounted for 69.5% of the total area after 1000s of the accident.

4.2 Effect of openings

In order to reduce the hydrogen concentration in the compartment, the lower left side of the steam generator compartment was changed to an opening structure without adding other equipment, and the results obtained are shown in Figure 13. More hydrogen flowed out of the compartment through the opening in the lower part of the compartment, which significantly reduced the hydrogen concentration inside the compartment. At 1000s of the accident, the area in the containment where the hydrogen concentration was higher than 4% was 42.2% of the overall area, which was a 27.3% decrease compared to the original one.





5. Conclusion

In this study, CFD numerical simulation is used to investigate the hydrogen transport behavior driven by cold-heat sources in the containment, and the main conclusions obtained are as follows:

(1) When the breach is small or the injection direction is horizontal, hydrogen will form a large circulation inside the containment mainly driven by momentum; while when the flow rate is small and the injection rate is small, hydrogen is mainly influenced by buoyancy, and is released upward to the top and then spreads to the sides.

(2) The sedimentation effect of condensation on the surface of heat exchangers can act as a deterrent to flow circulation in the opposite direction to that in the large space.

(3) The obstruction of hydrogen flow by the compartments tends to accumulate hydrogen in the compartments, and improvements to the compartment openings can significantly reduce the hydrogen concentration in the compartments.

In this study, the high-temperature gas in the breach and the heat exchangers are analyzed as the heat and cold sources, equipment such as sprinklers and hydrogen recombiners are not considered, nor is the heat exchange process between the containment wall and the gas. It still needs to be further verified for the complete hydrogen transport behavior in the containment.

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