Experimental and simulation analysis of hexane leak in pump room

Chenglong Zhou¹, Tao Chen*, Tao Chen¹, Zhipeng Li² and Xingfeng Li²

¹Department of Engineering Physics, Tsinghua University, Beijing, 100084, China
²Beijing GS Technology Co., Ltd, Beijing, 100084, China
*Corresponding author’s e-mail: chentao.a@tsinghua.com

Abstract. The technology of monitoring and tracing the unorganized emissions of VOCs in petrochemical parks is a research hotspot. For the VOCs leakage in the pump room of the aromatics extraction equipment, 6 distributed monitoring points are implemented to monitor the VOCs concentration. A 2-hour leak test is performed using n-hexane standard gas, and the process is simulated using computational fluid dynamics. The results show that there is a background value of n-hexane concentration in the pump room, which means that potential leakage occur. P36, P19, P18, and P15 were able to respond to the n-hexane leak, but the concentrations of P14 and P17 did not increase. The leakage sequence of simulation is the same as that obtained in the experiment. The concentration distribution is affected by the wall barrier and distance, and n-hexane will preferentially diffuse along the wall.

1. Introduction
The petrochemical industrial park has developed rapidly in recent years. While bringing huge economic benefits, the pollution problem is also becoming increasingly serious. Studies have shown that industrial sources are the largest source of Volatile organic compounds (VOCs) contributions[1-2]. VOCs can cause great harm to the atmospheric environment and human health, and have become a hot spot in international research. Emissions of air pollutants from petrochemical companies include organized and unorganized emissions. The monitoring and control measures of organized emissions are relatively complete. In contrast, the monitoring, evaluation and management of unorganized emissions is more difficult[3-4]. VOCs emissions caused by equipment leaks far exceed the processes of container storage, sewage treatment, transfer manipulation, and ventilation. The leakage of valves and connections accounts for more than 90% of the total leakage emissions[5]. Distributed monitoring technology installed inside the park is an effective method to monitor the unorganized leakage of VOCs[6]. It can monitor the concentration of VOCs in the park in real time. Once the concentration exceeds the standard, the system will alarm and reverse the source of the leak. And how to lock the leak source based on the monitoring point information is one of the key goals of distributed monitoring. For a fixed monitoring network, its response to leaks at different locations is inconsistent. The response characteristics can be used as the basis for traceability.

The factors that influence the leak process indoors and outdoors are different. Local wind field in the outdoor will dominate the diffusion of VOCs. For indoor environment, since most of them are windless, the diffusion is related to the indoor structure. In order to study the leakage of VOCs occurring indoors, a distributed monitoring network based on mass spectrometer was constructed for the pump room of
aromatics extraction equipment. The hexane leak in the pump room was simulated by standard gas test to analyze the response of the monitoring network. CFD method is applied to study the diffusion process.

2. Experiment design
The structure of the pump room is shown in Figure 1. The room contains a total of 21 pumps. VOCs leaks usually occur at connection locations such as flanges and valves on the pump. 6 monitoring points are arranged to monitor the VOCs concentration in the pump room in real time. The concentrations at the monitoring points is analyzed sequentially, and the analysis time for a single measuring point is 20s. The leak source was simulated with a concentration of 6023ppm n-hexane standard gas, the volume of the cylinder was 8L, and the rated pressure was 1.5M Pa. The standard gas tank is placed at P406B, and the leakage time is 2 hours. Its leakage flow is shown in figure 2.

![Figure 1. Distribution of pumps and monitoring points in the pump room](image)

![Figure 2. Change in n-hexane leak flow](image)

3. CFD method
The three-dimensional model of the pump room is shown in figure 3, which simplifies details that do not affect the diffusion process. ICEM is used to divide the structural grid, and the number of grids is 2 million (figure 4). The problem in this investigation is a three-dimension unsteady, natural convection flow. To reduce computing complexity, some reasonable assumptions are considered. The indoor airflow is modelled using the incompressible Navier-Stokes equations coupled with a Boussinesq approximation for thermal buoyance flows. Two separate continuity equations are solved for the air and C6H14 gas respectively. The simulated diffusion time is 2 hours and the time step is 0.2 s.
4. Results

4.1. Experiment analysis

Figure 5 shows the concentration of monitoring points over time from 1 hour before the start of leakage to 1 hour after the end of leakage. It can be found that before the start of the test, the n-hexane concentration at each monitoring point is not 0, and the concentration value at each point is not stable. The n-hexane background value indicates that some pumps were leaking. Once the standard gas leak began to leak, the concentrations at P36, P19, P18, and P15 increased significantly, while P14 and P17 did not increase significantly. Figure 1 (b) shows that two points P14 and P17 are far away from the standard gas position, and the leakage of the experiment did not affect the concentration fields at these two measurement points. The timing of the concentration increase at the four points affected by the leak is P36 to P18 to P19 to P15. Figure 6 shows the difference between the highest concentration value and the initial value during the experiment. It can be found that the increase in concentration at the four points is P36> P18> P15> P19. P36 is the point closest to the source of the leak, so it responds to the leak of the standard gas first and has the highest concentration. P15 is the far away from the leak source, so it responds to the leak at the latest. However, it is worth noting that the increase in concentration at P15 is greater than P19, which is closer to the leak source.
4.2. CFD simulation results

Figure 7 shows the n-hexane diffusion process obtained by simulation. It can be found that the concentration is highest at the leak source. The n-hexane diffuses from the leaking point along the wall on the same side, and spreads to the opposite pump meanwhile. And after 2 hours of leakage, n-hexane diffused throughout the pump room. In the longitudinal direction of the pump room, the concentration is highest at the source of the leak. The further away from the leak source, the lower the concentration. In the lateral direction, the concentration on the leak source side is higher than the concentration on the opposite side. It is consistent with the results obtained by the experiment. For example, the response time and concentration increase of P18 on the same side are prior to that of P19 on the opposite side, although the distance between these two points and the leakage source are very close. It shows that n-hexane diffuses gradually from near to far from the leakage source. Due to the obstruction of the pump room wall, the diffusion is not synchronous in each direction. VOCs leaked at P406b are preferentially diffused along the wall due to wall shielding. It should be noted that CFD simulation shows that all six monitoring points respond to the leakage. In the experiment, P14 and P17 did not respond. This may be because the CFD model does not consider details such as trenches and door joints, and VOCs may escape from these parts to the outside.

Figure 7. Concentration distribution of n-hexane in the pump room at different times
5. Results
In view of the indoor VOCs diffusion, the standard gas with concentration of 6023ppm n-hexane was used to simulate the leakage lasting for 2h. The leakage process is analyzed by CFD method. It can be found that:

1) There is a background value of n-hexane concentration in the pump room, which means that potential leakage occur.
2) P36, P19, P18, and P15 were able to respond to the n-hexane leak, but the concentrations of P14 and P17 y did not increase.
3) The leakage sequence of simulation is the same as that obtained in the experiment. The concentration distribution is affected by the wall barrier and distance, and n-hexane will preferentially diffuse along the wall.

Acknowledgments
This work was supported by the National Key R&D Program of China(No.2018YFC0808600).

References
[1] Wang H L, Nie L, Li J, et al. (2013) Characterization and assessment of volatile organic compounds (VOCs) emissions from typical industries. Chinese Science Bulletin 58.7: 724-730.
[2] Wei W, Wang S X, Chatani S, et al.(2008) Emission and speciation of non-methane volatile organic compounds from anthropogenic sources in China. Atmospheric Environment, 42(20):4976-4988.
[3] YANG X.(2000) Monitoring and evaluation methods for fugitive emissions of industrial waste gas. Chinese Journal of Public Health Engineering, 32-40
[4] LIAO D H.(2017) Discussion on non Pollution Emission and Monitoring Technology of Industrial Waste Gas. Modern Industrial Economy and Informationization, 7(12):48-49
[5] US Environmental Protection Agency.(1980) Assessment of atmospheric emissions from petroleum refining. EPA-600 /2-80-075A-075D, Cincinnati, OH:US EPA, 1980.
[6] Hutchinson M, Oh H, Chen W H.(2017) A review of source term estimation methods for atmospheric dispersion events using static or mobile sensors. Information Fusion, 2017, 36: 130-148.