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Risk Level Analysis of Petrochemical Hazardous Gas Leakage Based on Odour Recognition and CFD Simulation Technology

Wenjie Gu[a,b]

[a]College of Civil Engineering, Chongqing University, Chongqing 400045, China
[b]Key Laboratory of New Technology for Construction of Cities in Mountain Area (Chongqing University), Ministry of Education, Chongqing 400045, China
362923750@qq.com

Petrochemical enterprises have made an indelible contribution to the global modernization. However, as the high risk-level enterprises, once gas leak occurs, it will cause great harm to the surrounding environment and residents. At present, there still exists some weakness in China's research on petrochemical hazardous gas leak detection and risk classification is still weak. Based on odour recognition (rotten egg odour) and CFD simulation technology, this paper conducts analysis of risk levels for the hydrogenation process in petrochemical processing. The study has found that CFD can be used to simulate the concentration of harmful gas (H_2S) diffusion and characterize the severity of harmful gas leakage; the wind direction of the hydrogenation unit and the installation and arrangement of the equipment have an important impact on the leakage of harmful gases, and then CFD simulation can be used to analyse the risk level. This is of guiding significance for the placement of H_2S detector.

1. Introduction

Oil is a viscous, dark brown liquid, also called "industrial blood", which has made a huge contribution to modernization development (Zhang and Chen, 2010). Petrochemical enterprises, as an important part of social development, also provide huge energy and raw materials for various industries (Fu et al., 2016). Moreover, petrochemical enterprises are also more high-risky (Jungemann et al., 2012; Xie et al., 2014): the raw materials used by petrochemical enterprises are mostly hazardous chemicals (Bouazza & Vangpaisal, 2006); the processes involved in the production process also have the high-temperature and pressure, flammable and explosive features (Abed et al., 2012); Once an accident occurs in certain operation, it will inevitably cause irreparable damage to surrounding residents (Lee et al., 2015, Said, M., et al, 2016). This requires a scientific risk classification, in order to strengthen the management of high-level risks, and rationally arrange the gas detector, which shall reduce unnecessary spending by enterprises while improving the detection efficiency and reducing the risk of accidents.
At present, computer algorithms and CFD simulation software (Piazzullo, 2018) have been applied to carry out research work on hazard source identification and risk assessment of petrochemical equipment in foreign countries. In China, the traditional risk assessment method is used to evaluate the risk of gas leaks. In this paper, the odour recognition (rotten egg smell) and CFD simulation technology are used to evaluate the risk of petrochemical hydrogenation unit, which is of positive guiding significance for the placement of harmful gas detectors.

2. Research objectives and content

2.1 Research objective

In this paper, taking the diesel hydrogenation unit of petrochemical enterprises as the research object, the hazard source in the H_2S leakage is firstly identified, then the risk assessment is carried out, and finally the

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leak detection optimization is implemented on the basis of CFD technology.

2.2 Research content

According to the petrochemical production process, the equipment containing H_2S gas in the engineering process is firstly identified. The risk model is constructed, to obtain the wind field set using the local meteorological data and further construct the H_2S gas leakage probability set of the hydrogenation unit. At last, the CFD simulation technology is used to make risk classification of H_2S leaks (Kulkarni et al., 2018).

3. Hazard source identification of harmful gas

3.1 Diesel hydrogenation unit based on odour recognition

As more attention is paid to environmental protection by people, the low-sulfur diesel is the trend of oil refining. In the diesel refining process, the addition of hydrogen can remove the sulfur in the crude oil and achieve the purpose of reducing the sulfur content. During the desulfurization process, toxic and harmful substances such as H_2S shall be produced (Table 1).

Table 1: Distribution table of toxic substances in diesel hydrogenation unit

Facility\ Item	H_2S	NH_3	SO_2	Petroleum brain	Liquefied petroleum gas	Two methyl two sulphur
Reaction	√					√
Fractionating	√			√		
Gas desulphurization	√					
Solvent regeneration	√					
Acid stripping	√					
Sulfur recovery	√	√	√			
Hydroliquefied gas refining	√				√	
Storage and transportation	√					
Public and auxiliary facilities unit	√					

In the diesel refining process, the hydrodesulfurization and fractionation process flow chart is shown in Figure 1.

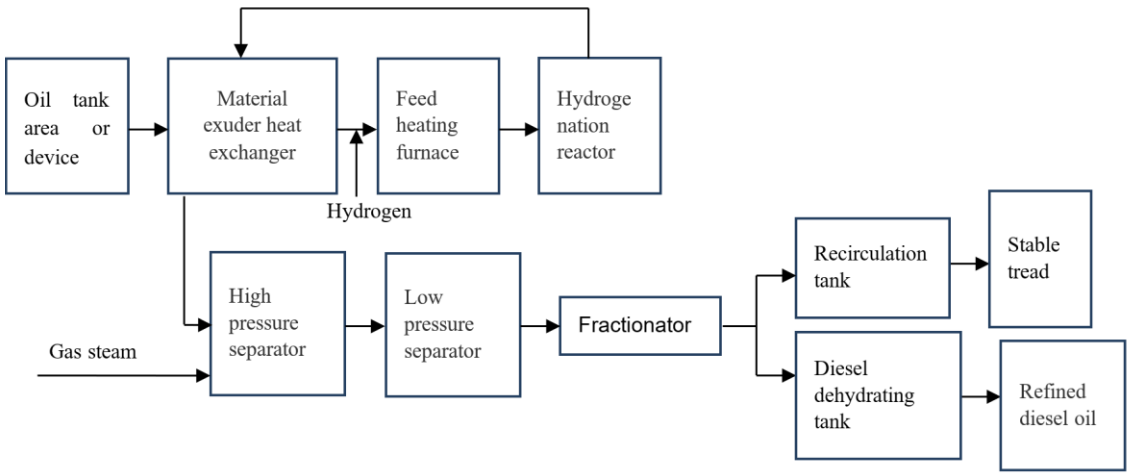


Figure 1: Hydrogenation of diesel oil and process flow chart of distributary system

It can be seen from Table 1 that H_2S is produced in all aspects of diesel hydrogenation. H_2S has a smell of rotten eggs, which will strongly stimulate the nervous system and mucous membranes of the human body and cause poisoning. Due to its high toxicity, H_2S should be key monitoring object of enterprises.

3.2 Hazard source identification based on odour recognition

Among the diesel hydrogenation units, the pressure-bearing equipment and containers are prone to leakage, mainly including reactors, heat exchangers, and storage devices. Table 2 lists the identified hazard factors that easily cause H_2S leakage in this diesel hydrogenation unit:

Table 2: Risk source identification table for H2S leakage equipment

No.	Equipment number	Device name
1	R1	Hydrogenation refined reactor
2	E1	Reactive outflow / mixed feed heat exchanger
3	M1	Thermal high pressure separator
4	H1	Hot air separation air cooler
5	E2	Heat separation / hydrogen mixture heat exchanger
6	M3	Cold high pressure separator
7	M6	Cyclonic Hydrocyclone
8	P1	Circulating hydrogen desulphurization tower
9	M2	Amine rich liquid flash tank
10	M4	Thermal low pressure separator
11	H2	Heat low split air cooler
12	M5	Cold low pressure separator
13	P2	Bottom line of stripper stripper for H_2S
14	E3	H_2S stripper rear cooler
15	M7	Recirculation tank of stripper stripping tower for H_2S
16	H3	Medium pressure steam water separator

3.3 Leak set of hydrogenation unit

Gas diffusion is affected by many factors, such as wind speed, wind direction, and atmospheric stability, etc. If the influencing factors are comprehensively analysed according to the weight, and the storage conditions of the leakage materials are also considered, such as storage state, leakage aperture, shape, etc., the achieved results shall make a more complete coverage of gas leak scenes.
Based on the identification results of H_2S leakage hazard source in rotten egg odour, the gas leakage model was established using the leak software. Then, the leakage probability of different leak source sizes was calculated to construct a leak set (Table 3).

Table 3: Leaked scene set array

Leakage \ Wind field	N 1.5m\s	S 2m\s	E 3.5m\s	W 3.7m\s
R1	R1-1	R1-2	R1-3	R1-04
E1	E1-1	E1-2	E1-3	E1-4
M1	M1-1	M1-2	M1-3	M1-4
H1	H1-1	H1-2	H1-3	H1-4
E2	E2-1	E2-2	E2-3	E2-4
M3	M3-1	M3-2	M3-3	M3-4
M6	M6-1	M6-2	M6-3	M6-4
P1	P1-1	P1-2	P1-3	P1-4
M2	M2-1	M2-2	M2-3	M2-4
M4	M4-1	M4-2	M4-3	M4-4
H2	H2-1	H2-2	H2-3	H2-4
M5	M5-1	M5-2	M5-3	M5-4
P2	P2-1	P2-2	P2-3	P2-4
E3	E3-1	E3-2	E3-3	E3-4
M7	M7-1	M7-2	M7-3	M7-4
H3	H3-1	H3-2	H3-3	H3-4

4. Risk classification at leakage points

4.1 Classification principle

The risk classification of leaks is a prerequisite for optimizing the gas detector arrangement. The leakage probability indicates the likelihood of an accident occurring, and the concentration of the diffusion field indicates the severity of the leak consequences. In this paper, the leakage probability and consequences are comprehensively analysed as a basis for risk level classification.

4.2 Physical model

Based on the contour of the simplified diesel hydrogenation unit, the grid model was built using the grid-based large scale (Figure 2 and 3).

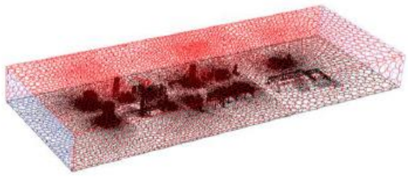


Figure 2: Grid model of diesel hydrogenation unit

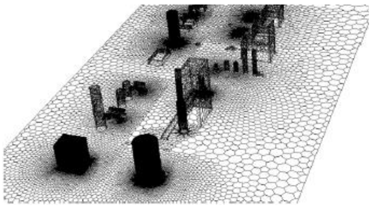


Figure 3: Partial enlarged drawing

4.3 Boundary condition

The boundary condition is calculated as:

$$V = \frac{1}{\tau}\delta^{'}\ln\left(\frac{z}{z_o}\right) \tag{1}$$

$$k = \frac{1}{\sqrt{C_\mu}}\delta^{'2} \tag{2}$$

$$\varepsilon = \frac{1}{\tau}\frac{\delta^{'3}}{z} \tag{3}$$

where V is the wind speed from the ground, δ' is the friction velocity, τ=0.4 is the Karman coefficient, Z_0=0.01m is the roughness, C_μ=0.09, and k and ε are the turbulent kinetic energy and coefficient.

4.4 CFD simulation calculation

In the process of discretization simulation calculation, discrete errors can be generated. If the grid density is high, the discrete error is relatively small, but the calculation cost is high. If the grid density is low, the calculation accuracy shall be not sufficient. Gambit software was used to set the grid scaling to 1:1.1, 1:1.2, 1:1.3, 1.4, and then different grid models were obtained. One of the leaks was used for verification. The results are as follows:

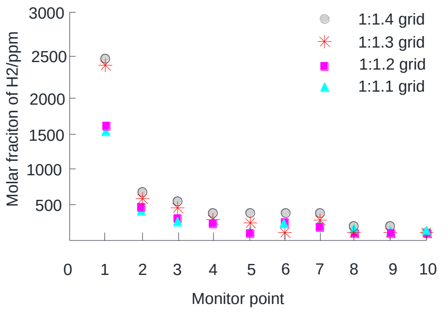


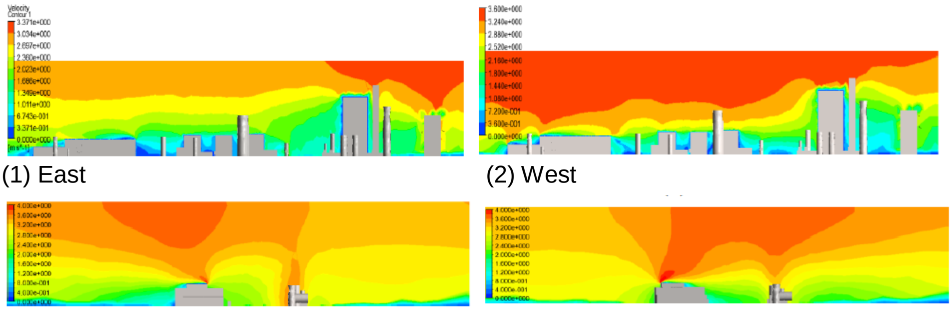
Figure 4: Comparison predicted by three kinds of mesh

It can be seen from Fig.4 that the monitoring points at the ratio of 1:4, 1:1.3 and the other two ratios differ greatly, and the difference between 1:1.1 and 1:1.2 is small. To save the calculation cost, 1:1.2 grid was adopted for simulation.

4.5 Ventilation effect simulation

The ventilation effect of the gas diffusion zone has an important influence on the collected concentration of harmful gases. Through the study of the spatial distributed wind field of diesel hydrogenation unit, the gas flow characteristics and wind field distribution at different locations were summarized to determine the risk level. According to the leakage scene set, the east, west, south and north winds were selected as the basic wind conditions for research.

Within the research region, the distribution of equipment pipelines in the east-west direction and the resulting large span have a great influence on the wind field. Moreover, the higher-located fractional device on the east side has an obvious blocking effect on the wind, significantly reducing the downstream wind speed. In case of toxic gas leaks downstream, it is easy to aggregate and cause an accident. Whereas, for west wind, it does not have this feature. In the southward and northward winds, due to the short distance between the equipment in the north-south direction, the wind direction and wind speed are also subject to drastic changes under the action of equipment and pipelines.



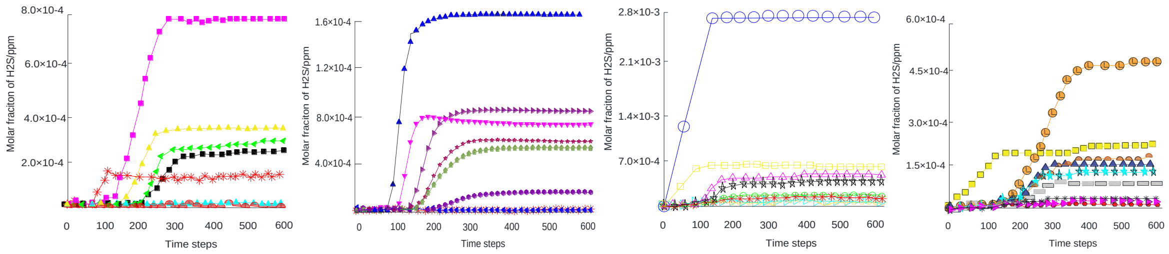
(1) East (2) West

(3) East (4) West

Figure 5: The distributed cloud map of the wind field in the vertical wind direction

It can be seen from Figure 5 that the wind direction and equipment layout have an important influence on the wind field distribution. The wind direction plays a leading role, while the layout of equipment facilities, pipelines, etc. interferes and swirls the local airflow. When the east wind springs up, the downstream wind speed is low or static wind area is large. Therefore, once the gas leaks, toxic and harmful gases are collected on the west side, which will pose a threat to the operators on duty. In addition, when the wind comes from the upstream, such as the north-south wind, due to the blockage of the equipment group, it will adversely affect the gas diffusion, which will also cause harm to the duty or resident personnel, once the gas is collected.

4.6 Classification of risk levels



Hydrofining Reactor Amine rich liquid flash tank Amine rich liquid flash tank Heat low split air cooler

Figure 6: Variation curve of H_2S concentration in different leakage sources

For the risk level classification of harmful gas leak, various uncertain factors must be considered in the leakage process. In order to reduce the calculation amount and determine the reasonable leakage simulation time, based on the risk identification of harmful gas leakage in the diesel hydrogenation unit, the four outermost leakages sources were selected for calculation in the longest diffusion wind. Table 2 lists the serial number of the four selected leakage sources: 1, 9, 11, and 15 respectively. Under the wind field conditions of maximum diffusion distance for the four leakage sources, 8 points were selected as the concentration monitoring points in the downstream wind direction of H_2S leakage area (Figure 6).
In the CFD simulation, the leakage time was set to 400s, the time step was 600, and the step size was 0.67s. It can be seen from Fig.6 that after the leakage occurs, the concentration of H_2S at each monitoring point increases from 0 to certain concentration, and after about 200 steps, it remains almost unchanged, that is, the leakage time is about 133s.

4.7 Classification results

Since the primary alarm threshold value of the H_2S alerter is set to 10 ppm in the relevant national regulations, this paper sets 10ppm as the threshold of H_2S.
Based on the simulation results, the risk level of the leaks was analysed, so as to obtain the risk matrix of each leakage source. The relative risk matrix was also made by comprehensively considering the occurrence probability and accumulating the risk matrix. Figure 7 shows that the higher the risk level, the greater the

potential risk; the more the number of risk levels, the greater the number of risk level areas; the comprehensive risk level of the diesel hydrogenation region can be obtained by superimposing the risks in each region. Fig.7 also indicates the possible leakage risks from different leakage sources, where the highest risk area is centred on the leakage source. When arranging the gas detectors, high-risk point should be fully considered. In addition, the heavier H_2S diffuses along the surface, so the point distribution should be made in the relatively concentrated places of personnel, such as the central control room.

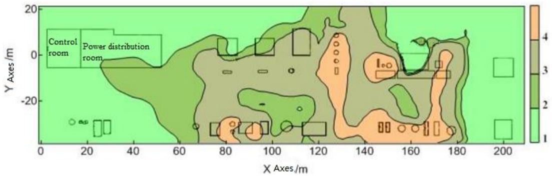


Figure 7: H_2S leakage comprehensive risk regional classification

5. Conclusions

This paper analyses the risk level of diesel hydrogenation unit based on odour recognition and CFD simulation technology. This is of positive guiding significance for the placement of harmful gas detectors. The following conclusions have been made: (1) Diffusion concentration field of harmful gas leakage can represent the severity of the leakage. The diffusion value of the harmful gas concentration was obtained by CFD simulation, thereby characterizing the severity of the leakage at the monitoring position. (2) The grid model was generated by Fluent software, to conclude that the 1:1.2 ratio can satisfy the calculation accuracy and also save the calculation cost. (3) The wind direction and equipment layout of the diesel hydrogenation unit have an important impact on the distribution of toxic and harmful gases. Through CFD simulation, the risk level of diesel hydrogenation can be obtained, which provides guidance for the placement of H2S detectors.

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