A Rapid Prediction Method for Chemical Clouds Diffusion with Terrain Effects Correction

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Abstract. A method for correcting analytic model of chemical clouds diffusion is proposed to take terrain effects into account. The calculation results show that the corrected model of clouds diffusion can describe the main diffusion features in complex terrains; furthermore, it has the advantages of rapid calculating and easy programming.

Introduction

Due to chemical plant accidental leakage and other reasons, it may release a large number of toxic chemicals into atmosphere, which will be a serious threat to human life and health. It is necessary to assess the harms of clouds for chemical accident emergency rescues. All above requires a rapid concentration prediction of chemical clouds diffusion. The concentration of toxic chemicals in the atmosphere can be predicted by the mathematical model which can study the mechanism of atmospheric diffusion and quantitative rule. The simplest and most rapid prediction model of clouds diffusion is based on the analytic method. In other words, by simplifying the quantitative relationship in the diffusion process, it is easy to get the analytical solution in mathematics and then use the experimental data to correct parameters. The current analytical model is based on the Gaussian model. The following formula is commonly used to calculate the Gaussian diffusion model for continuous point source diffusion [1].

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

In the formula, Q is the amount of release per unit time; u is the average wind speed; $\sigma y=\sigma y$ (x) and $\sigma z=\sigma z$ (x) is diffusion parameter; H is the height of source from the ground.

Under different stability, the selection of diffusion parameters can be found in references [2].

If we assume that the vertical diffusion coefficient changes exponentially with height, we can get a kind of analytic model, called Lachtman model [3].

The advantages of the analytical model, which can directly obtain the concerned concentration value at the coordinate and predict the clouds shapes distribution, are fast calculation speed and easy programming; furthermore, the programming is easy to realize. However, the main drawback is that calculation error is large in complex terrains and meteorological conditions owing to the introduction of the idealized assumptions in advance. Meteorological changes, such as wind direction and wind speed, can distort clouds shapes [4] in complex terrains. The analytical model based on the simplified assumptions can not take the influence of complex terrains into consideration, so the predicted clouds shapes that are different from the actual shapes mean no practical significance. The numerical model is usually used to predict [5] clouds diffusion under the condition of complex terrains. The basic principle of the numerical model is as follows: firstly, the spatial distribution of meteorological factors, such as wind speed, wind direction and temperature, is obtained through solving the basic equation of atmospheric dynamics by the numerical method; Then, the concentration distribution of the diffusion process of clouds can be calculated through solving atmospheric diffusion equation by the numerical method. The numerical prediction method has the advantage of strong theoretical basis and can comprehensively consider the effects of complex terrains on airflow and clouds diffusion, so the results of the calculation can reflect the actual situations. However, it is difficult to meet the need of rapid prediction for some reasons, such as complex theoretical modeling, complex solution algorithm, difficult programming and computational complexity.

Because of the shortcomings of current analytical model and numerical model, it is difficult to satisfy the need for rapid calculation of clouds diffusion under the condition of complex terrains. The purpose of this paper is to study the method of correcting the analytical model, which will take terrain effects on clouds diffusion into account and achieve both rapid prediction and certain accuracy to meet the actual need of chemical accident emergency rescues.

Modifying the Analytical Model of Atmospheric Diffusion

In order to find the key factor of model correction, the following is a brief analysis of the dynamic mechanism of terrain effects on airflow and atmospheric diffusion.

when the even and straight airflow encounters mountain block, climbing or bypassing may occur. Whether the airflow can climb over mountain block or not, it is closely related with the height of mountain, atmospheric stability, etc. The buoyancy of airflow is just enough to overcome gravity in neutral atmospheric stability, so the climbing process is smooth without bypassing. In stable conditions, airflow is inhibited and forced to bypass from the side, so airflow distortion occurs. Correspondingly, the shapes of clouds are also distorted. Under convective conditions, airflow is accelerated by buoyancy during the climbing process, and the leaving space is filled by the surrounding air. This results in wind direction changes and clouds deformation.

When bypassing the hillside, airflow must be excluded by the hillside, which inevitably results in changes of the concentration distribution of pollutants. Especially in the valley on both sides of the hillside, it can obviously make clouds become narrow and concentration rise. After leaving the valley, the clouds will expand to both sides, and concentration decreases.

It can be seen from the above analysis that terrain effects on atmosphere are possible to be taken into account properly by introducing a corresponding correction factor in the model.

As mentioned above, when straight airflow climbs over the hillside in neutral atmospheric stability, it will maintain the original direction, and its axis lifts the corresponding angle along the slope. There is no necessary to correct the model at this time. In stable conditions, airflow is forced to bypass the hillside, as it is difficult to climb the hillside. This results in that its axis decreases a certain distance compared with the neutral conditions. Correspondingly, clouds axis also decreases. The distance down has a direct relationship with terrain height and atmospheric stability. The greater the terrain gradient is, the more stable the atmosphere is, and the greater the distance down is. As opposed to clouds, the position of the calculated point is equivalent to raising the same distance. Therefore, the climbing correction factor is proposed as follows:

$$z_1 = z + f_z(z_g, S) \qquad (2)$$

In the formula, z is the height of the position of the calculated point from the ground; z_g is elevation; z_1 is the vertical coordinate that has taken climbing correction into account; $f_z(z_g, S)$ is climbing correction function; S is atmospheric stability factor. In the neutral conditions, $S = 0$; in the stable conditions, $S > 0$; in the convective conditions, $S < 0$.

Here, a coordinate conversion is performed. Since terrain is rugged, the relative coordinates are used in the vertical direction, which is defined as the height of the point from the local ground. It is convenient to calculate the concentration distribution of clouds and evaluate the chemical hazards in the relative coordinate system.

The key to determine the correction factor is to select the appropriate climbing correction function $f_z(z_g, S)$. According to the definition, the climbing correction function must meet the following constraints: in the neutral conditions, $f_z(z_g, S) = 0$; in the stable conditions, $f_z(z_g, S) > 0$; in the convective conditions, $f_z(z_g, S) < 0$. Furthermore, $f_z(z_g, S)$ must be a monotonically increasing function of both elevation and atmospheric stability.

The simplest form is to take the following formula:

$$f_z(z_g, S) = z_g S \,, \tag{3}$$

This satisfies the above basic constraints. Of course, the function $f_z(z_g, S)$ may actually be a complex non-linear form. Formula (3) can be seen as an approximate description under the conditions of undulating terrain and stable atmosphere which has not much deviation from neutral. As a preliminary study, the climbing correction function $f_z(z_g, S)$ in this paper is calculated according to formula (3).

When airflow is excluded by terrain, clouds become narrow, and the concentration increases. This effect can be taken into account by the principle of mass conservation. The specific method is to integrate the cross-section perpendicular to the wind axis, compare it with the concentration integral which does not consider climbing correction and define the terrain crowding correction factor.

$$f_a = \frac{\int c(x, y, z)dy}{\int c_1(x, y, z)dy} \tag{4}$$

In the formula, $c(x, y, z)$ is the concentration distribution that does not take climbing correction into account, yet, $c_1(x, y, z)$ is the concentration distribution that has taken climbing correction into account.

In this way, after two amendments, the concentration formula is:

$$c_1(x, y, z) = \frac{Q}{2\pi\sigma_y\sigma_z u}\exp[\frac{-1}{2}(\frac{y}{\sigma_y})^2]\cdot\left\{\exp[\frac{-1}{2}(\frac{z_1 - H}{\sigma_z})^2] + \exp[\frac{-1}{2}(\frac{z_1 + H}{\sigma_z})^2]\right\} \tag{5}$$

$$c_2(x, y, z) = f_a c_1(x, y, z) \tag{6}$$

In the formula, z_1 and f_a is respectively calculated by the formulas (2) and (4).

Test results

Using the corrected Gaussian model, the diffusion concentration distribution of the continuous point source and the instantaneous point source in the valley is calculated respectively. The meteorological conditions are as follows: wind speed 1.0m/s, atmospheric stability is stable, $S = 0.8$. The analysis of the range of the stability parameter S is as follows: Because chemical accidents are easy making serious effect under neutral and stable conditions, S is in the range of 0 to 1, where 0 is the neutral state and 1 is the most stable state. Terrain is set as follows: a circular and 100m high hill can play a certain role in blocking airflow; a valley is in the middle of two oval-shaped and 200m high hills.

Figure 1 shows the diffusion concentration distribution of clouds of the continuous point source which is 1m high from the ground. You can see clouds take the bypass because of the circular hills' blocking. As entering the valley, clouds narrow with the exclusion of terrain. After leaving the valley, clouds widen as terrain goes open. The view is consistent with the theory of atmospheric diffusion.

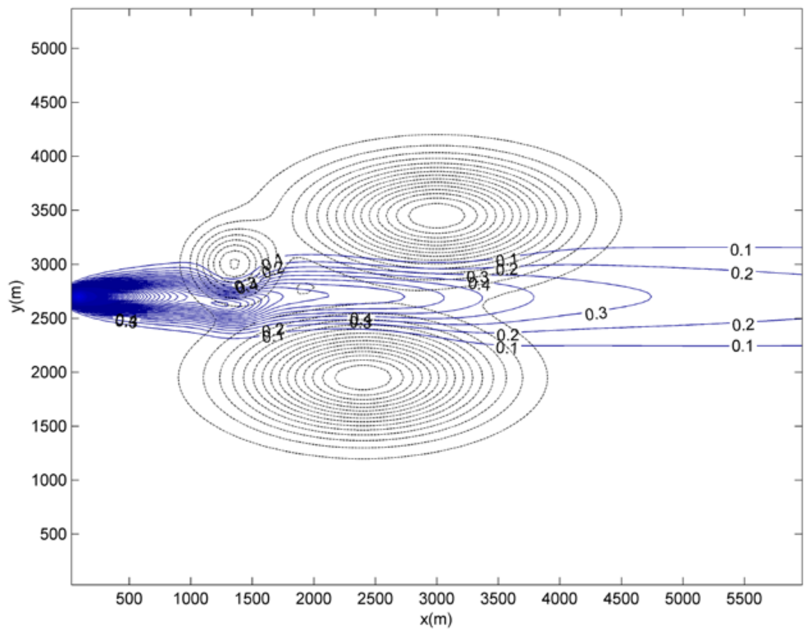

Fig.1 shows the concentration distribution of clouds of the continuous point source in the valley. In the figure, the dotted line is the terrain contour line, and the solid line is the iso-concentration line.

Fig.2 shows the concentration distribution of clouds of the instantaneous point source at different time (1000s, 1500s, 2000s and 3000s). It can be seen that clouds deform shapes and take the bypass when blocked by the hills. Besides, the front part of clouds narrow as entering the valley and widen after leaving the valley. These features are consistent with the theory of atmospheric diffusion.

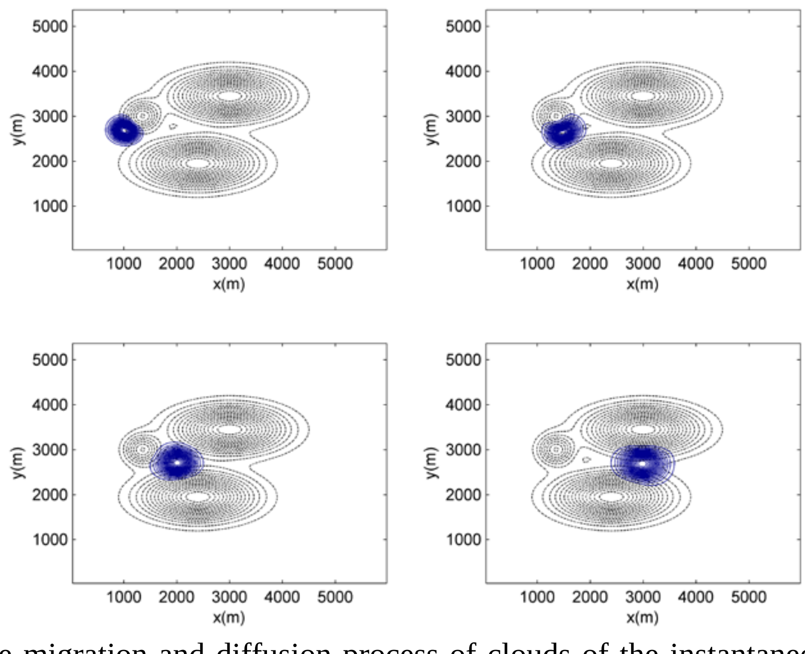

Fig.2 shows the migration and diffusion process of clouds of the instantaneous point source in the valley. The released point is in the center of the left boundary in the figure at initial moment.

Above the left: 1000 seconds after being released; above the right: 1500 seconds after being released; below the left: 2000 seconds after being released; below the right: 3000 seconds after being released.

In order to further test the applicability of the model, the actual terrain data are used to simulate under the simulated meteorological conditions which are the same as in the first two examples. As shown in Figure 3, there is a hill in the middle of the map. Under its influence, airflow bends direction and bypasses the hill, and then restores the original direction. This trend is consistent with the theoretical analysis.

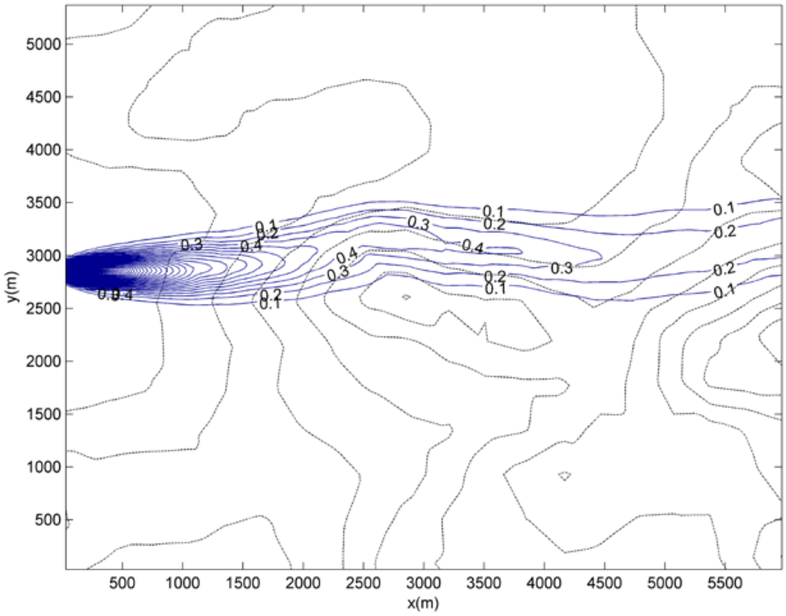

Figure 3 shows the concentration distribution of clouds which is simulated with the actual terrain data. In the figure, the dotted line is the terrain contour line, and the solid line is the iso-concentration line.

The above simulations are all realized by Matlab language programming. Using the Intel Core2 E8400 processor, it takes 0.55s for a single CPU to run an example, while 0.29s without considering terrain correction. The terrain correction method for the Gaussian diffusion model makes the calculation time double.

Conclusion

Based on the analysis of the mechanism of terrain effects on clouds diffusion, this paper puts forward an idea of correcting the analytical model, and makes a preliminary study on the correction method of clouds climbing, bypassing and terrain exclusion. By correcting the Gaussian diffusion model and considering terrain effects on clouds diffusion, the calculation results prove that it can reflect the main characteristics of clouds diffusion in complex terrains. Due to the complexity of the diffusion process of clouds, the method of correction factor has some limitations. For example, the phenomenon of large deformation and the splitting of clouds caused by the vertical wind direction shear can not be described only by correcting parameters, so the corrected Gaussian model can not replace the numerical model. However, in the situations that terrain undulation is not great and meteorological conditions are not very complex, the corrected analytical model can not only reflect terrain effects but also has the advantages of fast calculation speed and easy programming, which is expected to share a certain percentage in clouds concentration prediction, environmental simulation of chemical hazards and other applications. As this paper only conducts a preliminary study, the corrected model needs to make more theoretical researches on accuracy and scope of application besides experimental researches on atmospheric diffusion in complex terrains for verification and further development.

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