Gas Diffusion Model and Its Application based on CFD Theory

Yanbing Zhou 1, Beibei Liu 2,3, Qi Tang 4,*, Ping Qing 5, Han Li 5 and Xiaohong Zhang 2,3

1 Wuhan Deli Security Technology Co., Ltd., Wuhan, 430073, China;
2 School of Economics and Management, Beijing Institute of Petrochemical Technology, Beijing 102617, China;
3 Enterprise Development Research Center, Beijing Institute of Petrochemical Technology, Beijing 102617, China;
4 Faculty of Engineering, China University of Geosciences (Wuhan), Wuhan, 430074, China
5 School of Economics and Management, Huazhong Agricultural University, Wuhan, 430070, China

*Corresponding author e-mail: hudt@cug.edu.cn

Abstract. In order to reduce the loss and impact of the unexpected leakage of hazardous chemicals, the paper makes use of the computational fluid mechanics theory and applies the commercial software, FLOVENT, to imitate the steady state and transient state of six scenes of the diffusion scope and concentration change of NH3 and H2 in different wind directions and leak location; furthermore, it takes the simulated result as the basis to analyze the diffusion length and impact scope of the characteristic concentration, both of which will be the evidence for occupants evacuation.

Keywords: computational fluid mechanics, hazardous chemical, leak, diffusion, concentration.

1. Introduction
With the rapid economic development, enterprises are using more and more hazardous chemicals day by day. As many enterprises don’t do well in daily management on the storage, transportation and usage of a lot of hazardous chemicals, the leak of them, which can be caused by various factors, leads to fire, explosion and other accidents endlessly. In particular, there are always a lot of hazardous chemicals piled at the storage sites, where the accidents often cause greater negative influence on the society and environment. Therefore, the enterprise should enhance its daily control and management as well as take immediate measures to handle the leak and other accidents in order to minimize the loss and impact. Therefore, it’s needed to conduct the quantitative simulation on the leaked hazardous chemicals and then make up a proper emergency disposal scheme according to the simulated result, so as to reduce the accident loss to the minimum.

Since computer-aided engineering (CAE) tools have been developed prosperously throughout the world in recent years, computational fluid dynamics (CFD) which is one of the analytical techniques...
of CAE is applied to initiate the commercial software FLOVENT to imitate the steady state and instantaneity of six scenes of the diffusion scope and concentration change of NH\textsubscript{3} and H\textsubscript{2} in different wind directions and leak location (Spyros Sklavounos and Fotis Rigas, 2006; ZHONG Ying-jie, et al, 2003; ZHAO Xiang-di, et al, 2011; Gavelli F, et al, 2008) [1-4]; furthermore, it takes the simulated result as the basis to analyze the diffusion length and impact scope of the characteristic concentration, both of which will be the evidence for occupants evacuation.

2. Establishment of Analytical Model
Firstly, the simulation software of fluid mechanics is applied to simulate the maximum scope of influence when the concentration of the leaked gas in the 3D space of the factory reaches LC50, IDLH, ERPG-2 and TWA, respectively. The simulated result can be taken as the evidence for the enterprise to delimit the death zone, restricted zone, evacuation zone and polluted zone of the disaster prevention and emergence rescue. Moreover, the concentration changes with respect to time in the simulated result can be taken as the evidence for personnel evacuation (WANG Xue-qi, et al, 2013; Qiao Lin, 2012; HE Xiu-ying, 2007) [5-7].

2.1. Analysis process
In general, the analysis process of CFD is displayed as in Fig. 1.

2.2. Simulated Conditions
Firstly, the sit drawing is built into a 3D sit model by use of Pro/ENGINEER and FLOVETN (Ahn H T and Mikhail S, 2007; E Nourollah, 2009; CHENG Nai-wei, et al, 2012) [8-10]. Then, the concentration of NH\textsubscript{3} and H\textsubscript{2} at the site of the factory is simulated under the conditions of different leak locations, leak calibers, wind directions and wind speeds. Therefore, there are six events in all in this study (see Table 1). There are simulated in the ways of steady state and transient state, respectively in these six events. The simulation in steady state is done to know the maximum scope of influence of the leaked gas when it reaches the steady state, while the simulation in transient state is done to work out the time of rescue and distance of evacuation of the changes in concentration with respect to time. The transient state is simulated for 10min in total, with the result being output every 20s in the front 3min and every 30s in the later 7min. if the gas all out in 10min, flow velocity will be 77.5m/s and it leaks following the wind. Before the simulation of transient state is made, the pre-run of hr is set to made the wind field steady so as to have the model in a proper wind field.
Table 1. Simulated condition of various events

| Events | Location | Aperture/m | Gas   | Wind direction | Wind speed /m·s⁻¹ |
|--------|----------|------------|-------|----------------|------------------|
| 1      | Location 1 | 0.0254     | NH₃   | northeaster    | 2.14             |
| 2      | Location 1 | 0.0254     | NH₃   | southwester   | 1.10             |
| 3      | Location 2 | 0.1524     | NH₃   | northeaster    | 2.14             |
| 4      | Location 2 | 0.1524     | NH₃   | southwester   | 1.10             |
| 5      | Location 3 | 0.0254     | H₂     | northeaster    | 2.14             |
| 6      | Location 3 | 0.0254     | H₂     | southwester   | 1.10             |

In the setting of the computational domain, the model is simulated in the condition of 1atm and 20°C, in order to simulate the realistic influence of the surface boundary layer. Therefore, the height of the computational domain is assumed to be 200m and the direction of gravity is vertical to the ground (-Z), in order to calculate the two boundaries, set the wind speed and imitate the even direction of the air.

In the meantime, the medium is assumed to the air of 20°C. The flow field is supposed to be incompressible, with the flow being Newtonian fluid, viscosity coefficient fixed, thermal radiation unconsidered and buoyancy effect taken into account.

2.3. Analysis Grid
In order to gain the surface boundary layer effect, the mesh encryption is made close to the ground. To make the simulation of flow field effective, partial of the field area is encrypted. The grid of counted to be 816,715 in total.

3. Counting Process

3.1. Steady State Model
In this study, the air is the research object and the steady-state flow field the computing mode, so the applied governing equation is expressed in terms of tensor as follows: (Yoshihide Tominaga, et al, 2008) [11]

Equation of continuity:

\[
\frac{\partial \rho \mathbf{U}_j}{\partial x_j} = 0
\]  (1)

Equation of momentum:

\[
\frac{\partial}{\partial x_j} \left( \rho \mathbf{U}_i \mathbf{U}_j \right) =
- \frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial \mathbf{U}_i}{\partial x_j} + \frac{\partial \mathbf{U}_j}{\partial x_i} \right) \right]
\]  (2)

The speed and pressure are the sums of their respective time-average terms and disturbing terms, respectively.

\[
\mathbf{U}_i = \bar{U}_i + u
\]  (3)

\[
\bar{P} = P + p
\]  (4)

In the flow field, the average property of any variable is defined as follows:

\[
\Phi = \bar{\Phi} = \lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} \Phi \, dt
\]  (5)

The time average property of disturbing term
\[ \overline{\phi} = \overline{\psi} = 0 \]  
(6)

\[ \overline{\Phi \Psi} = \Phi \Psi + \overline{\phi \psi} \]  
(7)

\[ \overline{\phi \psi} = 0 \]  
(8)

The equation of the average property of disturbing terms with respect to time is as follows:

\[ \frac{\partial \rho U_j}{\partial x_j} = 0 \]  
(9)

\[ \frac{\partial}{\partial x_j} (\rho U_i U_j) = \]  

\[ -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \rho \mu u_i u_j \right] \]  
(10)

Where \( -\rho u_i u_j \) is called Reynolds stress item, which is an unknown term and solved in the turbulence model.

3.2. Turbulence Model

In this study the standard \( k - \varepsilon \) model of the turbulence model is adopted, which, based on the Boussinesq Approximation Reynolds stress, is expressed as (Sandra C K, et al, 2008) [12]:

\[ -\rho u_i u_j = \]  

\[ \mu_i \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left( \rho k + \mu_i \frac{\partial u_i}{\partial x_k} \right) \]  
(11)

Where the unknown term is \( \mu_i \), which is set as \( \mu_i = C_\mu \frac{k^2}{\varepsilon} \).

So \( k \) and \( \varepsilon \) can be gained from their respective transport equation, and the coefficient of each item is listed as follows.

\[ \frac{\partial}{\partial x_j} (\rho U_i k) = \]  

\[ \frac{\partial}{\partial x_j} \left[ \left( \mu_i + \frac{\mu_i}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] - \rho u_i u_j \frac{\partial U_i}{\partial x_j} - \rho \varepsilon \]  
(12)

\[ \frac{\partial}{\partial x_j} (\rho U_i \varepsilon) = \]  

\[ \frac{\partial}{\partial x_j} \left[ \left( \mu_i + \frac{\mu_i}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + \]  

\[ \frac{\varepsilon}{k} \left( - C_{\varepsilon 1} \rho u_i u_j \frac{\partial U_i}{\partial x_j} - C_{\varepsilon 2} \rho \varepsilon \right) \]  
(13)

\[ C_\mu = 0.09; \ \sigma_k = 1.0; \ \sigma_\varepsilon = 1.3; \ C_{\varepsilon 1} = 1.45; \ C_{\varepsilon 2} = 1.92. \]
4. Results analysis

In this study, the software FLOVENT is applied to imitate the steady state and instantaneous state of six scenes of the diffusion scope and concentration change of NH3 and H2 in different wind directions and leak locations; furthermore, it takes the simulated result as the basis to analyze the diffusion length and impact scope of the characteristic concentration, both of which will be the evidence for occupants evacuation (LENC Hai-qin, et al, 2012; Ye Dongfen, et al, 2012; LI Li, et al, 2013; ZHANG Yuan yuan, et al, 2013) [13-16].

As for NH3, we observe its scope of influence when its index concentration is 4837ppm (LC50), 300ppm (IDLH), 150ppm (ERPG-2) and 50ppm (TWA), respectively. As for H2, we observe its scope of influence when its index concentration is 8000ppm (1/5LEL).

In here, ERPG-2 is used to calculate the radius of the scope of influence, the lethal concentration 50% (LC50) to calculate the radius of the death zone, and the time weight average (TWA) to calculate the radius of the pollution zone.

4.1. Transient state simulation

Event One: wind flows in the direction of northeast at the speed of 2.14m/s; NH3 is leaked; and the accident happened at Site One. After an hour of pre-run, the wind field is almost steady.

Table 2. The position of the concentration of all indexes changing with respect to time (event one, source location:(-243, 72.2, 0.051), unit: m)

| Concentration | 4837 ppm | 300 ppm | 150 ppm | 50 ppm |
|---------------|----------|----------|----------|--------|
| Time/s        | x  | y   | z   | x  | y   | z   | x  | y   | z   | x  | y   | z   |
| 20            | -248 | 71.6 | 0.568 | -240 | 52.2 | 0.472 | -235 | 50.3 | 0.463 | -235 | 42.8 | 0.466 |
| 40            | -249 | 71.7 | 0.598 | -235 | 43   | 0.498 | -232 | 39.6 | 0.573 | -232 | 34.8 | 0.523 |
| 60            | -243 | 61.9 | 0.618 | -232 | 37.2 | 0.505 | -231 | 33.2 | 0.482 | -231 | 27   | 0.552 |
| 80            | -244 | 60.5 | 0.523 | -231 | 32   | 0.551 | -230 | 27.6 | 0.637 | -231 | 22.5 | 1    |
| 100           | -243 | 60.3 | 0.578 | -230 | 25.1 | 0.513 | -230 | 20.7 | 2.57  | -229 | 16.5 | 5.36 |
| 120           | -244 | 59.3 | 0.465 | -229 | 21.4 | 2.96  | -230 | 17.3 | 4.78  | -229 | 13.2 | 4.81 |
| 140           | -243 | 59   | 0.471 | -229 | 17.3 | 3.58  | -229 | 14.4 | 5.44  | -229 | 12.5 | 5.98 |
| 160           | -243 | 58.8 | 0.462 | -229 | 15.3 | 4.94  | -229 | 13.3 | 6.38  | -230 | 12   | 8.02 |
| 180           | -243 | 58.5 | 0.456 | -229 | 13.1 | 6.04  | -229 | 12   | 4.58  | -230 | 11.6 | 8.62 |
| 210           | -243 | 58.5 | 0.47  | -229 | 12.3 | 7.89  | -229 | 11.7 | 7.79  | -228 | 9.98 | 6.35 |
| 240           | -243 | 58.2 | 0.472 | -229 | 12.1 | 9.78  | -229 | 11.7 | 9.42  | -223 | 9.85 | 5.06 |
| 270           | -243 | 57.9 | 0.46  | -230 | 11.9 | 11.1  | -227 | 11.8 | 6.7   | -278 | 12   | 2.87 |
| 300           | -243 | 57.8 | 0.475 | -229 | 11.9 | 10.6  | -228 | 9.98 | 5.75  | -296 | 12.1 | 2.67 |
| 330           | -243 | 57.2 | 0.475 | -227 | 11.8 | 8.17  | -226 | 10   | 9.13  | -317 | 12.1 | 1.89 |
| 360           | -243 | 56.9 | 0.481 | -227 | 11.9 | 15.3  | -275 | 12.1 | 4.27  | -331 | 12.2 | 1.74 |
| 390           | -243 | 56.5 | 0.482 | -227 | 11.9 | 19.5  | -288 | 12.2 | 3.93  | -342 | 15.9 | 1.67 |
| 420           | -243 | 56.2 | 0.486 | -227 | 11.8 | 17.5  | -296 | 12.1 | 4.44  | -351 | 17.2 | 2.64 |
| 450           | -243 | 55.9 | 0.479 | -227 | 11.8 | 19.8  | -300 | 12.1 | 4.33  | -357 | 16.4 | 2.84 |
| 480           | -243 | 55.7 | 0.482 | -227 | 12.1 | 20.8  | -303 | 12   | 2.83  | -360 | 16.1 | 3.71 |
| 510           | -243 | 55.6 | 0.494 | -227 | 11.9 | 19.7  | -305 | 12.1 | 4.09  | -365 | 16.8 | 4.61 |
| 540           | -243 | 55.1 | 0.469 | -226 | 11.9 | 17.4  | -310 | 12.2 | 3.65  | -378 | 22.1 | 6.31 |
| 570           | -243 | 55.1 | 0.476 | -226 | 12.1 | 20.2  | -312 | 12.1 | 4.11  | -382 | 22.1 | 7.15 |
| 600           | -243 | 55   | 0.471 | -227 | 11.7 | 19.7  | -314 | 12.1 | 3.93  | -386 | 22.1 | 7.64 |
Table 3. The maximum influenced range of the concentration of all indexes changing with respect to time (event one, unit: m)

| Concentration | 4837 ppm | 300 ppm | 150 ppm | 50 ppm |
|---------------|----------|----------|----------|--------|
| Time/s        |          |          |          |        |
| 20            | 5.06     | 20.23    | 23.32    | 30.47  |
| 40            | 6.05     | 30.28    | 34.41    | 38.99  |
| 60            | 10.32    | 36.69    | 40.81    | 46.77  |
| 80            | 11.75    | 41.96    | 46.46    | 51.14  |
| 100           | 11.91    | 48.86    | 53.18    | 57.68  |
| 120           | 12.95    | 52.77    | 56.62    | 60.82  |
| 140           | 13.21    | 56.77    | 59.72    | 61.61  |
| 160           | 13.41    | 58.80    | 60.87    | 62.10  |
| 180           | 13.71    | 61.03    | 61.97    | 62.57  |
| 210           | 13.71    | 62.01    | 62.58    | 64.31  |
| 240           | 14.01    | 62.47    | 62.80    | 65.67  |
| 270           | 14.31    | 62.67    | 62.84    | 69.69  |
| 300           | 14.41    | 62.80    | 64.26    | 80.17  |
| 330           | 15.01    | 63.01    | 65.12    | 95.29  |
| 360           | 15.31    | 64.22    | 68.22    | 106.52 |
| 390           | 15.71    | 65.35    | 75.10    | 113.90 |
| 420           | 16.01    | 64.87    | 80.25    | 121.23 |
| 450           | 16.31    | 65.53    | 82.94    | 126.95 |
| 480           | 16.51    | 65.67    | 85.04    | 129.81 |
| 510           | 16.61    | 65.41    | 86.44    | 134.07 |
| 540           | 17.11    | 65.01    | 90.01    | 144.13 |
| 570           | 17.11    | 65.63    | 91.59    | 147.92 |
| 600           | 17.21    | 65.59    | 93.10    | 151.71 |

4.2. Imitation of steady state

In Table 4 are the maximum influenced ranges of the concentration of all indexes after the imitation of steady state; in figure 2 is the distribution diagram of the concentration of all indexes after the imitation of steady state. Compared with the imitation of transient state of the maximum influenced range and distribution diagram of the concentration of all indexes after 10min of leak, the imitation of the steady state is smaller in the maximum influenced range when the concentration is between 20 ppm and 4837 ppm, but its distribution range is bigger.

Table 4. The maximum range of the concentration of all indexes in the imitation of steady state (event one, unit: meter)

| Concentration | Location x | Location y | Location z | maximum influence distance |
|---------------|------------|------------|------------|---------------------------|
| 50            | -383       | 22.6       | 4.91       | 148.61                    |
| 150           | -349       | 29.5       | 1.75       | 114.29                    |
| 300           | -324       | 26.4       | 0.504      | 93.05                     |
| 4837          | -243       | 57.6       | 0.513      | 14.61                     |
Fig. 2 The maximum influenced range of the concentration of all indexes in the imitation of steady state (event one)

5. Conclusion
Quite different from the large-scale atmospheric diffusion, the diffusion of the leaked hazardous gas is affected not only by the storage status, storage condition and leak feature but also by the wind speed, wind direction and terrain, so the rule of the leakage diffusion can’t be described exactly with a single model. In this paper, only the hazardous gas diffusion model is preliminarily analyzed, but the research result can be used to help the enterprise to conduct the imitation of gas diffusion by using the flow field and model of 3D space, and the simulation result can be taken as the evidence for emergency rescue, so that appropriate measures can be carried out to minimize the loss when accidents happen.

References
[1] Spyros Sklavounos, Fotis Rigas. (2006) ‘Simulation of Coyote series trials-Part I: CFD estimation of non-isothermal LNG releases and comparison with box-model predictions’. Chemical Engineering Science, Vol. 61, pp. 1434-1443.
[2] ZHONG Ying-jie, DU Jin-yan, ZHANG Xue-mei. (2003) ‘CFD Technology and Application In Modern Industry’. Journal of Zhejiang University of Technology, Vol. 31, No.3, p. 284-289.
[3] ZHAO Xiang-di, YUAN Ji-wu, ZHAI Liang-yun, et al. (2011) ‘Leakage explosion consequence simulation based on CFD for liquid hydrocarbon tank farms’. OIL&GAS Storage and Transportation, Vol. 8, No.30, p. 634-651.
[4] Gavelli F, Bullister E, Kytomaa H. (2008) ‘Application of CFD (Fluent) to LNG spills into geometrically complex environments’. J Hazard Mater, Vol.159, No.1, p. 158-168.
[5] WANG Xue-qi, HAN Zhao-hui, SONG Dan-qing. (2013) ‘Simulation on Leakage Explosion Consequence of LPG Tank Farms Based on CFD’. Journal of Safety Science and Technology, Vol.9, No.2, p. 64-68.
[6] Qiao Lin. (2012) ‘the Research of Emergency Management System Based on the Gas Diffusion’. Chongqing University.
[7] HE Xiu-ying. (2007) ‘How to Improve the Liquid Hydrocarbon Spherical Tank Accident Emergency System Design’. Pet-nonchemical Safety Technology, Vol. 4, No. 23, p. 38-39.
[8] Ahn H T, Mikhail S. (2007) ‘Geometric Algorithms for 3D Interface Reconstruction’. Washington: Proceedings of 16th International Meshing Roundtable, p. 405-422.
[9] E Nourollah. (2009) ‘Simulation of Gas Pipeline Leakage Using the Characteristics Method’. 3rd International Conference on Electrochemical Process Simulation, Electrochemical Process Simulation, p. 119-130.

\[
\begin{array}{|c|c|c|}
\hline
\text{Con/ppm} & \text{Symbol} & \text{Distance/m} \\
\hline
50 & - & 148.61 \\
150 & - & 114.29 \\
300 & - & 93.05 \\
4837 & - & 14.61 \\
\hline
\end{array}
\]
[10] CHENG Nai-wei, SU Rui, ZHANG Yan-ling. (2012) ‘Study on 3D accident scene virtual simulation method of toxic gas diffusion’. 2012 (Shenyang) international academic symposium on safety science and technology, p. 476-479.

[11] Yoshihide Tominaga, Akashi Mochida, Ryuichiro Yoshie, et al. (2008) ‘AIJ guidelines for practical applications of CFD to pedestrian wind environment around buildings’. Journal of Wind Engineering and Industrial Aerodynamics, Vol. 96, No.10, p. 1749-1761.

[12] Sandra C K, De Schepper, Geraldine J, et al. (2008) ‘CFD modeling of all gas-liquid and vapor-liquid flow regimes predicted by the Baker chart’. Chemical Engineering Journal, Vol. 138, No.1-3, p. 349-357.

[13] LENC Hai-qin, SUN Hai-yan, WU Ze-hong, et al. (2012) ‘Research and implementation of diffusion simulation of hazardous bases leakage accidents’. Science of Surveying and Mapping, Vol. 37, No.4, p. 73-75, 78.

[14] Ye Dongfen, Ye Qiaolong, Luo Weichen. (2012) ‘A calculation approach and implementation of hazard chemical substance based on Gaussian diffusion model’. Computers and Applied Chemistry, Vol. 29, No.2, p. 195-199.

[15] LI Li, LIU Yongqian, YANG Yongping, HAN Shuang. (2013) ‘Short-term Wind Speed Forecasting Based on CFD Pre-calculated Flow Fields’. Proceedings of the CSEE, Vol. 33, No.7, p. 27-32.

[16] ZHANG Yuan yuan, ZHANG Ju-wei, SHANG Si-si, et al. (2013) ‘Research and Application on Diffusion Model of Leakage Gas’. Contemporary Chemical Industry, Vol. 42, No.4, p. 507-509.

[17] LI Yue, CHENG Shui-yuan, CHEN Dong-sheng, et al. (2013) ‘A renovated method for forecasting the consequences of the accidents by using the wind-changing direction with the time’. Journal of Safety and Environment, Vol. 13, No.2, p. 270-276.

[18] Tang Jing-yin. (2012) ‘Study on Designing and Implementing High Performance Atmospheric Dispersion Model and Source Back-Calculation Model for Hazardous Chemical Release’. Fudan University.

[19] Chen Cheng, Zhang Jingyi, Tony Qing, et al. (2013) ‘GIS-Based Desktop Emergency Drilling System’. Computer Applications and Software, Vol. 30, No.2, p. 242-244, 252.