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Simulation Analysis of Leakage and Diffusion of Liquid Chlorine Cylinder

Hui Jing

Nanjing City Vocational College, Nanjing, 210038 China
jh7625481@163.com

In order to study the influence of accidental leakage of liquid chlorine cylinder and chlorine diffusion, a 3D model of liquid chlorine cylinder for leakage diffusion is established according to the actual situation of chemical enterprises. Based on computational fluid dynamics (CFD) method, numerical simulation for chlorine diffusion in open space is carried out, and the influence of velocity on the leakage and diffusion of chlorine is discussed. Computing method is quantified by simulation results and poisoning accidents. Individual risk and social risk are used to characterize the risk size of the risk acceptor exposed to a particular risk field, which serve as a basis for determining whether the risk can be accepted. The results show that the external wind speed has a great influence on the chlorine leakage and diffusion process. The risk of death at each monitoring point gradually increases with time, and then the growth rate became stable.

1. Introduction

There are various forms of chemical leakage accidents, and the mechanism is very complex (Fukuda et al., 2015), especially for the low boiling point chemicals. For the convenience of storage and transportation, it is usually stored in tanks and other high-pressure containers in the form of liquefaction, high pressure and low temperature (Cong et al., 2015). When the storage container fails, toxic and harmful substances will leak into the atmosphere, which will lead to poisoning and environmental pollution. If a fire or explosion occurs, the consequences are more serious. The diffusion process of chlorine is complicated. Although large scale field experiments can collect real data of gas diffusion, the expenditure is huge and the repeatability is poor (Jiajia et al., 2016). Therefore, the simulation study on the accident consequence of liquid chlorine tank has important guiding significance for the safety production of enterprises and the emergency rescue under the condition of accident. Liquid chlorine cylinder is taken as the research object, and numerical simulation for liquid chlorine cylinder leakage and diffusion accident is carried out by using CFD method combined with Fluent software (Yu-nong et al., 2014). Reasonable suggestions are put forward to reduce the risk of chlorine diffusion poisoning.

2. Numerical simulation of liquid chlorine leakage and analysis of its influencing factors

According to the leakage equipment and leakage location of chlorine related equipment. The leakage may be liquid chlorine leakage, or gaseous chlorine leakage, or gas-liquid two-phase leakage (Abo-Elmagd et al., 2014). For liquid chlorine leakage, the liquid chlorine in the leaked substance may be flashing because of the environmental temperature much higher than the boiling point. The flash chlorine gas is diffused in the air (Ruoxia and Jinde, 2016). In order to investigate the most general process of chlorine leakage and diffusion, it is assumed that diffusion occurs in the ideal state of flat terrain without obstacles. In the gas diffusion process, without considering the thermodynamic gradient of heavy gas clouds inside, it is assumed that heavy gas clouds and boundary environment can reach thermal equilibrium in every moment (Ke, 2014).

2.1 Establishment of 3D physical model for liquid chlorine leakage

Considering the actual size of chlor-alkali production unit and building in chemical plant area, the three-dimensional space with 200m length x 50m width x 15m height is selected as the calculation area. The

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leakage source is a horizontal chlorine tank with a diameter of 3m and a length of 1.9m in the middle of the region. The height of the tank from the ground is 1m. The hexahedral mesh is divided into regions by using the professional pre-processing software ICEMCFD (Ahuva et al., 2014). The unstructured mesh is obtained by local mesh refinement of the leakage source and surface attachment, and the mesh number is 578309.
The finite element volume method is used to discretize the diffusion equation of chlorine gas. In the process of three-dimensional fluid diffusion, the discretization of the computational domain and the governing equation are expressed by t and b respectively. The corresponding two adjacent points are denoted as T and B. The discrete equation of the three-dimensional flow diffusion problem of chlorine under implicit integration scheme is assumed as follows (Shi et al., 2013):

$$a_p\Phi_p = a_W\Phi_W + a_E\Phi_E + a_N\Phi_N + a_S\Phi_S + a_T\Phi_T + a_B\Phi_B + b \tag{1}$$

In the formula, Φ is generalized variable. The implicit separation solver is used to calculate the discrete equations (Zhao and Zude, 2014). The first order upwind scheme is used for the discrete scheme of momentum, volume fraction and turbulent kinetic energy. The pressure and velocity coupling SIMPLE algorithm is used to calculate the velocity field and the pressure field by the continuity equation (Gang et al., 2017). Pressure relaxation factor, momentum relaxation factor, turbulent kinetic relaxation factor, dissipation rate relaxation factor and turbulence viscosity relaxation factor are set to 0.3, 0.7, 0.8, 0.8, 1, respectively.

2.2 Influence of different wind speeds on chlorine leakage and diffusion

In order to study the influence of atmospheric wind speed on the diffusion process, the external wind speed is set to 2m/s and 5m/s respectively, which is used to study the influence of different wind speeds on chlorine diffusion process. Figure 1, 2, 3 and 4 are the diagrams of the distance along the X direction and the distribution of chlorine concentration in the near ground. The wind speed are 2m/s and 5m/s, while the diffusion time are 30s and 100s.

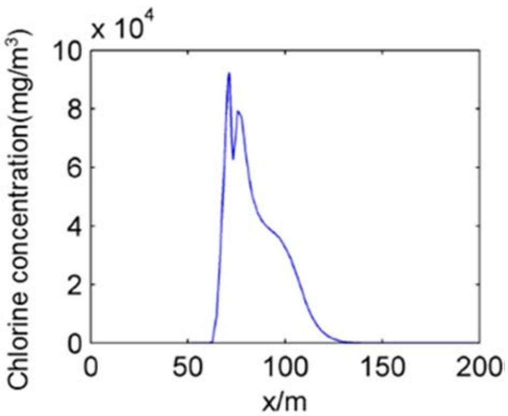

Figure 1: Relationship chlorine concentration with distance after 30s, the wind speed 2m/s

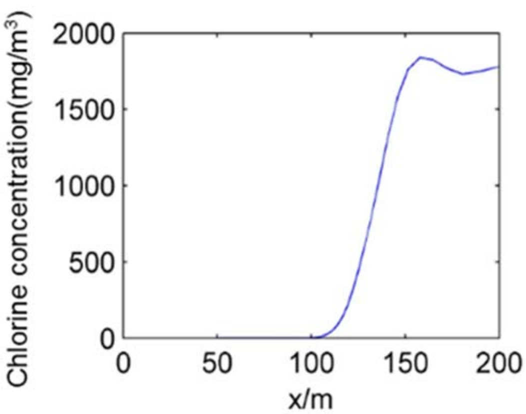

Figure 2: Relationship chlorine concentration with distance after 100s, the wind speed 2m/s

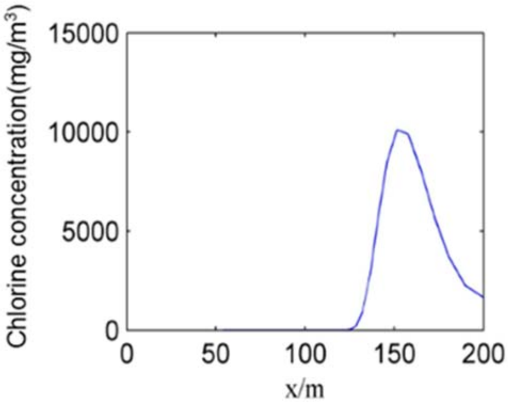

Figure 3: Relationship chlorine concentration with distance after 30s, the wind speed 5m/s

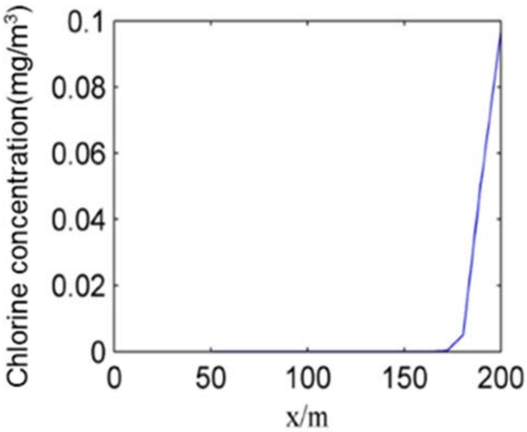

Figure 4: Relationship chlorine concentration with distance after 100s, the wind speed 5m/s

As shown in the figure, in the 30 seconds before the leakage of the tank, the chlorine concentration near the leakage point increases at a faster speed, and then the chlorine cloud diffuses and moves along the lower wind direction. With the increase of distance, the concentration of chlorine increases gradually.

As shown in figure 1, at 30s, the maximum diffusion distance of chlorine reaches about 150m. In figure 3, chlorine clouds have already spread to 200m. The results show that the diffusion velocity of downward direction of chlorine cloud is obviously accelerated with the increase of wind speed, and the concentration of chlorine decreases with the increase of wind speed. When the wind speed increases, the diffusion speed of the gas cloud downward direction accelerates, and the high concentration area also decreases at a faster speed. Although the gravity plays a dominant role in the gravity expansion stage, the diffusion velocity at the top of the gas cloud increases obviously due to the large wind speed (Elisabeth et al., 2016). At high wind speed, the bottom gas cloud moves faster under the action of gravity expansion in the early stage of diffusion. Moreover, the top gas cloud rapidly moves down to the wind direction by the high wind speed, forming the situation that the central gas cloud is turning inward in the wind direction. Subsequently, the gravity spreading effect gradually weakens until finally disappears, and the velocity at the bottom of the gas cloud decreases significantly. The velocity of the top gas cloud moves faster than that of the bottom gas cloud, leading to the state of head uplift (Blokker et al., 2014). At low wind speeds, the top of the gas cloud moves much slower than at the bottom. In addition, at the same release diffusion time, the diffusion distance of gas cloud downward wind direction is larger than that under low wind speed at high wind speed.

The above phenomena can be explained from two aspects: advection transport and turbulence action (Sofia, et al., 2013). First, the high wind speed intensifies the advection transport of gas clouds. Wind has an effect of downwind transport on gas cloud. The greater the wind speed is, and the more significant the transport effect is. This reduces the concentration of harmful gases at the lower wind direction. The advection transport of the atmosphere is weak at low wind speed. Therefore, the diffusion distance of the gas cloud downward wind direction is less than that of the high wind speed, and the high concentration gas cloud has longer residence time near the release source. Second, the atmospheric turbulence intensifies when the wind speed is high. As the wind speed increases, the pulse velocity increases (Sanchez et al., 2013). The concentration of chlorine gas cloud decreases with the increase of turbulent motion and turbulent diffusion. At low wind speed, the effect of gravity expansion on the advection of cloud is stronger than that of atmospheric velocity due to the larger initial Richardson number (Marc-Antoine et al., 2017). Therefore, the top gas cloud moves much slower than the bottom.

3. Individual risk assessment of chlorine leakage

Individual risk (IR) refers to the possibility that an unprotected person stays permanently in a certain place and dies because of an accident (Mahdi et al., 2017). The individual risk value at any point (x, y, z) in the computational domain can be calculated by formula (2):

$$IR(x,y,z) = P_f \times P(x,y,z) \tag{2}$$

In the formula, Pf is the probability of chlorine poisoning accident. Here is 7.13 x 10-4[59]. P (x, y, z) represents the individual mortality in space (x, y, z).
The concentrations of chlorine in space P1 (55,0,0), P2 (120,10,0), P3 (150,0,0), P4 (150,20,0), P5 (120,5,0), P6 (150,20,1.6), P7 (120,25,1.7) and P8 (45,0,0) are monitored. According to the formula (2), the individual risk of each point is calculated, and then the individual risk value is converted to death probability. Figures 5 and 6 show the changes between the death probabilities of each monitoring point and time.

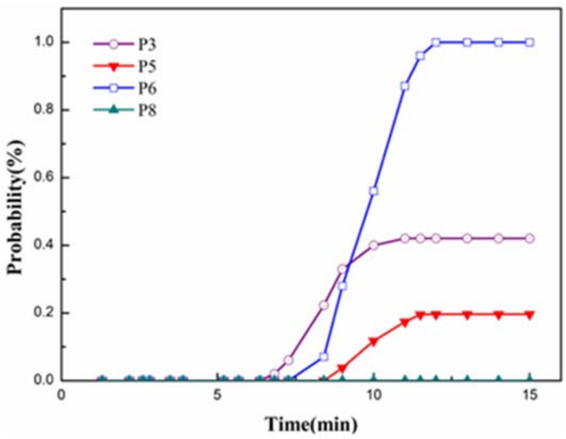

Figure 5: Variation mortality rate with time at monitoring points P1,P2,P4,P7

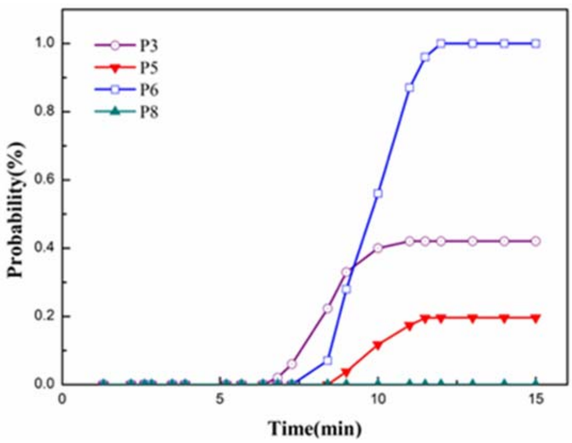

Figure 6: Variation mortality rate with time at monitoring points P3, P5, P6, P8

As shown in the figure, at the early stage of chlorine leakage accident, chlorine spreads at a higher speed, and the concentration of chlorine is first monitored at the monitoring point close to the leakage source. Under the influence of wind speed and topography (Dorval, 2016), the chlorine gradually diffuses down the wind. When the chlorine reaches the monitoring point far away from the leakage source, the chlorine concentration in the vicinity of the remote monitoring point increases gradually. With the stop of chlorine leakage, the chlorine concentration in each monitoring point near the leakage source gradually decreases. The greater the wind speed is, the faster the descent rate is, and the final concentration decreases gradually to zero. In the diffusion process, the greater the average concentration of chlorine is, the greater the death probability P at this point is. As shown in figure 5 and figure 6, the death risk P of each monitoring point increases gradually with the time t and reaches the maximum value, and then it is stable. Moreover, the location of the death rate varies greatly. From the above figure, the risk of poisoning at P1, P2, P4 and P7 points is larger, and the risk of P3, P5, P6 and P8 is relatively small, which is closely related to the diffusion law after chlorine leakage (Lizh et al., 2017). The closer to the leak point, the greater the exposure dose of chlorine is, and the greater the risk of death is. The risk of death increases gradually with the increase of time and reaches the maximum value, and then became stable. Moreover, the location of the death rate varies greatly.

4. Conclusion

Based on CFD method and the actual scene of chlor-alkali workshop in chemical enterprises, the leakage model of chlorine storage tank in 3D scene is constructed. The influence of wind speed on chlorine diffusion law is studied by using finite element software Fluent14.0. It is concluded that the external wind speed has a greater influence on the chlorine leakage and diffusion process. Computing method is quantified by simulation results and poisoning accidents. Individual risk and social risk are used to characterize the risk size of the risk acceptor exposed to a particular risk field, which serve as a basis for determining whether the risk can be accepted. The result shows that the closer to the leak point, the greater the exposure dose of chlorine is, and the greater the risk of death is. The risk of death increases gradually with the increase of time and reaches the maximum value, and then became stable.

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