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The Simulation Platform of Dangerous Chemical Gas Diffusion based on Gauss Plume Model

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With the development of chemical industry, petrochemical industry has already occupied an unshakable position in the national economy. Because of its unique advantages, the chemical industry park has greatly facilitated the development of various chemical enterprises. However, with the increase of enterprises in chemical industry parks, the safety management and emergency response of industrial parks become more and more important. Hazardous chemical gas leakage may occur in the production, storage and transportation of chemical products. Once the leakage occurs, it not only pollutes the environment, but also causes a large area of human and livestock poisoning. Therefore, it is very important to study the rule of chemical gas diffusion and make effective simulation. Through the accurate prediction of dangerous chemical gas diffusion, it can provide theoretical basis for the formulation of emergency plans, which can minimize the loss of life and property. In this paper, the research status of leakage and diffusion of dangerous gases at home and abroad is reviewed. Based on the improved Gauss plume model, a diffusion prediction simulation platform for hazardous chemical gas is proposed. Firstly, the several commonly used gas diffusion prediction models are introduced briefly. Secondly, a new prediction model based on Gauss plume model is proposed for the continuous leak of chemical gas. Finally, combined with the geographic information system (GIS), simulation experiment is carried out based on the improved prediction model. The experimental results show that the improved Gaussian plume model is more consistent with the actual diffusion.

1. Introduction

With the development of economic globalization, the competition between countries is becoming fiercer. In the national economic structure, petrochemical industry has already occupied an unshakable position in the national economy (Zhang, 2016). The relationship between the petrochemical industry and human beings is becoming closer. A wide range of chemical products are produced and consumed, most of which are dangerous chemicals. The chemical products with special properties have high requirements for production, storage and transportation. It is easy to cause leakage accidents due to uncertainties in human or environmental factors (Li, 2013). Once a leak occurs, the dangerous chemicals eventually turn into gases that diffuse in the atmosphere. If the spread can not be controlled in a timely and effective manner, it may cause incalculable harm to the surrounding residents (Peng et al., 2016).

With the attention of some countries to the speard of dangerous chemicals gases, many research teams have begun to build gas diffusion models through gas diffusion experiments. The gas diffusion model can describe the diffusion behavior of leakage in the atmosphere, and there are many gas diffusion models such as Sutton model, Gaussian plume model, Gauss puff model and so on. Generally speaking, the research methods of gas diffusion model are divided into two kinds. One approach is to build new models based on diffusion equations and boundary conditions, while a more common approach is to improve existing models. In order to solve the applicability of the existing models in the dynamic diffusion process, Wu and Long (2005) proposes a dynamic diffusion model based on differential diffusion equation and boundary conditions, which can evaluate the diffusion range of a chemical product after an instantaneous leak. Nevertheless, the model has too many limitations, so it is still at the theoretical stage. Briant (2011) improves the Gauss plume model and applies it to the concentration monitoring of exhaust gas pollutants in road traffic, which reduces the error of the model when the wind is not parallel to the road surface. Arystanbekova (2004) applies Gauss plume model to the

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concentration calculation of gas diffusion by using the Cartesian coordinate system to take the place of the single rectangular coordinate system. At the same time, his research also modifies the effective height of cloud. In view of the fact that liquid ammonia is easy to leak in the tank, Sun (2011) improves the Gauss puff model by taking into account the pressure change caused by leakage of liquid ammonia.

With the innovation and application of Internet technology, the integration of diffusion simulation theory and computer technology has become an inevitable trend. The emergence of geographic information system (GIS) accelerates the integration of GIS and real-time dynamic simulation, which greatly promotes the application of research results (Yi et al., 2008).

In this paper, the research status of leakage and diffusion of dangerous gases at home and abroad is reviewed. Based on the improved Gauss plume model, a diffusion prediction simulation platform for hazardous chemical gas is proposed. Firstly, the several commonly used gas diffusion prediction models are introduced briefly. Secondly, a new prediction model based on Gauss plume model is proposed for the continuous leak of chemical gas. Finally, combined with the geographic information system (GIS), simulation experiment is carried out based on the improved prediction model. The experimental results show that the improved Gaussian plume model is more consistent with the actual diffusion.

2. Gas diffusion model

There are many models about gas diffusion. After continuous development, there are several mature models of gas diffusion, and they are Sutton model, Gauss plume model, Gauss puff model, and FEM3 model. The Sutton model uses turbulent diffusion statistical theory to deal with turbulent diffusion problems. The model has a large error when simulating flammable gas diffusion. The FEM3 model is applicable to the diffusion of heavy gases for continuous source, and its simulation is more difficult because of the extensive calculation. Gauss model is relatively mature because of long-term theoretical proof and sufficient experimental data.

2.1 Sutton model

The Sutton model is mainly realized by means of the statistical theory of turbulent diffusion when the concentration distribution accords with the normal distribution. Because of a large number of experimental data, the application of Sutton model is very common. However, the model is not suitable for the simulation of flammable gas diffusion, otherwise there will be a great error. The model has been widely used in the field of environmental protection. The concentration distribution formula of the model is as follows.

$$c(x,y,z) = \frac{G \cdot e^{-\frac{y^2}{\lambda_y^2 \cdot x^{2-n}}}}{\pi \cdot \lambda_y \cdot \lambda_z \cdot V} \cdot [e^{-\frac{(z-h)^2}{\lambda_z^2 \cdot x^{2-n}}} + e^{-\frac{(z+h)^2}{\lambda_z^2 \cdot x^{2-n}}}] \tag{1}$$

In the formula, *G* refers to the amount of gas leakage, while *V* means the wind speed of the surrounding environment. λ_y and λ_z are respectively the diffusion coefficients on *y* axes and *z* axes.

$$\lambda_y = \sqrt{\frac{c^2 (v_y t)^{2-n}}{2}} \tag{2}$$

$$\lambda_z = \sqrt{\frac{c^2 (v_z t)^{2-n}}{2}} \tag{3}$$

The Sutton model is very poor in describing the diffusion of gases with flammable properties, and so it does not have very strong applicability.

2.2 Gaussian plume model

Gauss plume diffusion model is based on advection diffusion differential equation. When the wind speed and turbulent diffusion coefficient are relatively stable, the advection diffusion differential equation agrees with the standard normal distribution. This model has been widely used in non heavy gas cloud diffusion.

We assume that in the three-dimensional coordinate system, the origin is the emission point and the forward direction of *X* axis is the direction of the wind. In addition, *Z* axis is perpendicular to the horizontal plane. The coordinate system of Gauss model is as follows.

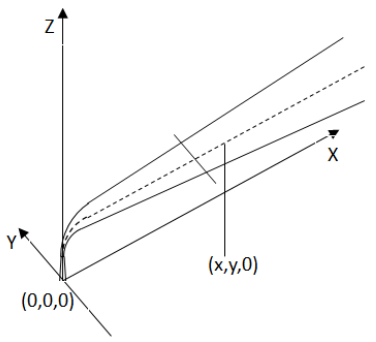

Figure 1. Coordinate system of Gauss model

Based on the assumption of the normal distribution, we can deduce that the concentration function of the leakage gas at any point below the direction of wind.

$$P(x,y,z)=f(x)\cdot\frac{1}{e^{ay^2}}\cdot\frac{1}{e^{bz^2}} \tag{4}$$

According to the theory of probability statistics, the expression of variance can be written as follows.

$$\begin{cases}\mu_y^2=\dfrac{\int_0^{\infty} y^2\cdot X\cdot dy}{\int_0^{\infty} X\cdot dy}\\ \mu_z^2=\dfrac{\int_0^{\infty} z^2\cdot X\cdot dz}{\int_0^{\infty} X\cdot dz}\end{cases} \tag{5}$$

Thus we can get the integral formula of the leakage velocity.

$$Q=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} v\cdot X\cdot dy\cdot dz \tag{6}$$

In the formula, μ_y and μ_z respectively indicate the standard deviation of the leakage gas in *Y* axis and *Z* axis, and v is the average wind speed of the surrounding environment. In conjunction with formula 4 and 5, we can obtain the following formula.

$$\begin{cases}a=\dfrac{1}{2\mu_y^2}\\ b=\dfrac{1}{2\mu_z^2}\end{cases} \tag{7}$$

Bring formulas 4 and 7 into formula 6, we can get the functions.

$$f(x)=\frac{Q}{2\pi v\mu_y\mu_z} \tag{8}$$

Finally, the formula for calculating the concentration is obtained as follows.

$$P(x,y,z)=\frac{Q}{2\pi v\mu_y\mu_z}\cdot\frac{1}{e^{(\frac{y^2}{2\mu_y^2}+\frac{z^2}{2\mu_z^2})}} \tag{9}$$

2.3 Gaussian puff model

The Gauss puff model is suitable for the scene that the Gas clouds are formed in a short time and the diffusion process lasts a long time. The model is based on the assumption that the leakage source is an independent cloud whose volume increases both in horizontal and vertical directions. Since the model can only be applied to transient diffusion, the practical application is relatively few. Gauss puff model is mainly divided into two kinds, one is suitable for the case of stable wind source, and another is suitable for no wind.
The formula with stable wind source is as follows.

$$P(x,y,z,t-t_i)=\frac{2Q}{(2\pi)^{3/2}\mu_x\mu_y\mu_z}\cdot e(-\frac{(x-v(t-t_i))^2}{2\mu_x^2}-\frac{y^2}{2\mu_y^2}-\frac{H_e^{\ 2}}{2\mu_z^2}) \tag{10}$$

By accumulating the above formula, we can obtain the following formula.

$$P(x,y,z,t)=\sum_{i=1}^{n}P(x,y,z,t-t_i) \tag{11}$$

The formula with no wind source is as follows.

$$P(x,y,z,t)=\frac{2Q}{(2\pi)^{3/2}\mu_x\mu_y\mu_z}\cdot e(-\frac{x^2}{2\mu_x^2}-\frac{y^2}{2\mu_y^2}-\frac{H_e^{\ 2}}{2\mu_z^2}) \tag{12}$$

The flow chart based on Gauss puff model is as follows.

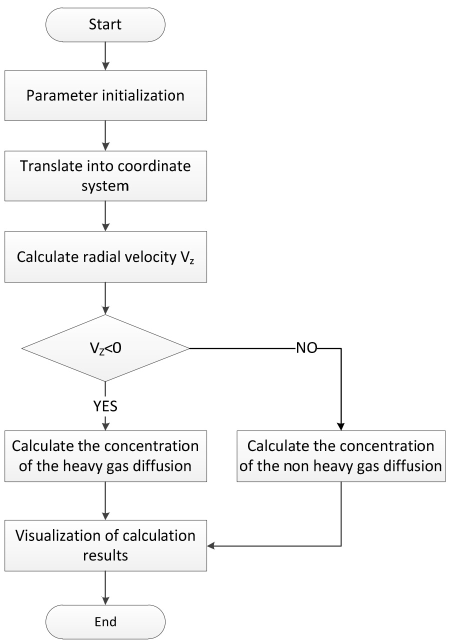

Figure 2. Flow chart based on Gauss puff model

3. Improved Gauss plume diffusion model

Gauss plume model has good simulation effect on the diffusion of gas when ambient turbulence and wind speed are stable. Because the premise of the model is that all the conditions are within the ideal and controllable range, so it can be seen as an idealized model. In this paper, the Gauss model is selected as the prototype of the diffusion simulation system, and the environmental parameters under various simulation conditions are analyzed. By introducing the thermal lifting action and the surface reflectance parameters, we optimize the Gauss plume model, which can improve the simulation accuracy.

3.1 Introduction of thermal lifting

Gauss plume model does not consider the effect of thermal lifting at the initial stage of gas leakage, which leads to the deviation in calculation of the effective source height. The effective source height of leaked

chemical gas is the distance from the center of the gas cloud to ground when the diffusion of the gas cloud is stable, which includes the height of the source of leakage and the height of the cloud lifting.
The formula of effective source height considering the ground uplift is as follows.

$$H = H_0 + \Delta h \tag{13}$$

Then the Briggs formula is used to obtain the final value of *Δh*

$$\Delta h = 30\left(\frac{F}{v}\right)^{\frac{3}{5}} \tag{14}$$

Where, F is the relation function of temperature and leakage velocity. Eventually, we get the effective source height of the leak source.

$$H = H_0 + 30\left(\frac{F}{u}\right)^{\frac{3}{5}} \tag{15}$$

3.2 Introduction of ground reflection

Gauss plume model does not consider the effect of surface reflection on concentration. When the gas particles are large enough, the reflection of the ground should be considered. In three-dimensional space, the concentration of point $R(x, y, z)$ should be considered as the sum of the concentration ignoring the action of the ground and concentration produced by the reflection of the ground. Assuming that the ground reflection coefficient is ε, and the diagrammatic sketch of ground reflection is shown in figure 3.

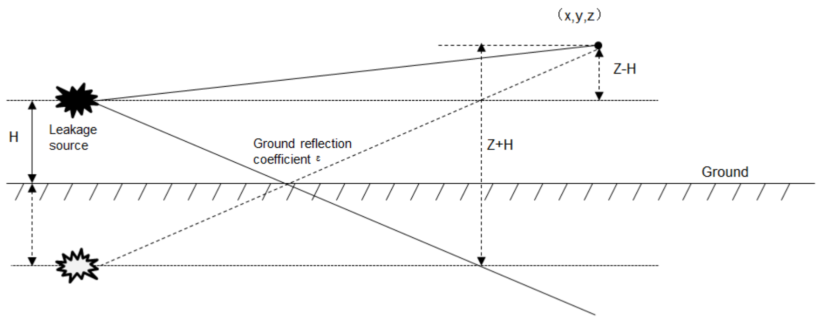

Figure 3. The diagrammatic sketch of ground reflection

The concentration formula caused by the ground reflection coefficient is as follows.

$$P(x,y,z) = \varepsilon \cdot \frac{Q}{2\pi v \mu_y \mu_z} \cdot \frac{1}{e^{(\frac{y^2}{2\mu_y^2} + \frac{(z+h)^2}{2\mu_z^2})}} \tag{16}$$

Considering the concentration ignoring the action of the ground and concentration produced by the reflection of the ground, we can get the concentration formula.

$$P(x,y,z) = \frac{Q}{2\pi v \mu_y \mu_z} \cdot \left[\varepsilon \frac{1}{e^{(\frac{y^2}{2\mu_y^2} + \frac{(z+h)^2}{2\mu_z^2})}} + (1+\varepsilon) \frac{1}{e^{(\frac{y^2}{2\mu_y^2} + \frac{(z-h)^2}{2\mu_z^2})}} \right] + \tag{17}$$

4. Simulation experiment and result analysis

In order to verify the simulation effect of the improved prediction model, we introduce GIS into the simulation platform for diffusion simulation. In order to show the prediction effect of the new prediction model intuitively, we use the original model and the improved model to analyze the simulation in the same environment. In the experiment, we defined the concentration of the leak source as 0.6 mg/m^3 and the ambient wind speed as 1.5

m/*s*. In addition, the coordinates of the leak source is defined as (0, 0, 0). Then, we get the impact range diagrams of the two models after 5 minutes and 8 minutes.

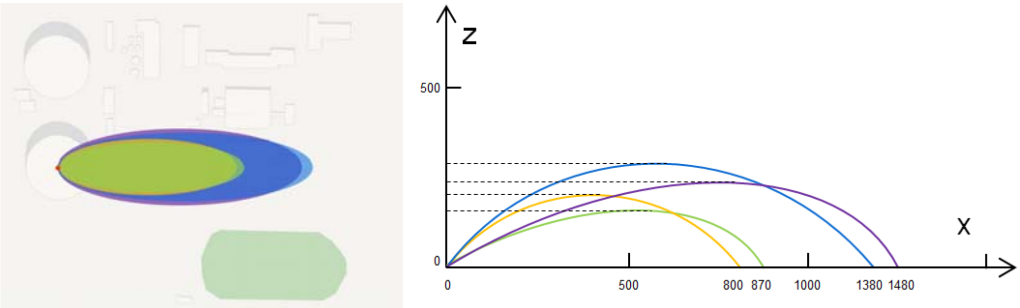

Figure 4. Simulation result and diffusion range diagram

From figure 4, we can get that the diffusion range of the two prediction models in different directions is highly coincident, which shows that the improved model can be used as non heavy gas prediction model. In addition, the improved simulation results are different from the traditional prediction models in both the down wind direction and the crosswind direction. This is because that the new prediction model takes into account the thermal lifting and the ground reflection. To some extent, the improved model can more effectively reflect the actual gas diffusion phenomenon.

5. Conclusion

While promoting economic development, the chemical industry also has a potential impact on the surrounding environment. In order to respond promptly to the leakage of chemical products in the process of production, storage and transportation, we need to make contingency plans in advance. The gas diffusion prediction model provides sufficient data support for the formulation of emergency plans. Compared with the traditional gas diffusion prediction model, the improved Gauss plume model can provide better evidence for the safety management department.

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References

Arystanbekova N.K., 2004, Application of Gaussian plume models mathematics and computers in simulation at instantaneous emissions, Mathematics and computers in simulation, 67, 451-458.
Briant R., Korsakissok I., Seigneur C., 2011, An improved line source model for air pollution dispersion from roadway traffic, Atmospheric Environment, 45, 4099-4107.
LI Y.Y., 2013, Improvement of Gauss plume model and its application in the simulation of hazardous chemicals leakage accident, 10-19.
Peng A.Q., Chu Z.W., Zhang S.L., 2016, Design and Implementation of a City Gas Pipeline Emergency-aidSystem Based on Gaussian Plume Model, Bulletin of Surveying and Mapping, 10, 110-112.
Sun D.L., Jiang J.C., Zhang G.M., 2011, Study on Liquid Ammonia Storage Vessel Release and Diffusion Models Improvement, Industrial Safety and Environmental Protection, 1(37), 27-29.
Wu X., Long C.J., 2005, Gas Diffusion Model and Its Application in Safety Assessment, Industrial Safety and Environmental Protection, 8(31), 50-52.
Yi G.X., Yang C.S., Ma J.L., 2008, Research and implementation of treatment system for leak- age and diffusion of hazardous material based on GIS, Journal of Safety Science and Technology, 4(5), 70-73.
Zhang X.Q., 2016, Design and implementation of gas diffusion simulation system for Industrial Park, 10-21.