Research on Fast Estimate Model for Concentration's Distribution of Chlorine Leakage of Moving Tank Car

Jinrong Zhang, Ling Wu, Haoxue Liu, Wenxuan Wang, Ping Li

Chang'an University, Xi'an, Shaanxi, 710064, China

Corresponding author is Jinrong Zhang

Abstract

In order to quickly estimate the toxic gas concentration distribution of liquid chlorine in moving tank car after leakage and predict possible outcome (scope and degree of the influence) of hazardous gas, the characteristics of liquid chlorine leakage in moving tank was analyzed in this paper, and then dynamic changing leaking speed, the tanker's moving direction and velocity were introduced according to the defects of Gaussian model, and finally the model of toxic gas diffusion after liquid chlorine leakage in moving tank car was build. The new model was simulated and analyzed by MATLAB. The simulation results showed that: this model can rapidly and effectively calculate toxic gas concentration distribution in different places and different time after leakage of liquid chlorine in moving tanker, and it can also simulate the dynamic transformation process of the toxic gas and provide technical support and theoretical basis for the prediction and assessment at the scene of the toxic gas leakage accident.

Keywords: MOVING TANK CAR, LEAKAGE OF LIQUID CHLORINE, CONCENTRATION DISTRIBUTION, GAUSSIAN MODEL

1. Introduction

Considering the convenience of the storage and transportation, usually chlorine is liquefied in low temperature with high pressure and stored in the tank or other high pressure container. There are some problems in most of tank cars after long-time use, such as the clamping parts of the tank car or safety accessories would loose because of the bumpy road or other unavoidable circumstances, individual parts was damaged and so on. If the driver does not often check vehicles' fault conditions and keep the tank car continue to run, the liquid chlorine in tank car will leak continuously. Leakage accident was not only a serious threat to human life but also to various spheres, such as water, air and soil. So appropriate emergency measures are needed timely after the accident to minimize the accident loss. But the precondition of these decisions is the accurate and fast estimation of liquid chlorine leakage pollution range, delimit warning zone and determine the scope of the evacuation of nearby residents. Therefore, it's necessary to calculate the toxic gas concentration distribution in the air during or after chlorine leakage of moving tank car, and it is the precondition and foundation of a series of emergency measures [1,2].

2. Analysis of Model

2.1. The Gaussian Model

At present, gas diffusion model such as Gaussian, BM model, Sutton model and 3D finite element model (FEM3) are widely applied [3]. Among them, Gaussian model was widely used due to mature, simple and efficient, and the calculation results agreed well with test value [4]. Gaussian model belonged to non heavy gas cloud diffusion model which was suitable for the diffusion of point source. It was divided into Gaussian puff model and Gaussian plume model. The former was suitable for instantaneous leakage and diffusion which meant leakage time was shorter than the diffusion time; the latter was suitable for continuous point source leakage and diffusion which meant leakage time and diffusion time was equal to or leakage time is longer than the diffusion time [5,6].

2.2. The Characteristic of Liquid Chlorine Leakage from Moving Tank

The process of liquid chlorine leakage from moving tank car is complex, and it can be roughly divided into 3 stages: the first stage was the continuous leakage in the driving process which started from the form of continuous leakage source and terminated when the driver found the danger and stopped immediately. In this process, the liquid showed continuous leakage and vehicle kept running continuously. The leaked material formed a linear concentration field along the road. The second stage was continuous leakage stage in the tank car's parking process which started when the driver found the danger and stopped immediately and terminated when the leakage was stopped or tank material was completely leaked. In this process, the continuous leakage of moving point source turned to continuous leakage of static point source. The last stage was the concentration decaying stage which started from the stop of the leakage and terminated after the danger has passed. In this process, the concentration constantly decayed. The duration of static point source in the second stage was usually short and the influence to the concentration of toxic gases in the surrounding region was small, so this stage could be ignored for the convenience of calculation in this paper.

The leakage of liquid chlorine from moving tank was continuous with limited storage, small spillage per unit time and not too long leakage time in the moving process of the tank. After the leakage of the gas, the outside air came in and the temperature went up. As a result, chlorine was quickly diluted by the air, the density difference between cloud of gas and air gradually decreased and the steady flow diffusion gradually showed dominance [7]. Therefore, in this leakage situation, considering the short time of gravity influence, it can also be calculated as neutral gas.

Compared to the common leakage from high-pressure storage tank of chemical plant or gas emissions from elevated point source [8-11], leakage of liquid chlorine from moving tank car mainly has the following features: firstly, the source of the leak was a moving point source, so the concentration distribution of chlorine gas in the air was related not only to wind speed, surface roughness, atmospheric stability, leakage rate and other factors outside, but also to the moving direction and speed of the vehicle; secondly, it is not a simple instantaneous leakage or continuous leakage, and the leakage time was typically between instantaneous and continuous leakage; thirdly, the Gaussian model assumed the leakage intensity Q was constant which was not consistent with the actual situation. The leakage intensity of liquid chlorine from tank showed dynamic changes with diffusion time. Therefore, the concentration distribution of toxic substance after liquid chlorine leakage from tank car could not be directly calculated by Gaussian puff model or the Gaussian plume model. In this paper the Gaussian model was improved based on the above characteristics.

3. The Improved Gaussian Model

The mathematical expression of Gaussian puff model [12,13] was showed as follows:

$$C(x,y,z)=\frac{Q}{(2\pi)^{\frac{3}{2}}\sigma_x\sigma_y\sigma_z}\exp\left[-\frac{(x-ut)^2}{2\sigma_x{}^2}\right]\exp\left(-\frac{y^2}{2\sigma_y{}^2}\right)\left\{\exp\left[-\frac{(z-H)^2}{2\sigma_z{}^2}\right]+\exp\left[-\frac{(z+H)^2}{2\sigma_z{}^2}\right]\right\} \quad (1)$$

Where,

$C(x,y,z)$: Gas concentration at a single point (x,y,z) in space, kg/m^3;

Q : Total weight of the releasing gas, kg;

$\sigma_x,\sigma_y,\sigma_z$: Diffusion standard deviation of leakage gas in the direction of x,y,z, m;

u: The average wind speed, m/s;

H : Height of valid source (the sum of emission height and lifting height), m.

Smoke emitted continuously from point sources can be regarded to be composed by numerous smoke units with infinite short time interval in order. Starting from the drain time, each puff moved along the direction of wind, the process of a puff diffusing was shown in Fig.1. The peak concentration axis was chosen as the coordinate axis of smoke diffusion to measure rate and scope of this pollutant diffusion. The average smoke flow of the whole sampling period was consisted of many instantaneous smoke flows.

The puff emitted at the moment $\hat{t}$ was researched. According to the statistical theory of diffusion, the 3D Gaussian diffusion equation of it in boundary conditions was shown as follows:

$$C_i(x,y,z)=\frac{Q_i}{(2\pi)^{\frac{3}{2}}\sigma_x\sigma_y\sigma_z}\exp\left\{-\frac{\left[x-u(t-\hat{t})\right]^2}{2\sigma_x^{2}}\right\}\bullet\exp\left(-\frac{y^2}{2\sigma_y^{2}}\right)\left\{\exp\left[-\frac{(z-H)^2}{2\sigma_z^{2}}\right]+\exp\left[-\frac{(z+H)^2}{2\sigma_z^{2}}\right]\right\} \tag{2}$$

Where,

$u(t-\hat{t})$: Distance of the puff transmission in the downwards direction;

The horizontal projection of leakage starting point was chose as the origin. The counting started from the start of leakage.

The weight of single puff emitted at the moment of $\hat{t}$ in the moving process of the tank car was $q(\hat{t})d\hat{t}$. The distance of the tank car was $v\hat{t}$ at this moment and the coordinates of leak point was $(v\hat{t}\cos\varphi, v\hat{t}\sin\varphi, H)$. Puff's moving direction was influenced by the wind, so the coordinate of the center of the puff was $(u(t-\hat{t})+v\hat{t}\cos\varphi, v\hat{t}\sin\varphi, H)$ at the moment of t. Then the concentration in (x,y,z) produced by this puff can be obtained after the coordinate transformation of the diffusion equation of Gaussian puff model.

$$dc=\frac{q(\hat{t})d\hat{t}}{(2\pi)^{\frac{3}{2}}\sigma_x\sigma_y\sigma_z}\exp\left\{-\frac{\left[x-u(t-\hat{t})-v\hat{t}\cos\varphi\right]^2}{2\sigma_x^{2}}\right\}\cdot\exp\left[\frac{-(y-v\hat{t}\sin\varphi)^2}{2\sigma_y^{2}}\right]\cdot\left\{\exp\left[\frac{-(z-H)^2}{2\sigma_z^{2}}\right]+\exp\left[\frac{-(z+H)^2}{2\sigma_z^{2}}\right]\right\} \tag{3}$$

Where,

$q(\hat{t})$: Leakage velocity at the moment of $\hat{t}$, kg/s.

v: Speed of the tank car, m/s;

φ: The angel between wind direction and the movement direction of the tank car, $(\varphi \le 90°)$;

Because the concentration of continuous point source in the place of (x,y,z) can be considered as the total effect of pollutant concentration within the period of tr of continuous release in this point, which was regarded as the sum of the emission of instantaneous discharge at the interval of Δt, so the integral can be obtained based on the equation (3). The total concentration of the point (x,y,z) of gas leakage in the period $(0,tr)$ caused by diffusion could be obtained.

$$C=\int_0^{tr} dc \tag{4}$$

Where,

tr: The total movement time in the leakage process, s.

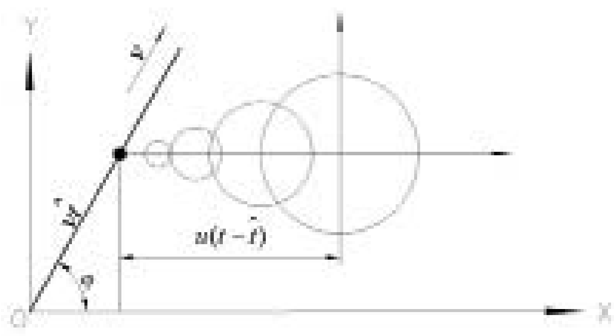

Figure 1. Diagram of single puff diffusion

4. The Standard Deviation of Diffusion of The Model

The standard deviation of Briggs diffusion was used in this paper as shown in Table 1 where A, B, C, D, E and F represented that the atmospheric stability's extreme instability, moderate instability, weak instability, neutral conditions, weak stability and moderate stability respectively [14].

Usually, standard deviation of diffusion decreased with the increase of atmosphere stability.

5.Application Example

The weight of tank car transported was 25 tons. The tank car travelled at a constant speed of 40 km/h at the direction of 30 degrees along with the positive direction of axis X. The speed of initial liquid chlorine leakage from tank car was 6.5 km/s which gradually decreased with the decrease of tank pressure [15] showed in the equation (5); the leak point was 1m high from the ground, and the leakage lasted 300s from the start to the end of the leakage. X axis was on the leeward, with the speed of wind being 2 m/s. The atmospheric stability was the B level and the terrain was open and flat; according to the " Allowable concentration of toxic substances in workplace air", the maximum allowable concentration (MAC) of chlorine in the air of workplace was 1 mg/m^3, immediate danger to life or health (IDLH concentration) was 30 mg/m^3, median lethal concentration (LC50) was 850 mg/m^3.

$$q(t)=q_0\left(1-0.007t^{0.5}\right) \tag{5}$$

After the leakage of liquid chlorine from moving tank car, simulation of hazard distance of gas in different time was shown in Fig.2 and Fig.3:

Table 1. Parameters of Briggs diffusion

Atmospheric stability	$\sigma_x=\sigma_y$	σ_z
A	$0.22x(1+0.0001x)^{-1/2}$	$0.20x$
B	$0.16x(1+0.0001x)^{-1/2}$	$0.12x$
C	$0.11x(1+0.0001x)^{-1/2}$	$0.08x(1+0.0002x)^{-1/2}$
D	$0.08x(1+0.0001x)^{-1/2}$	$0.06x(1+0.0015x)^{-1/2}$
E	$0.06x(1+0.0001x)^{-1/2}$	$0.03x(1+0.0003x)^{-1/2}$
F	$0.04x(1+0.0001x)^{-1/2}$	$0.16x(1+0.0003x)^{-1/2}$

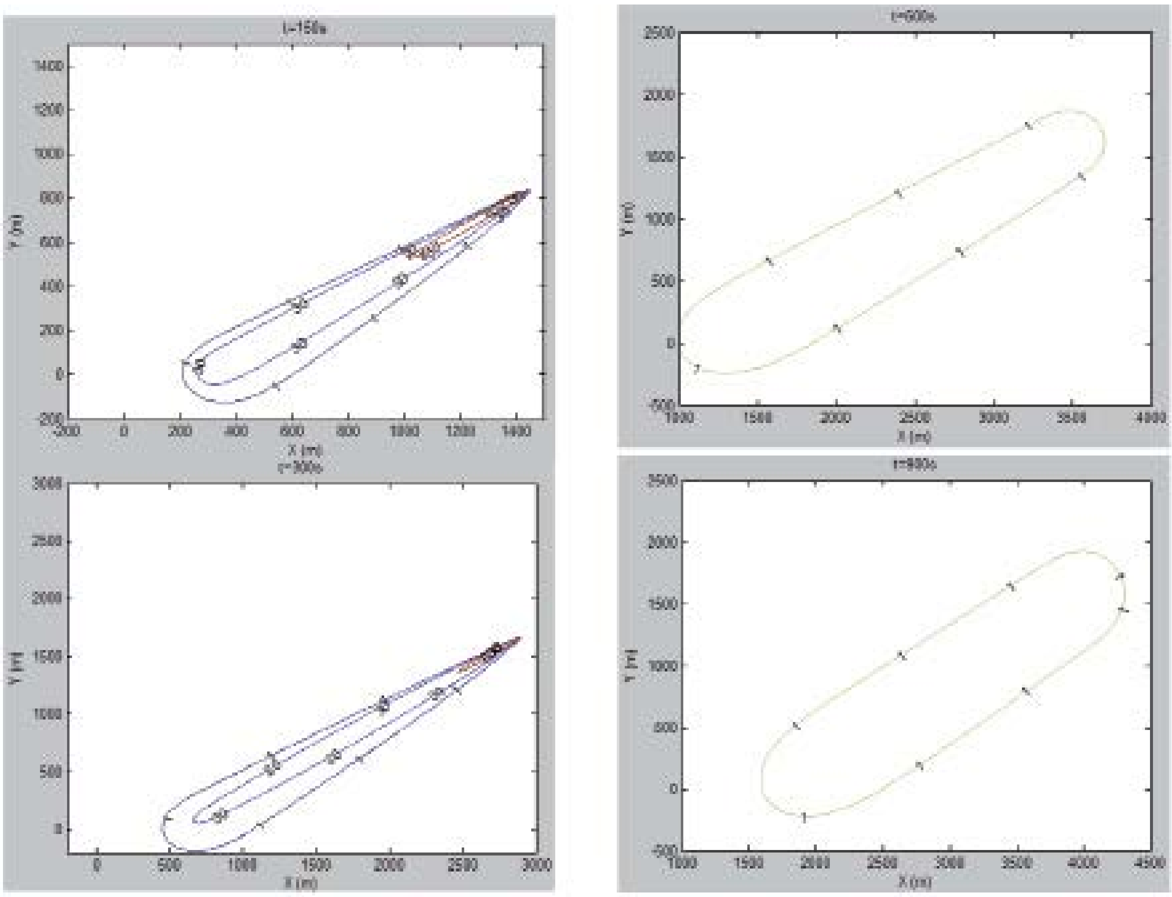

Figure 2. Contour curves of ground concentration in different time

(1) The diffusion of toxic gas was related to the moving direction of the tank car and to direction of leeward.

(2)When $t=150s$, the maximum concentration $7.4975\times104\,mg/m^3$ was reached at the coordinate of (1410,810,0) which was higher than LC50; when $t=300s$, the maximum concentration $7.3317\times104\,mg/m^3$ was reached at the coordinate of (2850,1640,0) which was higher than LC50 ; when $t=600s$, the maximum concentration $25.78\,mg/m^3$ was reached at the coordinate of (3340,1580,0) exceeding MAC , when $t=900s$, the maximum concentration6.67 mg/m^3 was reached at the coordinate of (3800,1500,0) exceeding MAC.

(3)At the period of $0\sim300s$, due to the decline of the leakage rate, the maximum concentration of gas diffusion values decreased slowly, but the influence scope of concentration gradually increased when time increased. After 300s, because of the stop of leakage, the maximum concentration value of gas diffusion

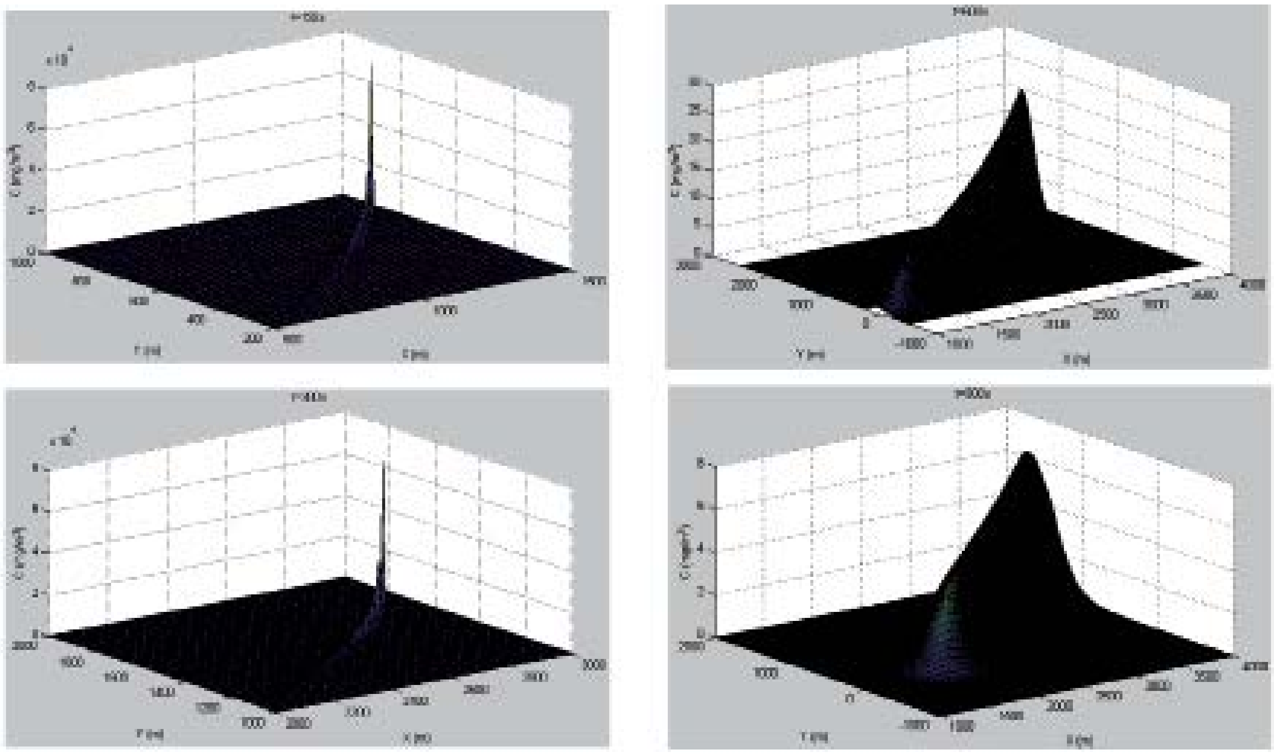

Figure 3. The ground concentration distribution in different time

decreased rapidly, and the influence region of concentration increased first and then shrank.

After the leakage accident, in order to take appropriate emergency measures we focused on the maximum concentration and time range possibly producing harm to some sensitive points. Assuming there were four sensitive points A, B, C and D on the flat ground with the coordinates (500,200,0), (1000,400,0), (1500,700,0) and (2000,900,0). Concentration curve with time was shown in Fig.4: Initial concentration of chlorine at the point A was 7.18×10^{-6} mg/m^3; the maximum value 501.1 mg/m^3 was reached when $t=103s$, and exceeding IDLH for 103s and MAC for 207s; initial concentration of chlorine at B point was 3×10^{-6} mg/m^3; the maximum value 125.3 mg/m^3 was reached when $t=212s$, exceeding IDLH for 127s and MAC for 322s; the maximum concentration of point C and point D were 83.2 mg/m^3 and 59.1 mg/m^3. But the duration of the concentration that exceeded MAC at the point D was much longer than the duration at point A, B and C, up to 384s. So we can conclude that the maximum concentration of chlorine value decreased in the direction of A,B,C and D, but the duration of the concentration that exceeded IDLH and MAC was gradually increasing.

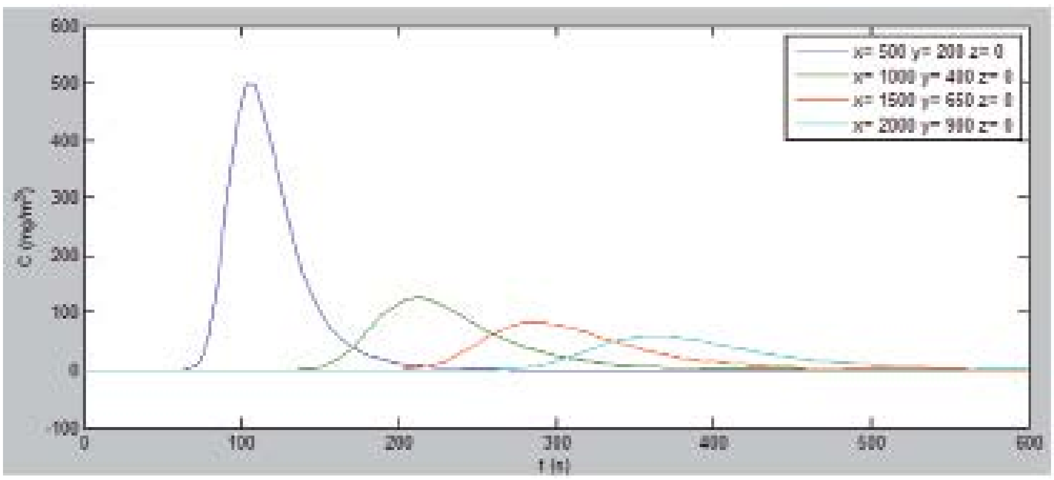

Figure 4. Concentration curves of sensitive points

Conclusion

(1) The fast method to estimate the concentration distribution of moving tank car toxic gas leakage accident based on the modified Gaussian model can estimate concentration of pollutants and the duration of harm quickly in emergency treatment such as chlorine leakage, according to tank car's direction of movement, speed, toxic gas leakage rate, wind speed and atmospheric stability and so on.

(2)There are many other uncertain factors affecting gas diffusion process, such as the changing wind speed, wind direction, complex terrain and so on. However, the model was built after being approximated and simplified which caused only an estimate value. Therefore, in the analysis of leakage accidents' consequences, corresponding modification should be made according to the actual situation.

References

1. LI Shi-wei, WANG Jian-qiang, ZENG Junwei. Improved Gaussian estimate model algorithm for radioactive gas diffusion. Application Research of Computers, 2012, 29(1):123-126
2. WANG Kongsen. Study on the method of fast estimating the concentration's distribution of chlorine leakage based on the Gaussian model. Journal of Safety Science and Technology,2012,8(9):33-37
3. Ghermandi, Grazia. Model comparison in simulating the atmospheric dispersion of a pollutant plume in low wind conditions. International Journal of Environment and Pollution,2012,48:69-77
4. Leeuwen CJV, Vermeire TG. Risk Assessment of Chemicals: An Introduction: 2 edition. Springer;2007.
5. Leelssy, Ádám. Dispersion modeling of air pollutants in the atmosphere: a review. Central European Journal of Geosciences, 2014,6:257-278
6. HE Ning, WU Zong-zhi, ZHENG Wei. Simulation of an improved Gaussian model for hazardous gas diffusion. Journal of Basic Science and Engineering, 2010, 18(4) : 571-580.
7. Bauer, Timothy J. .Comparison of chlorine and ammonia concentration field trial data with calculated results from a Gaussian atmospheric transport and dispersion model. Journal of Hazardous Materials, 2013, 254:325-335
8. M. A. Mcbride, A. B. Reeves, M. D. Vanderheyden, et al. Use of advanced techniques to model the dispersion of chlorine in complex terrain. Process Safety and Environmental Protection, 2001, 79 : 89 ～ 102
9. Aurelia Dandrieux, Gilles Dusserre, James Ollivier. Small scale field experiments of chlorine dispersion. Journal of loss prevention in the process industries, 2002, 15 : 5 ～ 10
10. WANG Dong-dong, LIUMao, LI Jian-feng, HE Wei-feng. CFD simulation of small-scale chlorine dispersion. Journal of Safety and Environment, 2008,8:126-130
11. Hanna, Steven R. CFD model simulation of dispersion from chlorine railcar releases in industrial and urban areas. Atmospheric Environment,2009,42:262-270
12. Ristic, Branko. Achievable accuracy in parameter estimation of a Gaussian plume dispersion model. IEEE Workshop on Statistical Signal Processing Proceedings,2014,209-212
13. Serena, P. On the accuracy of the Gaussian nonlinear model for dispersion-unmanaged coherent links. IET Conference Publications, 2013,2013:723-725
14. ROBINS A. Wind tunnel dispersion modeling some recent and not so recent achievements. Journal of Wind Engineering and Industrial Aerodynamics, 2003, 91 : 1777-1790.
15. Liu Kaizheng. Reaserch on Diffusion Model and Risk Estimation for Leakage of Toxic Gas Road Transportation by Tank Cars. Ph.D. thesis. Chang'an University,2011,101-105