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Dynamic Simulation and Quantitative Risk Assessment of Indoor Heavy Gas Diffusion

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Abstract. In order to study the dynamic diffusion process and risk of indoor liquid chlorine leakage, large-scale numerical simulation and risk calculation are carried out based on CFD method. Firstly, a full-scale model in 3km range is established based on CFD calculation, and then the chlorine diffusion process in six leakage scenarios is calculated and analyzed based on pool model. The individual risk and social risk of existing conditions and SIS increase are calculated respectively. The results show that the chlorine will diffuse slowly in the room when the small aperture leaks. In case of leakage of middle hole and larger hole diameter, chlorine gas will quickly fill the warehouse and leak to the outside of the warehouse. The influence of leakage pore size on the diffusion distance of chlorine is very obvious. The total diffusion distance of 900ppm chlorine is 24.2m-401.3m, and the diffusion time is 120s-670s respectively. Under the existing conditions, the individual risk and social risk do not meet the risk acceptance criteria. After sis is increased, the risk meets the acceptance criteria.

1. Introduction

Chlorine is a typical toxic heavy gas, which is highly dangerous to human body and environment [1]. The process of leakage and diffusion of liquid chlorine was studied, and its diffusion characteristics, accident influence scope and risk were quantitatively analyzed. There are three types of gas leakage and diffusion models: Gauss model, integral model and CFD model. Gauss model is sensitive to the transient change of diffusion environment and has poor adaptability. The integral model is suitable for the diffusion of free space without obstacles and can’t accurately simulate the real diffusion of indoor leakage [2-3]. For the leakage of liquid chlorine in the room, and involving gas-liquid two-phase flow, 2D software can’t achieve the simulation of accident consequences. CFD model performs well in the flow pattern and other aspects, and the simulation results of the model are roughly consistent with the observed turbulence pattern [4], which is suitable for simulating the leakage and diffusion of indoor heavy gas. Among many risk assessment tools, DNV SAFETI is the leading professional risk assessment software in the field of petrochemical industry [5].

Based on this, this paper simulates the leakage of chlorine gas storage bottle in a plant. A full-scale 3D model including bottle storage and surrounding main buildings is established. The maximum diffusion range and the shortest arrival time of chlorine in different leakage scenarios are calculated. At the same time, the existing conditions and the accident risk after adding safety measures are calculated quantitatively.

2. CFD simulation and mathematical control equation

2.1. Geometric model

FLACS is an advanced CFD security application tool. The atmospheric diffusion model in FLACS has been tested and verified in various cases [6-8].

The length of liquid chlorine warehouse in a factory is about 97m, the width is about 16m, and the height is 10m. There are about 300 steel cylinders in the warehouse, each with a volume of about $0.8m^3$. The full-scale three-dimensional physical model is established by using the FLACS pre-processing program CASD, and the model scale is 1:1, as shown in Figure 1.

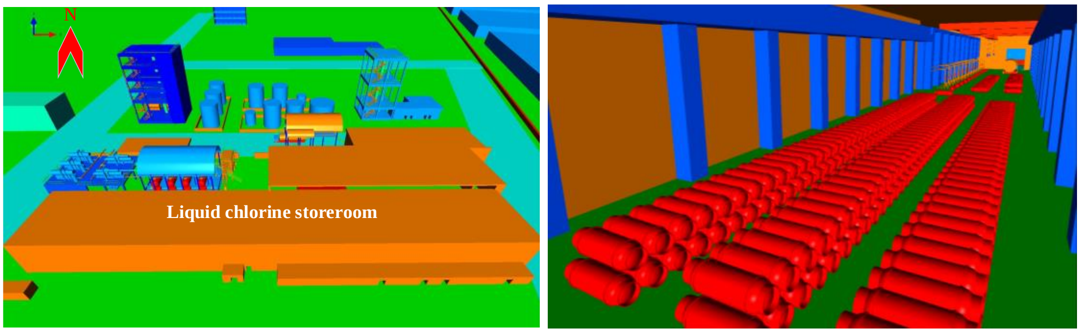


Figure 1. 3D model of liquid chlorine warehouse and steel cylinder

2.2. Turbulence model

In the simulation of plant accident scenario, FLACS is based on the turbulence model based on RANS equation [9]. Different closure methods of Reynolds time averaged equations make up different turbulence models. At present, the most widely used turbulence model is k - ε model. The standard k - ε model is formed by introducing an equation of turbulent dissipation rate ε on the basis of K equation of turbulent kinetic energy. The forms of K equation and ε equation are as follows:

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho u_i k)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right]+G_k-\rho\varepsilon \tag{1}$$

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x_i}(\rho u_i\varepsilon)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x_i}\right]+\frac{\varepsilon}{k}(C_{1\varepsilon}G_k-C_{2\varepsilon}\rho\varepsilon) \tag{2}$$

Where ρ is the density, t is the time, K is the turbulent kinetic energy, u is the velocity, μ is the turbulent viscosity of the fluid, ε is the energy dissipation rate of the turbulent flow, and GK is the turbulent kinetic energy caused by the average velocity gradient.

The wind direction of the plant area is NNE, the relative turbulence intensity is 0.05, and the turbulence length is 0.001M. After the leakage of liquid chlorine, a liquid pool will be formed on the ground. Therefore, POOL model is used in the calculation.

3. Simulation of leakage and diffusion process of liquid chlorine

3.1. Leakage scenario

3.1.1. Toxic hazard concentration. There are two kinds of lethal concentrations of chlorine in the existing literature. One is $300mg/m^3$ (about 95ppm), but the exposure time of personnel is not specified.

Second, when the concentration of chlorine in the air reaches 0.09%, people will die after inhaling it for 5-10 minutes [9]. After comprehensive consideration, 0.09% is regarded as the dangerous concentration of concern (recorded as C_d).

3.1.2. Meteorological conditions. Average wind speed in the plant area is 1.3m/s. Wind direction is NNE (22.5 °). Pasquall-Gifford stability is F. See Table 1 for calculation scenarios.

3.1.3. Simulation scenarios. The pressure is 1MPa and the temperature is 25℃. Leakage pore size is divided into three categories: 5mm, 25mm and 50mm. Leakage time of 5mm aperture includes 180s and 600s, 25mm aperture includes 180s and 300s, 50mm aperture is divided into 60s and 180s

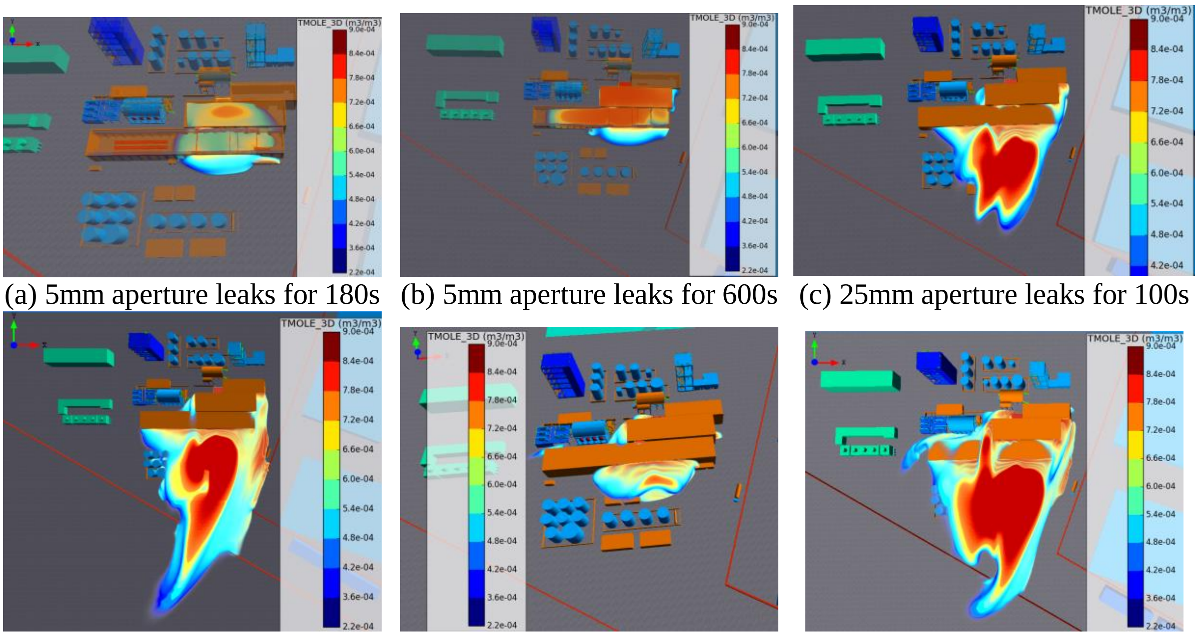
3.2. Calculation of flash diffusion process
Liquid chlorine, as an industrial pressurized, low-temperature liquid, will flash when released to the atmosphere [10]. The end of the near-field region is defined as the position where all the liquid in the jet changes phase. Flash releases can be considered jet leaks in FLACS. The flash program in FLACS is used to calculate the source term of all droplets after evaporation. See table 1 for calculation results.

Table 1. Calculation results of flash jet

Leakage aperture(mm)	Flash distance(m)	Jet area(m^2)	Jet temperature(℃)
5	1.2	6.8	-70.5
25	6.1	1.7	-70.5
50	12.3	6.7	-70.5

The results of flash calculation show that the flash distance increases with the increase of the leakage aperture. The jet area did not show a linear change with the change of the leakage aperture.

3.3. Simulation results and analysis
The leakage and diffusion process of liquid chlorine in different scenarios is calculated by using the FLACS post-processing program flowvist, as shown in figure 2.



(a) 5mm aperture leaks for 180s (b) 5mm aperture leaks for 600s (c) 25mm aperture leaks for 100s

(d) 25mm aperture leaks for 300s (e) 50mm aperture leaks for 60s (f) 50mm aperture leaks for 180s

Figure 2. Diffusion process of liquid chlorine with different leakage aperture and leakage time

After the liquid chlorine leaks from the steel cylinder in the liquid chlorine warehouse, the maximum diffusion distance and corresponding diffusion time of the chlorine gas with concentration of concern are shown in table 2.

Table 2. Simulation results of leakage and diffusion of cylinder warehouse unit (C_d = 0.09%)

Aperture(mm)	Leakage time(s)	The longest distance(m)	Flash distance(m)	Total distance(m)	Diffusion time(s)
5	180	23.0	1.2	24.2	120
	600	25.0	1.2	26.2	300
25	180	187	6.1	193.1	410
	300	210	6.1	216.1	435
50	60	234	12.3	246.3	360
	180	389	12.3	401.3	670

In case of small aperture leakage (5mm), chlorine gas will slowly spread to the whole plant with time change after indoor leakage, resulting in the increase of indoor toxicity concentration. Among them, the indoor concentration at 180s of leakage is about 540ppm, and the whole warehouse is not filled. The maximum diffusion distance of C_d concentration is 23m. The indoor concentration can exceed 900ppm after 600s of leakage, and the whole warehouse is full. At this time, the maximum diffusion distance of C_d concentration is 25m. Due to the leakage of small pore, the leaked chlorine is mainly distributed in the room. Therefore, the leakage of chlorine through the door of the warehouse is less, and the diffusion distance is not different.

When the middle hole leaks (25 mm), the diffusion of chlorine is faster. The leakage time has great influence on the total diffusion time and the maximum downwind distance of the gas cloud. The maximum diffusion distance of C_d at 180s and 300s is 187m and 210m respectively.

In case of large aperture leakage (50 mm), the leakage time has a significant effect on the total diffusion time and the maximum downwind distance of the gas cloud. The leaked chlorine gas quickly fills the whole warehouse and spreads to the outside. The maximum diffusion distance of C_d is 234m and 389m at 60s and 180s respectively.

The simulation results show that the liquid chlorine, as a heavy gas, has a wide range of diffusion and is difficult to dissipate for a long time. In the aspect of overall change, the influence of leakage aperture on diffusion range is very obvious.

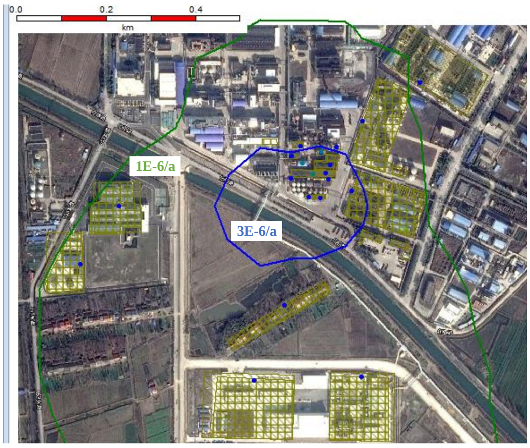
4. Risk of liquid chlorine leakage

4.1. Leakage frequency

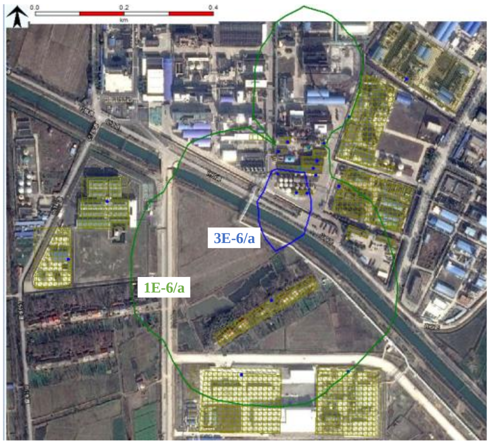
The leakage frequency database of DNV leak is used as the basic leakage frequency. At the same time, equipment correction factor (0.234) and management factor (0.5) are considered for correction. The corrected leakage frequency of 5mm, 25mm and 50mm is 4.5e-3, 3.2e-4 and 6.6e-5/a respectively.

4.2. Individual risk

The personal risk under the existing process conditions mainly considers the personal death risk of important sensitive points. It is expressed as the contour line of annual death risk (IRPA). Under the current operating conditions, the safety measures in the liquid chlorine warehouse are mainly the emergency shut-off valve. In this condition, the effective cut-off time is longer, and the individual risk is shown in figure 3 (a). As can be seen from the figure, the current risk is very high and has a great influence range. Therefore, independent safety instrument system (SIS) is considered. After adding SIS system, the leakage time can be greatly reduced and the effectiveness of emergency cut-off can be improved. The failure probability of SIS system emergency interlock cut-off is one order of magnitude lower than that of remote cut-off. The increased individual risk of SIS is shown in figure 3 (b).



(a) Individual risk of existing conditions



(b) Individual risk after SIS increase

Figure 3. Contour distribution of individual risk

The personal risk outside the battery limit of the liquid chlorine warehouse is significantly reduced by adding the SIS system of emergency shutdown. Only a few areas within the battery limit are within the contour range of 3 × 10-6 / year. There is no risk contour line of 1.0 × 10-5 / year and 1.0 × 10-3 / year. The main sites outside the battery limit are located outside the contour range of 3 × 10-6 / year. On the whole, individual risk is in the acceptable range.

4.3. Social risks

Social risk is represented by F-N curve (a certain number of deaths corresponds to cumulative accident frequency). The social risks under the original process conditions and the increase of SIS are shown in Figure 4.

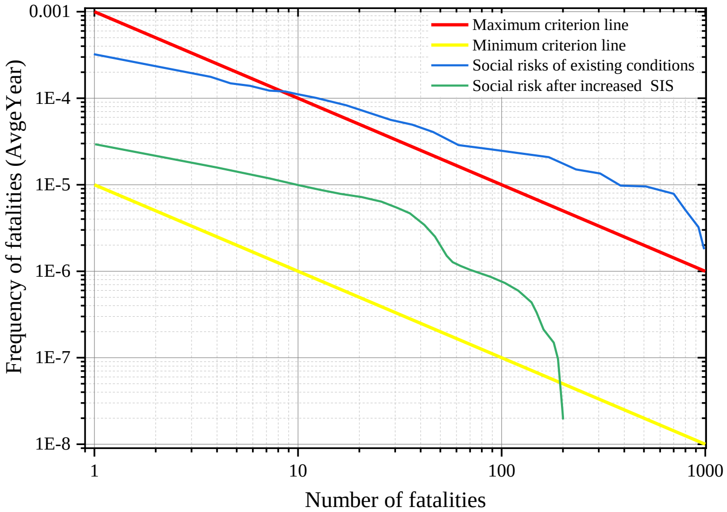


Figure 4. Social risks under existing conditions and SIS increase

It can be seen from the figure that the overall social risk is high under the existing conditions. When the death toll is more than 8, the cumulative death frequency is more than 1.2e-4/year. The FN curve is higher than the upper limit standard of the lowest possible area (ALARP area) and is in the risk unacceptable area.

After SIS increased, the social risk curve decreased to ALARP area. The risk is acceptable. It shows that the increased safety measures can effectively reduce the risk.

5. Conclusion

According to CFD technology, a three-dimensional model of liquid chlorine warehouse is built. The dynamic diffusion process of liquid chlorine in six different leakage scenarios was calculated. The main conclusions are as follows:

(1) The three-dimensional model based on CFD can effectively simulate the leakage of liquid chlorine under indoor conditions. When the pore size is small, chlorine will diffuse slowly in the room, and only a small part of chlorine will leak out through the door of the warehouse. In case of leakage of middle hole and larger hole diameter, chlorine gas will quickly fill the warehouse and leak to the outside of the warehouse.

(2) Compared with the leakage time, the influence of the leakage aperture on the diffusion distance of chlorine gas is more obvious. In six leakage scenarios, the total diffusion distance of C_d concentration is 24.2m-401.3m. The corresponding diffusion time is 120s ~ 670s. Therefore, it is very important to prevent the leakage of larger pore diameter for the prevention of chlorine accident.

(3) The individual risk and social risk under the existing conditions do not meet the risk acceptance criteria. With the increase of SIS, the leakage time can be greatly reduced, the reliability of leakage detection can be improved, and the risk can be significantly reduced.

Acknowledgments

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