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The Simulation System of Hazardous Chemical Gas Diffusion in Plant Based on Cellular Automata

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Generally speaking, the process of production, transportation and storage in petrochemical, pesticide, energy and other chemical industry involves the regulation of hazardous chemicals. If not well managed, it will cause leakage accidents, and even bring great harm to nearby residents and the environment. The accurate prediction of diffusion range in the first time can effectively help us to organize the evacuation of people in affected areas, which is of great significance to reduce casualties and property losses. In this paper, a simulation system of dangerous chemical gas diffusion in plant based on cellular automata is proposed. Firstly, in this paper, we introduce the principle and basic structure of cellular automata. Secondly, this paper gives a brief introduction to the Gaussian plume model, which is an excellent gas diffusion model. Thirdly, the three-dimensional model of cellular automata based on Gaussian plume model is proposed. The distribution of the cellular at present is predicted by the state of neighbor cellular in three-dimensional coordinates. Finally, the experimental results are compared with other algorithms in this paper, and the comparison results show that the improved 3D cellular automata model has better simulation results.

1. Introduction

Leakage of toxic or flammable gases will caused great harm to the environment and people. Once a large amount of volatile gas is released into atmosphere, it will hard to prevent the spread effectively. Thus, analyzing the diffusion law of dangerous chemical gas and predicting the impact range have important theoretical value and practical significance. A good forecasting system can not only provide a scientific guidance for the construction of emergency rescue system and emergency management in chemical industry park, but also provide the decision basis for the relevant management departments (Li, 2013)).
In recent years, domestic and foreign scholars have done a lot of research work, and great progress has been made in simulation system of dangerous chemical gas diffusion, such as ALOHA, SLAB, DEGADIS and SAFETY. The former ministry of chemical industry develops the leakage simulation system for hazard analysing (Wu et al., 2001). In addition, the china academy of safety science develops disposal system for diffusion accident of hazardous chemical gas (Yi et al., 2008).
In this paper, we propose a simulation system of dangerous chemical gas diffusion in plant based on cellular automata. Firstly, this paper introduces the principle and basic structure of cellular automata. Secondly, this paper gives a brief introduction to the Gaussian plume model, which is an excellent gas diffusion model. Thirdly, the three-dimensional model of cellular automata is proposed by introducing Gaussian plume model. The distribution of the cellular at present is predicted by the state of the neighbour cellular in three-dimensional coordinates. Finally, the experimental results are compared with other algorithms in this paper, and the experimental results show that the improved 3D cellular automata model has better simulation results.

2. Basic theory and method

2.1 Cellular Automata

Cellular automata is a method to simulate complex phenomena through a simple operation rule after a simple connection of many simple components (Zhu, 2013). The essence of cellular automata is a dynamic system which evolves in discrete time points in a cellular space composed of discrete cells (Chopard, 1998; Ochoa et al., 2016). The basic structure of cellular automata consists of five parts and they are cellular, cellular space, neighbour, evolution rule and state.

(1) Cellular

It is the basic unit of cellular automata, which is also called cell or element. Normally, the cell has only one state variable, and it can also increase the state variable according to the specific situation.

(2) Cellular space

Cellular space is a collection of all cells distributed in space. At present, the research of cellular automata model is mostly concentrated in one dimension, two dimensions and three dimensions. For one-dimensional cellular automata, the partition of cellular space is only a case of banding. For two-dimensional and multidimensional space, the cellular spaces can be represented in many shapes such as triangle, square and hexagon. Here, the square is the most widely used.

(3) State

The state of a cell in some moment is usually described by a discrete set which can be expressed binary set {0, 1} or discrete set $\{S_0, S_1, S_2 \ldots S_i \ldots S_n\}$

(4) Neighbor

When the cellular is updated, the space of the other cells which directly affect the state of the current cellular in next time is called the neighbour of cellular. In principle, all cell neighbours should be the same size. Usually the cellular automata has two kinds of neighbours, they are Von Neumann neighbour and Moore neighbour. In the two-dimensional cellular space, Von Neumann neighbour is composed of the current cellular and other cellulars which come from the direction of east, west, south and north. Moore neighbour consists of the current cell and the other 8 cells. Compared with Von Neumann neighbour, Moore neighbour is also calculated from the directions of northeast, northwest, southeast and southwest.

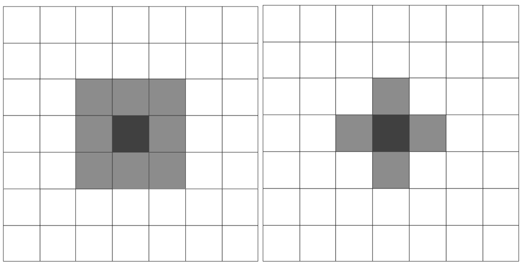

Figure 1: Von Neumann neighbour and Moore neighbour

(5) Evolution rule

Generally speaking, the transfer rule is a state transition function which determines the cellular state of the current time according to the state of cellular and neighbour state at last moment.

$$s_{mn}^{t+\Delta t} = \sum_{i,j \in N} f(s_{mn}^{t}, s_{ij}^{t}) \cdot w_{ij} \tag{1}$$

In the above formula, *f*() means the transfer rule, which plays a decisive role in cellular automata model. S_{mn}^{t} is the current state of the cell whose coordinates is (*m*, *n*) and S_{ij}^{t} is the state of neighbour (*i*, *j*). In addition, w_{ij} is the weighting coefficient of cellular (*i*, *j*) and it satisfies the following formula.

$$W = \sum_{i,j \in N} w_{ij} = 1 \tag{2}$$

2.2 Gaussian plume model

The Gaussian model includes Gaussian plume model and Gaussian puff model. The plume model is suitable for continuous diffusion of point source, which is mainly used in complex terrain area. The plume model considers the influence of the wind speed. On the contrary, the puff model is suitable for short time diffusion such as sudden transient gas leakage (Pai et al., 2001). In this paper, the research is mainly based on Gaussian plume model. The basic equation of Gaussian plume model is as follows.

$$C(x,y,z) = \frac{U_s}{2\pi v \sigma_y \sigma_z} e^{-\frac{y^2}{2\sigma_y^2}} \left(e^{-\frac{(z-H_r)^2}{2\sigma_z^2}} + e^{-\frac{(z+H_r)^2}{2\sigma_z^2}}\right) \tag{3}$$

In the formula, $C(x, y, z)$ means the mass concentration of leakage gas at moment t where the coordinate of cellular is (x, y, z). In two-dimensional cellular space, the formula can be expressed as follows.

$$C(x,y,0)=\frac{U_s}{2\pi v\sigma_y\sigma_z}e^{-\frac{y^2}{2\sigma_y^2}}\left(e^{-\frac{(z-H_r)^2}{2\sigma_z^2}}+e^{-\frac{(z+H_r)^2}{2\sigma_z^2}}\right) \tag{4}$$

Where, v means the wind speed of the surrounding environment, H_r is the effective height of the source. σ_x, σ_y and σ_z are respectively the diffusion coefficients in x, y, z directions. l, m, r, w are environmental impact parameters.

$$\sigma_z = K(z_0)\cdot l\cdot x^m \tag{5}$$

$$\sigma_y = K(z_0)\cdot 10^r\cdot x^w \tag{6}$$

$$K(z_0)=(10\cdot z_0)^{\frac{1}{0.533x^{0.22}}} \tag{7}$$

z_0 is the characteristic parameter of diffused surface layer.

$$z_0 = 0.041h \tag{8}$$

The Gauss plume model is mainly suitable for the scene that wind speed is steady and the diffusion range is less than 5km. In addition, the simulation results show that the model performs well when the wind speed is in the range of 1m/s-15m/s.

3. Cellular automata based on Gaussian plume model

In this paper, a three dimensional cellular automata model is proposed based on Gaussian plume model in order to simulate the motion of hazardous chemical gas in x, y, z directions. When the density of the dangerous chemical gas is equal to the air density, the motion in z direction can be ignored and the model can be simplified as a two-dimensional cellular automaton model. The three dimensional cellular automata based on Gaussian plume model is under the assumption of Von Neumann neighbour.

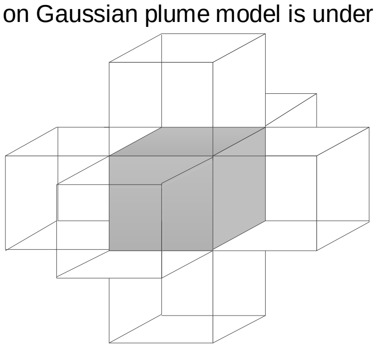

Figure 2: Three-Dimensional Cellular Automaton Mode

(1) The definition of cellular

Assuming that A_d is the diffusion area cellular whose coordinate is (x, y, z) and A_c means the area of a cellular.

$$D(x,y,z)=\frac{A_d}{A_c} \tag{9}$$

According to the results of the calculation, there will be the following scenes.

Case 1: $D(x, y, z)<1$. It indicates that the current cell region is partially diffused.

Case 2: $D(x, y, z)=0$. It indicates that the current cell region is not spread.

Case 3: $D(x, y, z)\geq 1$. It indicates that the current cell region is fully spread.

By setting the threshold $T=0.7$, the cell state is treated with two values.

$$\begin{cases} A(x,y,z)=0 & 0 \le D(x,y,z) < T \\ A(x,y,z)=1 & \mathrm{T} \le D(x,y,z) \end{cases} \tag{10}$$

When $D(x, y, z)$ reaches the threshold T, the region can be considered to be fully diffused.
(2) The determination of transfer rule
Since the current state of the cellular is determined by the state of last moment and the diffusion rate of the neighbour, the following formula can be used to represent the cell.

$$d_{x,y,z}^{t+\Delta t} = f(A_{x,y,z}^{t}, v_{x-1,y,z}^{t}, v_{x,y-1,z}^{t}, v_{x,y,z-1}^{t}, v_{x+1,y,z}^{t}, v_{x,y+1,z}^{t}, v_{x,y,z+1}^{t}) \tag{11}$$

When the neighbour cellular $D(x\text{-}1, y, z)$=1, the diffusion area of current cellular from direction (x-1, y, z) can be expressed by $\frac{v_{x-1,y,z}^{t} \cdot r \cdot \Delta t}{r^2} = \frac{v_{x-1,y,z}^{t} \cdot \Delta t}{r}$.

Thus the diffusion area formula from six directions can be get as follows.

$$\begin{aligned} d_{x,y,z} = {} & \frac{v_{x-1,y,z}^{t} \cdot \Delta t}{r} \cdot a_{x-1,y,z} + \frac{v_{x,y-1,z}^{t} \cdot \Delta t}{r} \cdot a_{x,y-1,z} + \frac{v_{x,y,z-1}^{t} \cdot \Delta t}{r} \cdot a_{x,y,z-1} + \frac{v_{x+1,y,z}^{t} \cdot \Delta t}{r} \cdot a_{x+1,y,z} \\ & + \frac{v_{x,y+1,z}^{t} \cdot \Delta t}{r} \cdot a_{x,y+1,z} + \frac{v_{x,y,z+1}^{t} - 1 \cdot \Delta t}{r} \cdot a_{x,y,z+1} \end{aligned} \tag{12}$$

4. The simulation system of dangerous chemical gas diffusion based on cellular automata

The simulation system of dangerous chemical gas diffusion in plant based on cellular automata is made up of four parts, and they are remote monitoring part, network communication part, the data processing server and monitoring platform.

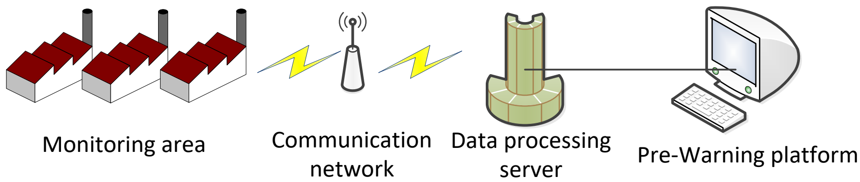

Figure 3: The simulation system of dangerous chemical gas diffusion based on cellular automata

The remote monitoring part is composed of a large number of chemical gas sensors which are distributed in any position of the factory. The sensor includes sensor module, data processing module, communication module and battery module. Firstly, the sensor module is mainly responsible for collecting the data information of the monitored area and signal conversion. Secondly, the processing module is mainly responsible for data storage and processing of node information. Thirdly, communication module is mainly responsible for sending and receiving node data and exchanging control information with other nodes. At last, the battery module is mainly used to provide enough energy for the normal operation of sensor nodes.
The network communication mainly refers to communication lines, which can be wireless or wired. The network communication part is mainly responsible for the data transmission between the monitoring platform and the sensor network. Compared with wireless communication, wired transmission is more stable and secure.
The data processing part mainly refers to the high performance data processing server, which is thought to be the brain of the system. It is mainly used for 3D modeling and data acquisition and analysis. The simulation algorithm directly determines the accuracy of the whole system.
The monitoring platform is mainly used for human-computer interaction, and it can not only display the operation of the factory, but also can send commands to other parts.

5. Experiment and result analysis

According to dangerous gas diffusion model based on cellular automata, we divide the physical space of the factory into grids. The experiment is carried out under the condition that each grid area is 2m×2m and each grid corresponds to a cellular. In order to verify the performance of the cellular automata model proposed in this paper, we use BM model and Sutton model to do the experiment under the same experimental conditions. The BM model is composed of a series of experimental data of gas leakage, which is considered as the empirical model. The Sutton model is a model of dealing with diffusion problems by using the theory of turbulent diffusion statistics.

In this experiment, the verification of the three models is carried out at the same time, and the results are recorded for data analysis.

The experiment will be carried out in two scenarios.

(1) The accuracy of the diffusion model is verified in the case that the sensor is fixed and the ambient wind speed is gradually enhanced.

(2) The accuracy of the diffusion model is verified in the case that the ambient wind speed is fixed and the number of sensors is increasing.

In order to evaluate the prediction accuracy of the model, the absolute value of the difference between the predicted area and the actual diffusion area is calculated. Finally, we can get the proportion of the absolute value in actual diffusion area.

$$\varphi = \frac{|V_f - V_a|}{V_a} \cdot 100\% = \frac{|\sum_{x,y,z \in P} a_{x,y,z} \bullet v_{x,y,z} - V_a|}{V_a} \cdot 100\% \quad (13)$$

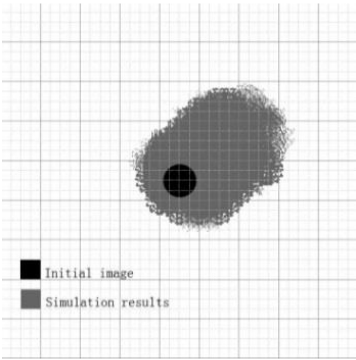

Figure 4: Simulation of gas diffusion after 30 seconds

The figure 4 shows the effect of chemical gas diffusion after 30 seconds in the case of ambient wind speeds of 0.5m/s when the density of the chemical gas is the same to air. It can be seen that the diffusion of chemical gas is relatively slow due to the low wind speed. At the same time, the distribution of chemical gas is also very close.

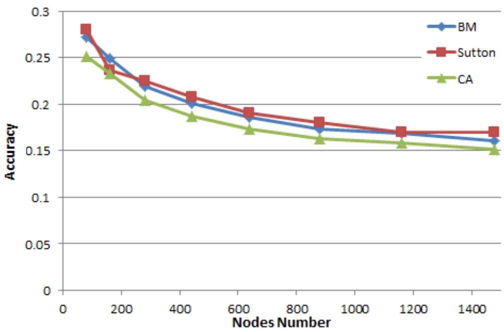

Figure 5: Curve of node number and precision

In figure 5, we can see the change curve of the prediction accuracy and the number of sensor nodes. With the increase of the number of sensor nodes, the prediction error is getting smaller and smaller. However, when the node density reaches a certain number, the influence of the number of sensors on the prediction error is no longer obvious. From the total accuracy change curve we can see that compared with BM and Sutton model, the gas diffusion model based on cellular automata has better prediction accuracy.

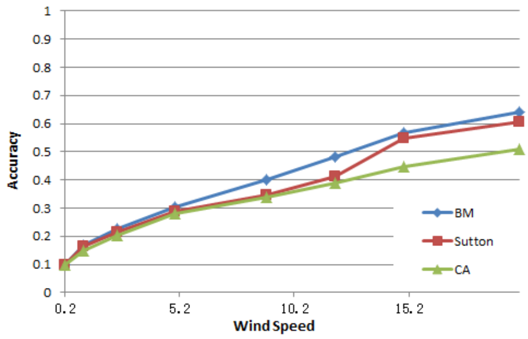

Figure 6: Curve of wind speed and precision

In figure 6, we can see the change curve of the prediction accuracy and the wind speed. With the increase of wind speed, the prediction error is also increasing. The prediction model can not have good prediction accuracy under high wind speed because it does not consider the instability of airflow and the influence of building structure. Generally speaking, compared with the other two forecasting models, the prediction model based on cellular automata has a better advantage in accuracy.

6. Conclusion

In this paper, we analysis the mathematical models of gas diffusion process and propose a simulation system of dangerous chemical gas diffusion in plant based on cellular automata. By introducing Gauss plume model into cellular automata, we realize the prediction of the diffusion range. The experimental results show that the improved gas diffusion model has higher prediction accuracy compared with other prediction models. We believe that with the development of information technology, more and more new prediction model will be put forward and applied to practice, which will promote the safety management in chemical industry.

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