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A SIMULATION METHOD OF SITE SELECTION FOR LIQUID AMMONIA TANKS

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Abstract
To decrease liquid ammonia leakage-induced casualties of ammonia chemical enterprises, a simulation comparison method of liquid ammonia toxicity leakage and crowd evacuation was proposed, a spatial model was constructed with Pyrosim software, using 8 liquid ammonia tanks as a layout example. The ammonia diffusion path under eight leakage scenes was analysed with FDS software by setting eight ammonia leakage points. The personnel evacuation model was built with the Pathfinder software, obtaining the crowd evacuation time under the eight scenes. Finally, the optimal site for liquid ammonia tanks in this case was determined through a comparison of ammonia diffusion path and evacuation time. Results show that among the eight candidate sites for ammonia tanks, the Leakage Scene 4 shows the longest time (78 s) for diffusion to the two evacuation exits, which is longer than the crowd emergency evacuation time (73 s) in the scene. Therefore, the Leakage Scene 4 can be used for the setting of liquid ammonia tanks. The obtained conclusions provide a safe suggestion for the scientific planning of the liquid ammonia storage sites of chemical enterprises.

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Key Words: Ammonia Leakage, Gas Diffusion, Crowd Evacuation, Site Selection for Liquid Ammonia

1. INTRODUCTION

During the production of ammonia in chemical enterprises, the potential risks of accidents increase dramatically with the intensifying complication of technological process [1]. The frequent occurrence of great safety accidents caused by dangerous chemical products brings serious threats to the ecological environment and the physical health and property safety of humans. As the raw material or the final product in industrial production, ammonia is a typical inflammable and explosive toxic gas. Leakage and diffusion accidents of ammonia easily cause mass deaths and casualties, such as fire disasters, explosions, and toxication [2]. Research on emergency management science pointed out that none of the existing systems has 100 % safety state, and all of them only have as much as safety preventive measures [3]. Therefore, establishing a scientific and reasonable plan of ammonia tanks in chemical enterprises, decreasing the deaths and casualties of operators in ammonia leakage accidents, and increasing emergency evacuation efficiency during ammonia leakage have important scientific values and practical significance in ensuring maximum safety.

Countries mainly select sites for liquid ammonia tanks in accordance with the relevant documents of national safe production and supervision departments in safety design for ammonia production and processing industry [4], such as China's *Comprehensive Evaluation Guidelines of Chemical Industrial Parks*, America's *Process Safety Management of Highly Hazardous Chemicals,* and *Chemical Management and Storage Management Measures* issued by Japan's Chemical Engineering Association. These relevant safety design standards and evaluation methods can prevent the occurrence of liquid ammonia leakage and decrease relevant deaths and casualties to some extent. However, the relevant standards are mainly

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formulated based on influences to surrounding environment, chemical properties, and ammonia production technology. This approach ignores the crowd evacuation ability and efficiency after liquid ammonia leakage. Scholars in the academic circle of safety planning for liquid ammonia tanks carried out experimental study and theoretical analysis on the diffusion laws of toxic gases produced by liquid ammonia, as represented by Burro test [5] and Thorney Island test [6]. Nowadays, scholars have mainly focused on horizontal small-sized pressure vessel structures and the influences of potential safety hazard checking, leaking hole size, leaking height, and environmental wind speed on leakage diffusion [7]. These studies analysed the influencing factors and diffusion modes of gas leakage and diffusion, verified existing mathematical models, and provided data supports for these models. Although ammonia leakage and diffusion have become one of the research hotspots in the simulation field, only a few scholars carried out related simulation analysis and investigated site selection for liquid ammonia tanks according to factory layout and evacuation efficiency with considerations to the crowd evacuation simulation results of liquid ammonia production and processing enterprises.

In this study, a site selection test method of liquid ammonia tanks based on simulation analysis was proposed to offset the shortages of existing studies and avoid crowd deaths and casualties in case of ammonia leakage. On the basis of repeated comparisons of ammonia diffusion time under different site selections and crowd evacuation time under emergency states, the ammonia tank sites of liquid ammonia production and processing enterprises can be planned scientifically to determine the ammonia diffusion laws and crowd evacuation efficiency. The results can provide decision-making references for the safety design of chemical enterprises.

2. STATE OF THE ART

After toxic gas leakage, the great premise of personnel evacuation is to calculate the path and concentration of gas diffusion. Choosing an appropriate gas diffusion model is the key in calculating toxic diffusion. With the continuous occurrence of gas leakage accidents in the chemical industry many scholars began to study gas diffusion. Using the Gaussian plume model as basis, Zhang et al. [8] investigated the diffusion risks of dangerous chemical products (e.g. liquid chlorine and liquid ammonia) during air transmission and after transportation and analysed the transportation risks of dangerous chemical products by applying several technologies. Kitabayashi et al. [9] carried out a wind tunnel simulation of pollutants and gas diffusion under complicated terrains. By focusing on the fast crowd transfer and evacuation path optimization under coupled wind and disaster conditions, Chen et al. [10] propose a toxic gas diffusion model of cellular transmission upon toxic leakage accident. Wang [11] built small- and large-sized models for horizontal ammonia tank leakage and toxic gas and simulated the local leakage and overall diffusion conditions of horizontal liquid ammonia tanks using the component transport model based on Fluent software. Zhou et al. [12] design a set of gas diffusion Gaussian models applicable to industrial ammonia leakage and studied and proposed the wireless sensor network ammonia leakage source positioning method and monitoring system based on Zig Bee. Horiguchi and Numazawa [13] reproduced the influences of toxic gas leakage and diffusion on human health by combining computational fluid dynamics and the physiological pharmacokinetics model and proposed the safety evaluation method of toxic gas leakage. Havens et al. [14] simulated and measured two CO_2 diffusion speeds and concentrations with uniform intervals and consistent surface roughness by changing the CO_2 release speed and wind speed in neutral stable boundary layer and concluded that CO_2 plume concentrations were distributed along the vertical wind direction. In summary, existing studies mainly concentrated in the simulation analysis of ammonia diffusion laws [15] and relevant physicochemical parameters [16] and proposed safety plans and designs of chemical enterprises. Although numerical simulation methods have the advantages of low cost, high repetition rate, short time consumption, parameter presetting, and strong comprehensive analysis ability, they require relatively detailed physical diffusion process and spatiotemporal data. The diffusion models in existing studies have relatively complicated calculations and give insufficient considerations to ammonia diffusion laws in a single zone of different chemical enterprises and scientific site selection for major hazard sources (e.g. liquid ammonia tanks). A simulation test requires the accurate physical boundary conditions and mathematical description of research objects.

After toxic gas leakage, safe crowd evacuation has attracted increasing research attention. Helbing et al. [17] divided evacuation activity into panic and normal states, which were studied respectively, and carried out a simulation test to verify the comparison data. They found that the physical state of personnel has significant influences on evacuation results. Ye and Lyu [18] introduced the toxic load value of evacuation path into the ant colony algorithm by establishing the path evaluation function, carried out adaptive strategy adjustment by using the heuristic method, improved the heuristic function of the algorithm, and proposed the evacuation path planning under the toxic diffusion background. Sime [19] proposed the ORSET model and comprehensively analysed distribution features in buildings by considering psychology, architecture, fire alarm, and evacuation index facilities. The minimum evacuation time was calculated to guide the safe evacuation of personnel under emergency conditions. By comprehensively considering the spatial structure layout of civil airplanes and combining cellular automaton with Pathfinder simulation software, Guo et al. [20] concluded the optimal emergency evacuation strategy of civil airplanes under emergency events. Deng and Gai [21] established an evacuation analysis system in major toxic leakage accident zones based on GIS, analysed business and data processes in regional evacuation, simulated the evacuation effect, and proposed a new evacuation mode. Liu and Zhu [22] proposed an exit selection model with considerations to crowd congestion and toxic damages and analysed the influences of emergency exit intervals, gas parameters, and seven different positional leakage points on evacuation time and number of people at different exits. By comprehensively considering weather conditions, leakage intensity, and evacuation personnel information, Seo et al. [23] proposed the risk evaluation model of emergency evacuation path based on neural network in the context of toxic gas diffusion. The optimal evacuation path was determined by integer programming, and the safest path for single evacuation personnel was proposed. In summary, existing studies mainly adopted crowd test and simulation. Research perspectives focus on crowd emergency evacuation path selection and planning problems under emergency events. Although the above studies contributed to the formulation of emergency evacuation scheme and the optimization of the evacuation efficiency of chemical enterprises, only a few comprehensively considered the diffusion problems of toxic and harmful gases. Combining the spatial structural design in different factories and the sample size of evacuation people, the site selection for major risk sources such as liquid ammonia tanks was determined through a multiscale simulation comparison. The diffusion modes of toxic and harmful gases are relatively complicated and vary significantly among different chemical substances. Therefore, combining enterprise production layout and evacuation ability and carrying out a comparison analysis of the multiscale site selection of major hazard sources are necessary to analyse the site selection for great risk sources in different types of chemical enterprises.

To address the shortage of existing studies, the present work simulated the ammonia diffusion time of eight sites for liquid ammonia tanks according to the spatial layout structure of chemical enterprises by using Pyrosim simulation software modelling based on the ammonia diffusion analysis theory of chemical enterprises. Combined with the crowd evacuation efficiency of Pathfinder simulation software, the proposed method can scientifically select sites for ammonia tanks that can guarantee the safety of operators to the maximum extent under the emergency event of ammonia leakage. This study aims to provide decision-making references to major hazard safety planning designs for chemical enterprises.

3. METHODOLOGY

3.1 Ammonia leakage mode setting and calculation of leakage volume

The three major modes for liquid ammonia leakage and diffusion sources are as follows [24]: vertical upward leakage of ammonia vapor from small holes in liquid gas storage tanks, vertical upward release of steam cloud from middle holes in liquid gas storage tanks, and gas tank explosion or breakage to form steam clouds after transient leakage. Statistical analysis of previous liquid ammonia accidents revealed that leakage is mainly the result of wall corrosion-induced ruptures, valve aging or poor connector sealing, and pipeline breakage. These accidents are mainly of continuous leakage mode. Hence, most leakage accidents can be viewed as ammonia continuous point leakage mode caused by different pore diameters. In the calculation of the toxic leakage volume, the leakage rate is related with flowing state of gas. The flowing state equation is:

$\frac{P_0}{P} \succ \left[\frac{2}{k+1}\right]^{\frac{k}{k-1}}$ indicates the subsonic flowing state, and the corresponding leakage volume is:

$$Q_m = C_{dg} AP \sqrt{\frac{kM}{RT}\left(\frac{2}{k-1}\right)\left(\frac{P_0}{P}\right)^{\frac{2}{k}}\left[1-\left(\frac{P_0}{P}\right)^{\frac{k-1}{k}}\right]} \tag{1}$$

$\frac{P_0}{P} \prec \left[\frac{2}{k+1}\right]^{\frac{k}{k-1}}$ indicates the supersonic flowing state, and the corresponding leakage volume is:

$$Q_m = C_{dg} AP \sqrt{\frac{kM}{RT}\left(\frac{2}{k-1}\right)\left(\frac{P_0}{P}\right)^{\frac{k+1}{k-1}}} \tag{2}$$

where Q_m is the gas leakage rate (kg/s), C_{dg} is the gas leakage coefficient, k is the specific heat ratio of diffusion gas, M is the molecular weight of gases, R is a gas constant J/(mol·K), P_0 is the gas pressure in pipelines (Pa), P is the environmental pressure (Pa), T is the gas temperature (K), and A is the area of leakage holes (m^2).

3.2 Hypotheses

The practical leakage and diffusion of liquid ammonia are a very complicated process involving liquid evaporation phase transition, gas–liquid phase mass and heat transfer, and other conditions. For the simplification of this process, some hypotheses are proposed:

(1) After gas is leaked into air, ammonia does not chemically react with air.

(2) No heat exchange with external environment is considered in the calculation field. The external temperature is assumed to be 298 K.

(3) The gas is the ideal gas and observes the ideal gas equation.

(4) Air is viewed as incompressible fluid in the turbulent state.

(5) The speed is constant after leakage and does not change with time.

On the basis of the above research hypotheses, the toxic gas leakage conditions are all rectangular fracture with a side length of 0.3 m from the top centre of liquid ammonia tanks. After tank fracture, liquid ammonia is volatilized into ammonia gas. Without considering the influences of other factors, the ammonia diffusion rate was set as 1.83 m/s.

3.3 Numerical simulation scenes and parameter setting of ammonia leakage in chemical enterprises based on Pyrosim

Physical model setting of chemical enterprise spaces: A chemical enterprise in Zhenzhou City, Henan Province of China was chosen for this study. This chemical enterprise has one liquid ammonia tank and seven fermentation tanks. The factory is designed as a single floor with one liquid ammonia tank, accessory tanks, fermentation tanks, shoe-changing room, men's dressing room, women's dressing room, men's room, women's room, archives room, raw material warehouse, raw material channel, raw material preprocessing room, and preprocessing product room. The liquid ammonia tank and fermentation tanks were placed in a 2 × 4 rectangle at north side of the factory. The locations were named. Tanks in the first row from right to left were numbered No. 1 – No. 4, and those in the second row from right to left were numbered No. 5 – No. 8 (Fig. 1).

The chemical enterprise has four evacuation exits. The gate size in the east is 3.6 m (width) × 3.2 m (height), and the worker entrance size is 1.2 m (width) × 2.5 m (height). The side gates in the east and west are both 1.6 m (width) × 2.5 m (height) in size. For management convenience, two side gates are generally closed, and the remaining doors and windows are open. The tank is 3 m high and 5 m in diameter, making it a 5.5 m (length) × 5 m (width) × 2 m (height) rectangle. Devices in the raw material processing room were simplified as six rectangles with a size of 2.4 m (length) × 1.2 m (width) × 1.5 m (height). Shelves in the raw material warehouse were simplified as seven rectangles with a size of 5 m (length) × 1 m (width) × 2 m (height), and those in the archives room were simplified as five rectangles with a size of 5.6 m (length) × 0.8 m (width) × 2 m (height). Given that ammonia is a colourless gas, tracer particles surround the fractures of the liquid ammonia tank. The ammonia diffusion path is reflected by the flowing direction of tracer particles.

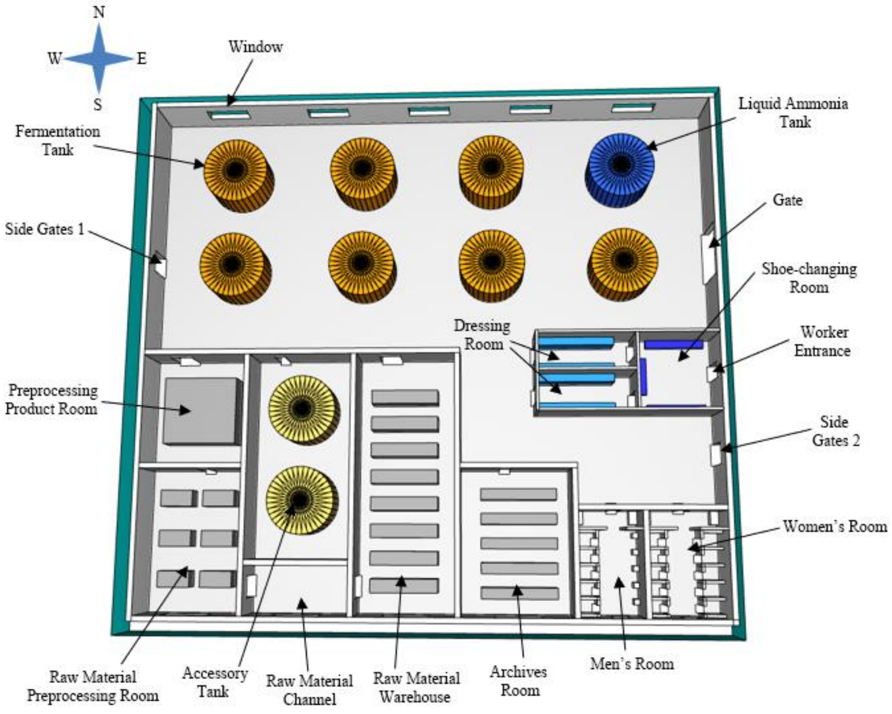


Figure 1: Physical model of the factory zone of the ammonia chemical enterprise.

Determination of the network model: The main factory space of this chemical enterprise is rectangular. It was simplified as a cubic model of 45 m (length) × 41 m (width) × 4 m (height). The grid parameters are shown in Table I. The minimum grid size is 0.5 m × 0.5 m × 0.5 m, and the total grid number is 59,040.

Table I: Setting of grid parameters.

Axis	Min (starting point)	Max (end point)	Grid number
X	-1	44	90
Y	-1	40	82
Z	0	4	8

3.4 Crowd evacuation model setting in the factory based on Pathfinder

Personnel distribution conditions and design of escaping speed: According to field survey, most workers of this chemical enterprise are adult men. In this study, the workers were divided into 75 % men and 25 % women. According to different job types and locations, the personnel distribution in the chemical enterprise is shown in Table II.

Table II: Personnel distribution in the chemical enterprise.

Regions	Men	Women	Regions	Men	Women
Tank zone	15	2	Raw material channel	1	0
Archives room	2	3	Raw material preprocessing room	3	3
Raw material warehouse	4	1	Preprocessing product room	1	0
Accessory tank room	2	0	Men’s room	1	0
Dressing rooms	1	0	Women’s room	0	1
Total: 40, including 30 men and 10 women.					

The normal walking speed of adult men is in the normal distribution of 1.35±0.2 m/s and that of adult women is in the normal distribution of 0.98±0.2 m/s. Therefore, the walking speed of workers in this chemical enterprise was chosen as the random distribution speed in the above ranges.

Human body size and design of reaction time: According to the body size of Chinese adults and the shoulder width data of different groups and with considerations to gender ratio, age, and work clothes in the enterprise, the men’s shoulder width was distributed randomly within 0.41–0.45 m and that of women was distributed randomly within 0.38–0.42 m.

An ammonia leakage detection alarm was set above the liquid ammonia tank in the chemical enterprise. When liquid ammonia leaks, the ammonia gas first spreads upward. At this moment, the detection alarm will come in contact with ammonia gas and send alarms. Moreover, the liquid ammonia tank is only 1 m away from the roof. The time from liquid ammonia leakage to ammonia gas detection and then to alarm triggering can be ignored. After the alarms are sent, workers on duty make emergency evacuation responses accordingly and the response time is 0 s. Given that workers in other regions are far away from the leakage site, the response time was randomly chosen as 0–8 s for personnel evacuation.

Behavioural mode selection of Pathfinder: Pathfinder contains two different simulation modes: Steering and SFPE. During simulation based on “Steering” mode, workers move along their own paths. With considerations to the influences of barriers, doors, and mutual impacts on path movement, avoidance behaviours occur among workers without their flow being limited by doors. During simulation based on “SFPE” mode, worker movement is mainly restricted by walking speed and worker flowing rate of doors. Congestion, in which multiple persons occupy the same space, might occur. The simulation results were mainly used for benchmark comparison. With comprehensive considerations to practical situations, the “Steering” mode is close to the behaviours of workers in real scenes. Hence, the “Steering” model was chosen for simulation in this study.

With the above parameter settings and field survey conditions, the personnel evacuation model of the chemical enterprise in this study was determined (Fig. 2).

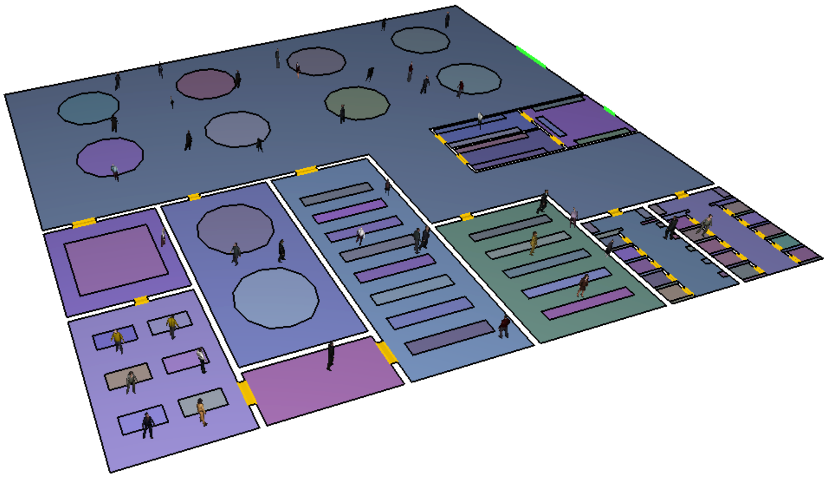


Figure 2: Personnel evacuation model in the study case.

3.5 Evacuation scene design

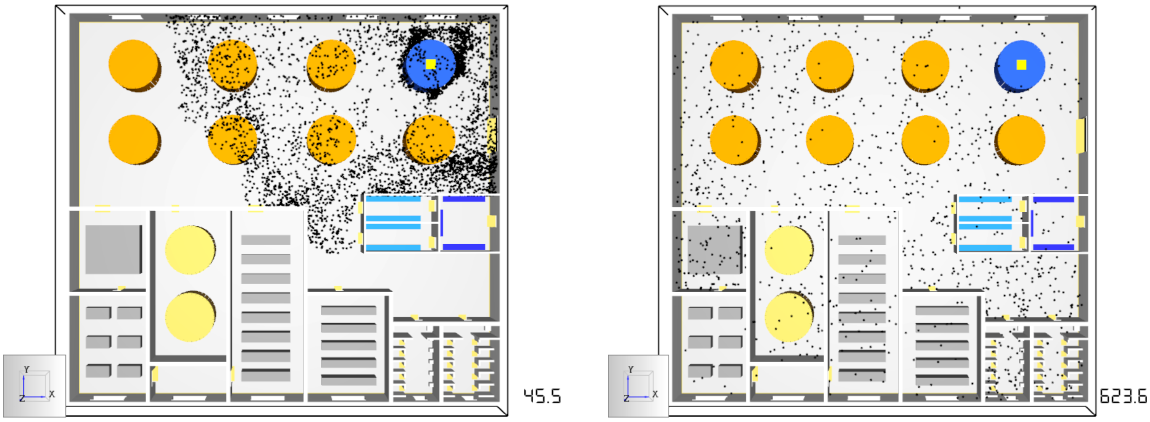
The physical model of the factory zone of this chemical enterprise was built by Pyrosim. According to ammonia leakage scenes under different conditions, different initial conditions were set and FDS was operated for the dynamic simulation of ammonia leakage and diffusion. The dynamic operations of presetting leakage scenes were carried out. The operation processes vary significantly with building size and grid number.

In this study, eight leakage scenes were set according to eight liquid ammonia tank positions in the chemical enterprise. In Scene 1, the liquid ammonia tank is at Position 1, and the fermentation tanks occupy Positions 2–8. In Scene 2, the liquid ammonia tank is at Position 2, and the fermentation tanks occupy the remaining positions. The rest of the scenes were set in the same way. Each scene was subjected to 2 h of simulation time to obtain ammonia leakage and diffusion simulation results under different scenes.

4. RESULT ANALYSIS AND DISCUSSION

4.1 Numerical simulation results of ammonia leakage based on Pyrosim

Leakage simulation results of Scene 1: In Scene 1 where the liquid ammonia tank was at Position 1, top fracture occurred. Ammonia gas diffused to the nearby windows and outdoor spaces, then to the factory gate, and finally to external regions. It continued to spread in the factory zone to the doors of dressing rooms and raw material warehouse (Fig. 3 a).

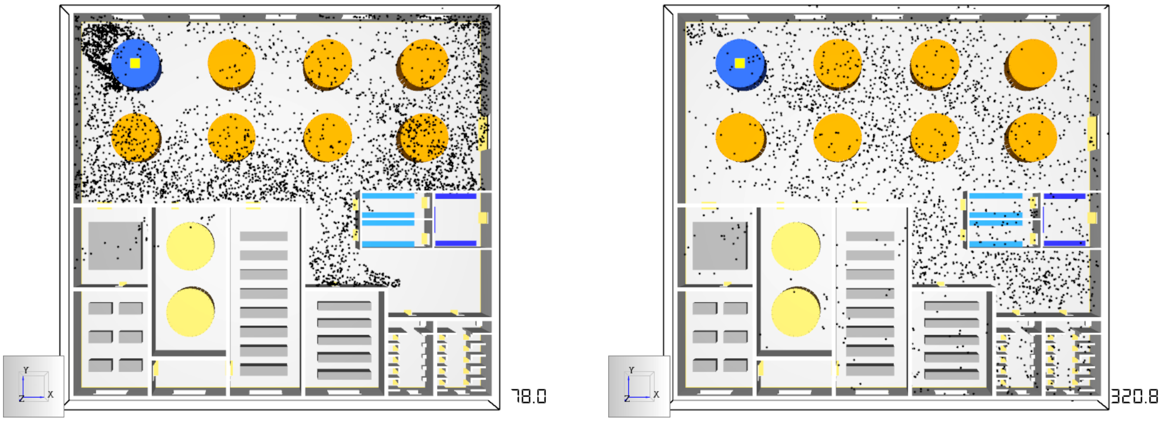


a) b)

Figure 3: Diffusion condition of ammonia diffusion in Scene 1 at 45.5 s and 623.6 s.

At 45.5 s, the ammonia gas has diffused to two excavation exits. Later, the ammonia gas spread in the raw material warehouse, diffused to the door of the accessory tank room, and spread in this room. Meanwhile, ammonia gas spread to the channel to men’s and women’s rooms. Later, ammonia gas arrived at the west wall and began to spread in the preprocessing product room. Finally, ammonia gas successively diffused to women’s room, men’s room, dressing rooms, raw material preprocessing room, shoe changing room, and raw material channel. As shown in Fig. 3 b, ammonia gas has diffused to all rooms at 623.6 s.

Leakage simulation results of Scene 4: In Scene 4 where the liquid ammonia tank was at Position 4, top fracture occurred. Ammonia gas diffused to the two evacuation exits at 73 s (Fig. 4 a). It diffused to the maximum indoor area at 320.8 s but not to the raw material preprocessing room and raw material channel (Fig. 4 b).



a) b)

Figure 4: Diffusion condition of ammonia diffusion in Scene 4 at 73 s and 320.8 s.

Owing to paper layout, only the analysis results of ammonia gas diffusion in Scenes 1 and 4 are presented. From the observation and data analysis of the eight leakage scenes, the times for ammonia gas to diffuse to the two evacuation exits and maximum indoor area were acquired (Table III).

Table III: Time for ammonia gas to diffuse to two conditions under different scenes.

Simulation scenes	**Time of diffusion to two evacuation exits**	**Time of diffusion to maximum indoor area**
Scene 1	45.5 s	623.6 s
Scene 2	37.0 s	675.7 s
Scene 3	51.9 s	299.6 s
Scene 4	78.0 s	320.8 s
Scene 5	39.2 s	632.1 s
Scene 6	32.8 s	365.5 s
Scene 7	50.8 s	402.7 s
Scene 8	69.8 s	522.8 s

4.2 Crowd emergency evacuation simulation results based on Pathfinder

Crowd emergency evacuation results of Scene 1: In Scene 1 where the liquid ammonia tank is at Position 1, top fracture occurred. Liquid ammonia volatilized into ammonia gas after coming in contact with air and began to diffuse around to trigger the alarm. The two workers near Position 1 and between Position 1 and the gate escaped from the gate, and the other workers escaped from the worker entrance. The crowd evacuation at 45.5 s of evacuation when the ammonia gas spread to the two evacuation exits is shown in Fig. 5. At this moment, 36 workers were evacuated successfully. However, 4 workers have not entered the dressing rooms. The total evacuation time was 75.8 s.

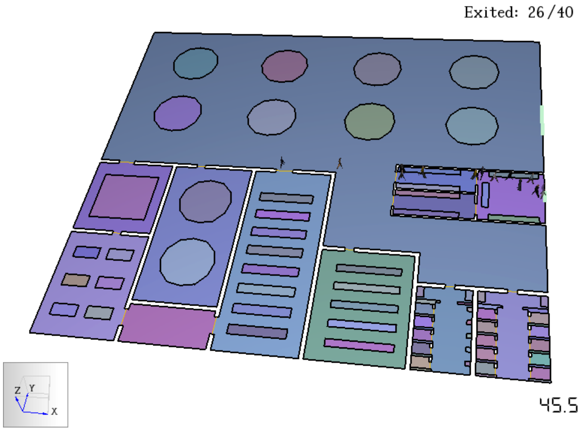


Figure 5: Conditions of crowd evacuation to 45.5 s in Scene 1.

Crowd emergency evacuation results of Scene 4: In Scene 4 where the liquid ammonia tank is at Position 4, top fracture occurred. Seventeen workers in the tank region escaped from the gate, and the others escaped from the worker entrance. The crowd evacuation conditions at 73 s when ammonia gas diffused to the two evacuation exits are shown in Fig. 6. At this moment, 40 workers were evacuated successfully and all workers left the factory zone.

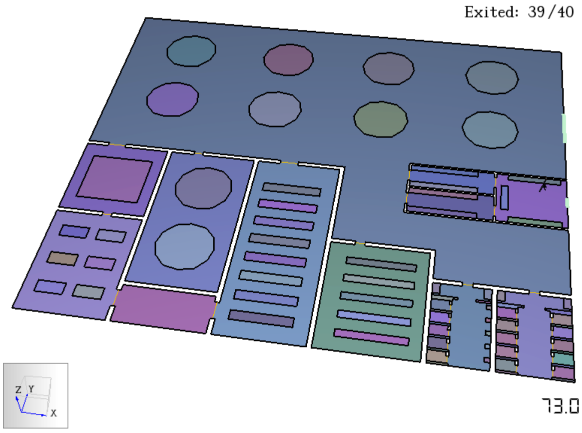


Figure 6: Conditions of crowd evacuation to 73 s in Scene 4.

Owing to paper layout, only the crowd evacuation results of Scenes 1, and 4 are presented to analyse crowd evacuation efficiency. From the observation and data analysis of the eight scenes, the crowd evacuation results in the time when ammonia gas diffused to safe exits under different scenes were acquired. The results are shown in Table IV.

Table IV: Time of ammonia gas diffusion to evacuation exits in different scenes.

Simulation scenes	Time of diffusion to evacuation exit	Number of non-evacuated workers when ammonia gas diffused to the evacuation exit
Scene 1	45.5 s	4
Scene 2	37.0 s	5
Scene 3	51.9 s	3
Scene 4	73.0 s	0
Scene 5	39.2 s	5
Scene 6	32.8 s	7
Scene 7	50.8 s	2
Scene 8	69.8 s	3

4.3 Site selection for the liquid ammonia tanks based on the combination of ammonia leakage and crowd evacuation simulation results

According to simulation results of ammonia leakage, the time it takes for ammonia gas to diffuse to the two evacuation exits was the longest in Scene 4, and the time for ammonia gas diffusion to the maximum indoor area was the longest in Scene 2. Hence, the early indoor diffusion speed of Scene 4 was the lowest, which is conducive for the early safe evacuation of workers after the discovery of ammonia leakage. The global indoor diffusion rate of Scene 2 was the lowest, which is beneficial for workers to cope with ammonia leakage in the factory zone after they withdrew from the factory.

Simulation results of the crowd evacuation efficiency under ammonia leakage conditions showed that the ammonia gas diffuses to the gate in a short time in Scene 1 because the liquid ammonia tank is close to the gate. As a consequence, most workers can only escape from worker entrance and the evacuation efficiency is low. In Scene 2, ammonia gas diffused to the two evacuation exits in a short time, trapping or poising the evacuating workers. Hence, the evacuation efficiency is low. In Scene 3, most workers in the tank region evacuated from the gate and were far away from the two evacuation exits, resulting in a good evacuation effect. In Scene 4, all workers in the tank region escaped from the gate and were the farthest to the two evacuation exits. When ammonia gas diffused to the two evacuation exits, all workers were already evacuated, exhibiting the best safe evacuation effect. In Scene 5, the liquid ammonia tank is the nearest to the gate, which is disadvantageous for the escape of the workers in the tank region. Most workers have to escape from the worker entrance, resulting in a low safe evacuation efficiency. In Scene 6, the liquid ammonia tank is the nearest to the door of dressing room and is on the evacuation path toward the gate. This position is the most disadvantageous for personnel evacuation, and the safe evacuation efficiency is the lowest. In Scene 7, although ammonia gas diffused to two evacuation exits at a later time, the liquid ammonia tank is relatively close to doors of three rooms toward the raw material warehouse. Ammonia leakage will block the door later, and most workers in the room will inhale ammonia gas during escaping, thus leading to a low safe evacuation efficiency. The phenomenon in Scene 8 is close to that in Scene 7, and most workers from various rooms such as the accessory tank room will inhale ammonia gas during escaping, causing a low safe evacuation efficiency.

The safest approach is to set the liquid ammonia tank at Position 4. The phenomenon in Scene 3 is relatively close to that in Scene 4. Hence, setting the liquid ammonia tank at Position 3 can also be considered. The ammonia leakage in Scene 6 is the most dangerous, and this scene is the most disadvantageous for personnel evacuation. Hence, Position 6 is the most inappropriate position for liquid ammonia tank.

5. CONCLUSION

A simulation analysis on ammonia leakage and diffusion laws for typical spatial layouts of eight liquid ammonia tanks based on Pyrosim software is carried out to select the most appropriate site for the liquid ammonia tanks of chemical enterprises. With the use of the Pathfinder software, the time for ammonia gas diffusion to the safe exit and time for emergency crowd evacuation under different scenes are compared. Moreover, the crowd evacuation efficiency under different scenes is analysed. Based on the principle of maximum safety, the optimal site for the liquid ammonia tank in the chemical enterprise is determined. Some major conclusions could be drawn:

(1) Combined with the fluid mechanics equation of ammonia leakage and diffusion, the results of Pyrosim simulation objectively disclose the ammonia diffusion laws and diffusion time when the liquid ammonia tank is at different positions through reasonable model meshing. The time for ammonia gas to diffuse to safe exits also varies when the liquid ammonia tank is

at different regions of the chemical enterprise. Scientific planning of major hazard sources can provide sufficient time for crowd evacuation in case of ammonia leakage.

(2) According to the field survey of spatial structural layout in ammonia production and processing enterprises, the emergency crowd evacuation efficiency under emergency events such as ammonia leakage can be simulated using the Pathfinder software and considering the practical number of operators in the enterprise. The evacuation time under emergency state can be decreased to some extent by analysing evacuation laws and path.

(3) From the simulation analysis results of ammonia leakage and diffusion, the diffusion laws of toxic gas from liquid ammonia tank leakage and crowd evacuation time in the eight scenes in the case study are simulated. The evacuation time in Scene 4 is 73 s, which is shorter than the time of ammonia gas diffusion to the safe exits (78 s). Research conclusions can provide new ideas for the site selection of liquid ammonia tanks in chemical enterprises.

The built simulation model is based on the top fracture of the liquid ammonia tank, a common ammonia leakage accident. Moreover, this case study chooses a middle-sized ammonia gas production enterprise. The following are recommended research directions in the future. For the analysis of large-scale ammonia chemical enterprises with several liquid ammonia tanks and several fermentation tanks, multiple groups of ammonia leakage and diffusion simulation analysis models under different scenes must be set up for the accurate site selection of liquid ammonia tanks. In addition, the simulation analysis results of ammonia gas diffusion under different natural wind speeds will be involved in follow-up studies.

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