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Numerical Simulation for Delimiting Ammonia Leakage Diffusion Risk Zone

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Based on CFD-Fluent software platform, leakage diffusion of ammonia storage tank area is simulated, Main study on wind speed and leakage direction of influence on ammonia leakage diffusion process as well as the range of severe and moderate risk zone. The results show that the wind speed affected gas parameters such as diffusion area, jet distance, and concentration, different leakage direction caused different degree of status, and leakage against the wind is the most unsafe condition. Through the numerical simulation of ammonia leakage diffusion process, correctly judging the behaviour of leak occurrence, development and influence scope, provide scientific guidance for delimiting warning zone after the accident.

1. Introduction

As raw material or final product in industrial production, ammonia frequently appeared in people's field of vision. In the process of transportation or use, Leakage diffusion accident of ammonia caused by lack of management, operational errors and external environment, leaded to fire, explosion, poisoning and other accidents. Research the process of ammonia Leakage diffusion, obtain diffusion area, provide theoretical basis for emergency rescue and evacuation plan (Rolf, 2014).

In recent years, with the development of computer hardware, the CFD (Computational Fluid Dynamics) method is used to simulate the hazardous gas leak diffusion process by researchers at home and abroad. In view of the liquefied petroleum gas storage tank, Zhao Bo etc. (Zhao, 2012; Xing et al., 2014) simulated the thermal response of tanks under the condition of external heat, studied mechanical response and failure mechanism of tank in fire environment. Research has shown that rate of temperature and pressure rise of tank medium grows faster as heat flux increases, Tank wall temperature rise rate also increase. (Deng et al., 2012; Guo et al., 2013; GOUSSEAUP et al., 2011) simulated gas diffusion process under the condition of complex topography Using CFD technology combined with experiment method, results show that CFD simulation can reflect the flow characteristics of the gas. (NasimShishehgaran et al., 2014; Yu et al., 2013), simulated Liquefied gas through the different shape and height hole, The difference of holes affect pressure and temperature of liquefied gas leakage And then change the leakage flow coefficient; Cheng Mengmeng etc. established CFD simulation mode of different leak location of the buried gas pipeline, On the part of the natural gas pipeline Results show that the top part, bottom part and the part of the leeward side of the natural gas pipeline, hazardous area of bottom part is biggest; J. Malet etc. with boundary conditions controlling simulated layering of lightweight gas confined in a container by CFD According to the result of simulation, when lightweight gas was injected to upper portion of dense gas, the stratification of the gas is determined by the nature of the upper filling gas, the boundaries between different gas density associated with the injection speed.

With research deepening, more scholars pay attention to the application of numerical simulation in the actual production process. Based on the results of simulation, analysis instantaneous concentration distribution, study wind speed, leakage point location, direction and such f-actors, estimate dangerous gas concentration range after leakage, set the alert area.

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2. Numerical model and numerical method

2.1 Calculated work condition

Take ammonia leakage diffusion process for example, the application of CFD method was discussed. Set the size of simulation area: 120m×60m×40m (shown in Figure 1), Cylindrical tank ammonia, and radius: 4m, high: 8m. Study the influence of leakage on the surrounding area, set tank in central regions of geometric model, the center of tank coordinate points is (60, 30, 4).

Set the simulated wind speed respectively 0m/s, 2m/s, 5m/s, the direction of wind is the X axis. Tank leakage hole radius: 0.01m, the leakage rate: 50m/s. To study the effect of different leakage direction on diffusion, the leak direction has three situations: X axis, X axis negative direction, Y axes.

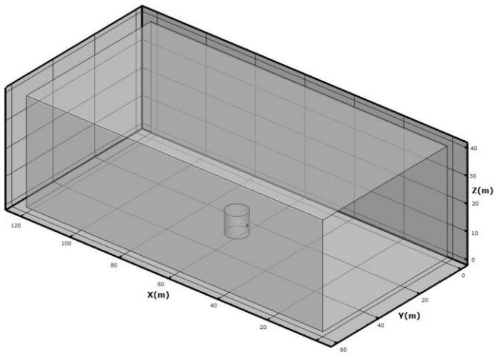

Figure 1: The geometric model of calculate the area

This paper established for calculation watershed, the storage tank and ground is set to no-slip wall boundary conditions, boundary type of Wind inlet and leakage inflow wall is inlet velocity, boundary type of air outlet wall is pressure outlet. The initial conditions of calculation area is set as same as the atmospheric conditions, that is a standard atmospheric pressure, temperature of 273k.

Grid generation directly affected calculation speed and accuracy. On CFD simulation of ammonia leakage diffusion computing, grid generation was conducted for Calculation Region. Grid model adopted tetrahedron or hybrid grid generation method, the minimum grid size is 0.25mm, the largest grid size is 0.9mm, the grid number is 629556.

2.2 Numerical model and numerical method

During the production process, most of dangerous gas diffusion is single multicomponent problems without any chemical reaction. Diffusion process shall follow the law of momentum conservation, mass conservation and energy conservation.

(1) Continuity equation

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial X_j}\left(\rho u_j\right)=0 \tag{1}$$

In this equation, uj is the three directions (X, Y, Z) of velocity component (m/s), t(s) is time, for the mixture density (kg/m3).

(2) The momentum conservation equation

$$\frac{\partial\left(\rho u_j\right)}{\partial t}+\frac{\partial}{\partial X_j}\left(\rho u_i u_j\right)=-\frac{\partial P}{\partial X_i}+\frac{\partial}{\partial X_j}\left(u_t \frac{\partial ui}{\partial X_j}\right)+\left(\rho-\rho_\alpha\right) g_i \tag{2}$$

In this equation, P is the absolute pressure, ut is fluid turbulent viscosity. gi is the gravitational acceleration in direction(X,Y,Z).

(3) The energy conservation equation

$$\frac{\partial(\rho T)}{\partial t}+\frac{\partial}{\partial X_j}\left(\rho u_j T\right)=\frac{\partial}{\partial X_j}\left(\frac{u_t}{\sigma_T} \frac{\partial T}{\partial X_j}\right)+\frac{cp_x-cp_a}{cp}\left[\left(\frac{u_t}{\sigma_c}\right) \frac{\partial W}{\partial X_j}\right] \frac{\partial T}{\partial X_j} \tag{3}$$

In this equation, T is fluid temperature, is constant, average 0.9~1.0, cp is mixed fluid specific heat at constant pressure, is leaking material constant pressure specific heat, is specific heat at constant pressure of air.

(4) Component mass conservation equation

$$\frac{\partial(\rho\omega)}{\partial t}+\frac{\partial}{\partial X_j}\left(\rho u_j\omega\right)=\frac{\partial}{\partial X_j}\left(\rho D_1\frac{\partial\omega}{\partial X_j}\right) \tag{4}$$

In this equation, ω is components quality fraction, Dl is fluid.
(5) Turbulent flow model
Turbulent k equations

$$\rho\frac{dk}{dt}=\frac{\partial}{\partial X_i}\left[\left(u+\frac{u_t}{\sigma_k}\right)\frac{\partial k}{\partial X_i}\right]+G_k+G_b-\rho\varepsilon-Y_M \tag{5}$$

Turbulence dissipation rate ε equation:

$$\rho\frac{d\varepsilon}{dt}=\frac{\partial}{\partial X_i}\left[\left(u+\frac{u_t}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial X_i}\right]+C_{1\varepsilon}\frac{\varepsilon}{k}\left(G_k+C_{3\varepsilon}G_b\right)-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} \tag{6}$$

In this equation, is turbulent kinetic energy caused by mean velocity gradients, is turbulent kinetic energy caused by buoyant effect, is compressible turbulent pulsating expanding influence on the total dissipation rate. As default value constant, =1.44, =1.92, =0.09, Turbulent kinetic energy k and turbulent Brandt number of dissipation rate is respectively =1.0, =1.3.
In this paper, the three-dimensional non-steady numerical simulation, choose standard k-з turbulence model, in order to calculate a better algorithm convergence, pressure-velocity coupling is chosen SIMPLEC, momentum, turbulence kinetic energy and turbulence dissipation are chosen a first order discretization method.

3. Example analysed

Based on acute short term exposure limit concentration, the harm of ammonia can be divided into three levels: concentration is 0.004mol/L~0.02mol/L, caused mild poisoning exposuring 30min, with irritation nausea, headache. Concentration is 0.02mol/L~0.04mol/L, caused moderate intoxication expositing 28min, with cough and obvious discomfort; concentration is greater than 0.04mol/L, caused severe intoxication exposuring 30min, with strong irritation, endanger life and cause death immediately. When the concentration, endanger life and cause death immediately.
The main areas of human activity is on the ground with high degree risk, Once ammonia leakage diffusion accident happening, will cause serious consequences. Chinese average height is 168cm, choosing leakage time 28min, distance from the ground 1.7m, analyze gas concentration diagram.

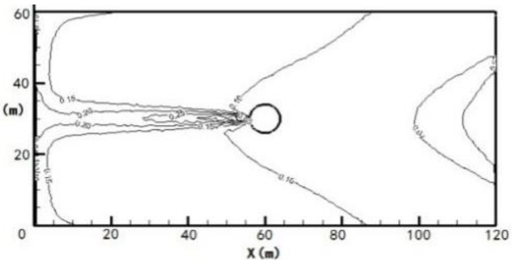

Figure 2: Contours graph of ammonia concentration when wind speed is 0m/s.

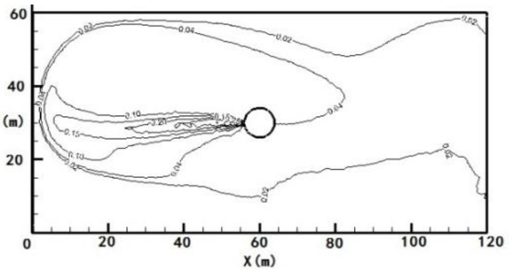

Figure 3: Contours graph of ammonia concentration when wind speed is 2m/s.

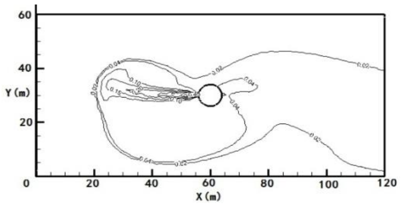

Figure 4: Contours graph of ammonia concentration when wind speed is 5m/s.

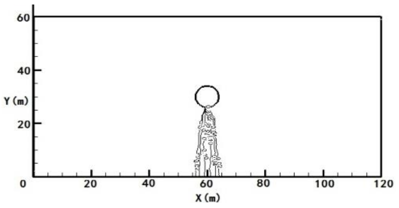

Figure 5: Contours graph of ammonia concentration when wind speed is 0m/s.

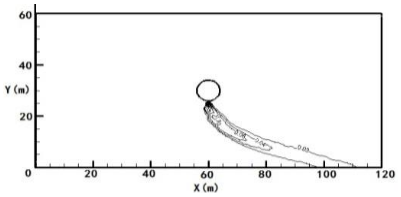

Figure 6: Contours graph of ammonia concentration when wind speed is 2m/s.

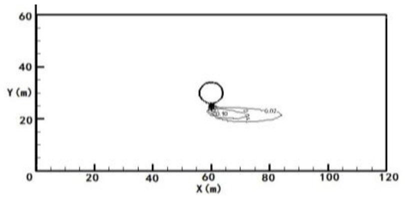

Figure 7: Contours graph of ammonia concentration when wind speed is 5m/s.

Storage tank burst under external force, substances inside escaped quickly from leakage hole, gas leaked along the direction of diffusion. When leakage direction with wind in the opposite, small leakage diameter, strong internal pressure, Ammonia rapid gasified with a lot of kinetic energy and spewed from leaking hole, It can be seen from the diagram, jet line around density is larger, with the jet distance increasing, the density of contour Lines gradually decreases, it shows that gas concentration near the stream line area is the largest, gas concentration gradually decreases away from the stream line area of (figure 2).When the surface leakage perpendicular to Wind velocity, Main impetus of ammonia gas cloud diffusion is natural wind, Winds will intensify mass transfer between air and ammonia. The ammonia diffuses along with the wind. With increase of wind speed, distance of gas injection is shorter, concentration of gas is lower, and the influence scope is narrower. When the wind speed is 2m/s, jet distance is 60m (figure 3). When the wind speed is 5m/s, jet distance shortened to 40m. Because the wind speed is weaker relative to contrary wind leakage (50m/s), the leakage gas cloud diffuse along the wind direction overcoming wind resistance (figure 4).

When leakage direction perpendicular to the wind, under no wind condition, gas with larger initial kinetic energy leaked from leakage hole, with vertical injection status, along the axis of symmetry of X=60m to both sides in free diffusion, at X=60m, gas concentration reaches the maximum value (figure 5).

When wind velocity increases to 2m/s, gas on contraction distribution is no longer shown symmetry, but gas concentration on leeward is higher than upwind direction. It can be seen region of influence of gas concentrations obvious shifted to downwind area. Angle between Jet direction and X axis is 45 degrees, horizontal distance of Gas diffusion is 50m. When the wind speed continues to increase to 5m/s, gas deflection angle increases, the angle between jet direction and X is nearly 90 degrees, gas diffusion transverse was reduced to 25m, due to enhancement of gas turbulence, gas concentration reduced, risk reduced (figure 6).

When the direction of leakage is the same with the wind direction, at static wind, the gas is ejected from the leak port, and continues to spread along the injection orientation, and the scope of the gas between X=100m to X=60m. Then, the horizontal distance is 40m and the longitudinal distance is 10m (Figure 7). Under the action of the wind, when the wind velocity increase to 2m/s, the gas spread downwind. Then, the horizontal distance increases to 60m and the longitudinal distance is approximately 10m (Figure 8). When the wind velocity continues to increase until 5m/s, the horizontal distance reduces to 30m compared to the wind velocity of 2m/s and the longitudinal distance also reduces to is 5m. This illustrates that when the wind speed increases, the wind not only accelerated the velocity of the gas transported downwind, but also gas concentration were diluted, which lowers the concentration and risk of gas to some extent.

When the direction of leakage is contrary to the wind direction, at static wind, almost the entire area of the ammonia concentrations are in the range of 0.04mol/L. Contacting these area for 30min will lead to coughing, a strong sense of stimulation, even life threatening, severely harm; When the wind velocity increased to 2m/s, the range of severe hazard area is an ellipse approximately. The major axis of the ellipse is 80m, the minor one is 45m, and the area is 2826m2. The range of moderately hazardous area is a rectangle. The length, width and area of the rectangle are 120m, 40m and 4800 m2 respectively. When the wind velocity continues to increase until 5m/s, the range of severe hazard area is a rectangle approximately that’s 45m long, 30m wide, and the area of the rectangle is 1250m2. The range of moderately hazardous seems like a “S”, and the area of the “S” region is 4000 m2. These show that with increasing wind speed, the severe hazard area and moderate hazard area is reduced.

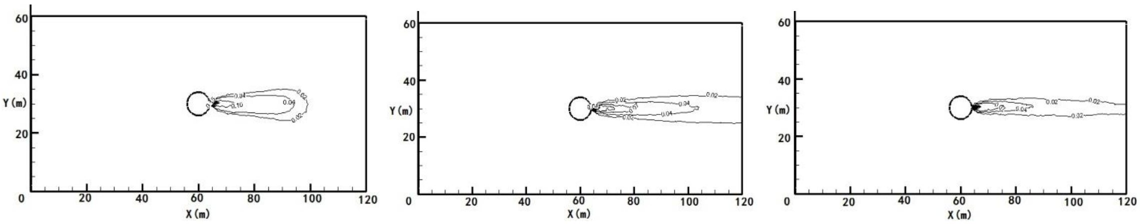

Figure 8: Contours graph of ammonia concentration when wind speed is 0m/s, 2m/s, 5m/s

When the direction of leakage is perpendicular to the wind direction, at static wind, the range of moderately hazardous area is a rectangle. The length, width and area of the rectangle are 25m, 10m and 250m2 respectively. When the wind velocity increased to 2m/s, the range of severe hazard area is a rectangle that’s 25m long, 5m wide, and the area of the rectangle is 125m2 approximately. The range of moderately hazardous area is a rectangle that’s 50m long, 5m wide, and the area of the rectangle is 250m2. When the wind velocity continues to increase until 5m/s, the range of severe hazard area is an ellipse approximately. The major axis of the ellipse is 10m, the minor one axis is 5m, and the area is 39.25 m2. The range of moderately hazardous area is an ellipse which the major axis is 25m and the minor one is 5m and the area is 98.13m2. These show that, when dangerous gases diluted with the action of wind, the extensive severe hazard area and moderately hazardous area is reduced.

When the wind direction is the same as the direction of leakage, the severe danger zone is an ellipse which has an area of 52.5m2, and the lengths of the major axis and minor axis are 30m, 7m, respectively. Moderate risk area is an ellipse with an area of 274.75m2, and the lengths of the major axis and minor axis are 35m, 10m, respectively.

When the wind velocity increased to 2m/s, the range of severe hazard area is an ellipse which the major axis is 40m and the minor one is 4m and the area is 125.6m2. The range of moderately hazardous area is a rectangle approximately that’s 55m long, 7m wide, and the area of the rectangle is 385m2. When the wind velocity continues to increase until 5m/s, the range of severe hazard area is an ellipse. The major axis of the ellipse is 20m, the minor one axis is 3m, and the area is 41.7m2. The range of moderately hazardous area is an ellipse approximately which the major axis is 55m and the minor one is 5m and the area is 215.88m2.

Direction of leakage is a key factor to hazardous areas after the accident. When the direction of leakage is contrary to the wind direction, the gas expand maximum to gas clouds great harmed to a large scale and gather upwind. With the concentration of gas increases gradually, the risk increases and the threat of surrounding environment increases. When the direction of leakage is perpendicular to the wind direction, the concentration of gas clouds has higher level downwind, but it is lower when the direction of leakage is perpendicular to the wind direction and the impact of gas clouds on the region upwind is not obvious. When the direction of leakage is the same with the wind direction, with the action of wind gas and air mixed well, and the concentration of dangerous gases is diluted. In this state, the concentration in this area is smaller and the risk is also relatively lower. Visible, wind leakage is the worst status to security, while vertical and wind leakage is less dangerous relatively.

4. Conclusion

Based on CFD software in this paper, numerical simulation research was carried on the leakage diffusion state of ammonia storage tank. To simulate the wind speed and direction of leak affected leakage diffusion, obtained the most dangerous area and scope, Conclusions are as follows:

(1) When leakage direction opposite to the wind, with wind speed increasing, the area of 0.04mol/L ammonia concentration is range from 7200m2 to 1250m2; When leakage direction perpendicular to the wind, with wind speed increasing, the area of 0.04mol/L ammonia concentration is range from 250m2 reduce to 39.25m2; When leakage direction opposite to the wind, with wind speed increasing, the area of 0.04 mol/L ammonia concentration is range from 52.5m2 reduce to 41.7m2. When the wind speed is 5m/s, jet distance shortened to 40 m. because the wind speed is small relative to the speed of wind leakage (50m/s), the leakage gas cloud delivered along upwind direction overcoming wind age.

(2) Under different wind speed conditions, when
leakage direction opposite to the wind, the scope of the severe danger zone is largest, goes perpendicular with goes perpendicular or the same in both cases, the severe danger area is smaller, the scope of that wind leakage under the condition of the highest risk, should strengthen the guard. It shows that risk is highest under the condition of wind age leakage, should be strengthen prevention.

(3) Wind strengthens the effect of air turbulent, augmented function of Wind transporting, prompted ammonia spreading down the wind. With wind speed increasing, diffusion distance increases downward wind, the jet deflection angle increases. So the factory construction should choose Annual minimum frequency on the wind, less risky areas shall be set on the upper side of the risky areas.

References

Deng H.F., Chen G.M., Zhu Y., Fu J.M., Liu D.X., 2012, Simulation and test of gas leakage diffusion law under the condition of complex topography [J]. Journal of China University of Petroleum (Edition of natural science), 36(1); 122-135.

Gousseau P., Blocken B, Stathopoulos T., van Heijst G.J.F., 2011, CFD simulation of near field pollutant dispersion on a high-resolution grid: a case study by LES and RANS for a building group in downtown montreal [J]. Atmospheric Environment, 45:428-438. doi:10.1016/j.atmosenv.2010.09.065.

Guo D.P., Yan H., Yao R.T., Xiao X.F., Fan D., 2013, Comparative analysis of t numerical and wind tunnel simulation, complex building effecting on near field diffusion [J]. experimental fluid mechanics. 27(2): 56-62.

NasimShishehgaran, Marius Paraschivoiu., 2014, CFD based simulation of hydrogen release through elliptical orifices [J]. International Journal of Hydrogen Energy. 35 (39): 20350-20356. doi:10.1016/j.ijhydene.2014.03.226.

Rolf K. Eckhoff., 2014, Boiling liquid expanding vapour explosions (BLEVEs): A brief review [J]. Journal of Loss Prevention in the Process Industries. 32: 30-43.

Xing Z.X., zhao L., Ou H.X., Hao Y.M., 2014, LNG storage tank thermal response source term storage tank design based on FLUENT software platform, Journal of China Safety Science. 24(2):41-45.

Yu H.F., Li X.G., Sui H., Li H., 2013, CFD Simulation of Orifice Flow in Orifice type Liquid Distributor [J]. China Petroleum Processing and Petrochemical Technology, 15 (3): 70-78.

Zhao B., Bi S.M., 2012, Numerical simulation of tank pressure and temperature response on fire environments [J]. Journal of petroleum (petroleum processing), 28(3): 512-516.