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Grey Mathematics Model for Atmospheric Pollution Based on Numerical Simulation

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Urban air environment is a complex system with multiple objectives, multi levels and multiple factors. In this paper, the grey analysis of atmospheric environmental system is carried out, and the grey differential equation of air pollution is established, and the calculation method analysis and model verification of the grey numerical model are carried out. The relationship between the model parameters and the numerical solution is mainly analyzed, and the concentration field of the pollutant diffusion in the unsteady state is plotted. In this paper, the atmospheric environment system is analyzed from the grey system theory, and a more objective grey mathematical model is set up to carry out the Grey Numerical Simulation of the air pollution diffusion in urban area. It is of great practical significance to the flexible management and decision of air pollution control.

1. Introduction

Atmospheric pollution is defined such that some substances in the atmosphere reach a high-enough concentration and are active for a sufficient time to undermine the normal survival and development of humans and ecosystems, and cause great harm to human body, ecology and materials. It is attributed to both natural and human factors. Air pollution will pose great threat to human health. It is estimated that, worldwide, there are 1.1 billion urban residents who are exposed to the environment with ultrahigh concentration of sulfur dioxide that far exceeds the standards required by the World Health Organization (WHO) standards (Yurii, 2014). Compared with the existing air simulations, the gray mathematics simulation method for atmospheric pollution can regard all relevant parameters and input and output information in the atmospheric environment system as gray variables (i.e., a range), and operate them in accordance with the algorithm specified by gray mathematics (Wu, 2016). In doing so, the "inaccuracy" and "incompleteness" of the original information such as the internal structure, parameters and boundary conditions in the atmospheric environment system can be better responded to, so that the results obtained by the model are more flexible and actively serve for decisions (Li et al., 2015; Cassidy et al., 2008; Reddy and Rao, 2005). The study in this paper is of great significance to master the temporal and spatial distribution characteristics of urban air pollution, scientifically control air pollution and effectively implement environmental management.

2. The basic Grey Numerical Model of air pollution

2.1 Grey analysis of atmospheric environment system

The atmospheric environment system as an open and complex system continuously interacts and exchanges materials and energies with the outside world. From the perspective of impact factors, the output of the atmospheric environment system, that is, the concentration of pollutants, is the result of comprehensive effect of natural and human factors. In the diffusion nature of the atmospheric medium, the actual diffusivity of atmospheric medium is quite complicated, and most of them are heterogeneous and anisotropic, that is, the recognition of the parameters is gray for the whole system (Wang and Zhang, 2013). From the boundary of the atmospheric environment system pollution area, in the evaluation of atmospheric environment quality, the plane infinite boundary and homogeneous medium are often taken to simplify the calculation. In fact, the simulated domain boundary is often limited and constantly changing, so that the boundary of atmospheric environment pollution gets grey (Fan et al., 2015). The above analysis proves that the atmospheric environment system is an extrinsic gray system. In this sense, when inquiring into some characteristics of atmospheric environment system, we should take a full consideration to the finiteness of the obtained system information, and build a more objective model with the gray system idea, that is, a gray mathematics model.

2.2 Establishment of Grey Differential Equation of Air Pollution

It is presumed that atmospheric pollutants can blend with the atmospheric environment. There are similar hydrodynamic characteristics between the pollutants and the atmospheric environment particles. As discussed above, based on the grey parameters and variables of atmospheric pollution, the principles of mass conservation and energy conservation are applied to derive the gray differential equation relevant to it as follows (Feng, 2014), as shown in Fig. 1.

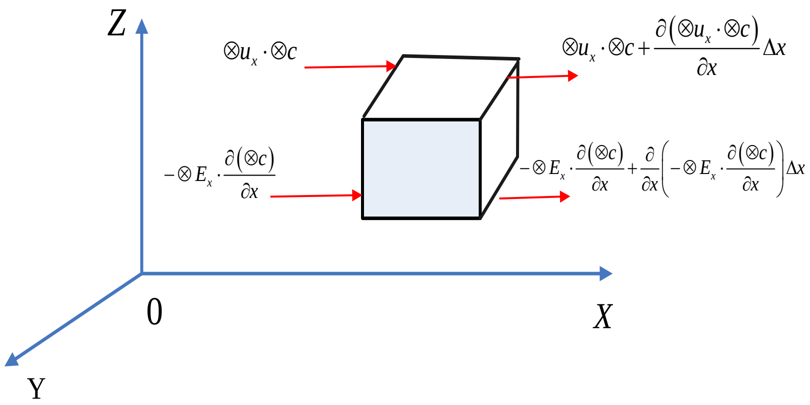

Figure 1: Mass balance in volume element

The mass of the pollutants input into the volume element per unit time in the X direction is as follows:

$$C_j \in \{C_1, C_2, \ldots, C_n\} \tag{1}$$

The mass of the pollutants output from the volume element per unit time in the X direction is as follows:

$$C_j \in \{C_1, C_2, \ldots, C_n\} \tag{2}$$

The variable quantity of pollutants in the X direction per unit time is as follows:

$$\begin{aligned}
&\left[\otimes u_x \cdot \otimes c + \left(-\otimes E_x \cdot \frac{\partial(\otimes c)}{\partial x}\right)\right]\Delta y \Delta z \\
&-\left[\otimes u_x \cdot \otimes c + \frac{\partial(\otimes u_x \cdot \otimes c)}{\partial x}\Delta x + \left(-\otimes E_x \cdot \frac{\partial(\otimes c)}{\partial x}\right) + \frac{\partial}{\partial x}\left(-\otimes E_x \cdot \frac{\partial(\otimes c)}{\partial x}\right)\Delta x\right]\Delta y \Delta z \\
&= -\left[\frac{\partial(\otimes u_x \cdot \otimes c)}{\partial x} + \frac{\partial}{\partial x}\left(-\otimes E_x \cdot \frac{\partial(\otimes c)}{\partial x}\right)\right]\Delta x \Delta y \Delta z
\end{aligned} \tag{3}$$

Similarly, the variable quantities of pollutants in the Y and Z directions per unit time are as follows:

$$-\left[\frac{\partial(\otimes u_y \cdot \otimes c)}{\partial y} + \frac{\partial}{\partial y}\left(-\otimes E_y \cdot \frac{\partial(\otimes c)}{\partial y}\right)\right]\Delta x \Delta y \Delta z \tag{4}$$

$$-\left[\frac{\partial(\otimes u_z \cdot \otimes c)}{\partial z} + \frac{\partial}{\partial z}\left(-\otimes E_z \cdot \frac{\partial(\otimes c)}{\partial z}\right)\right]\Delta x \Delta y \Delta z \tag{5}$$

If the atmospheric pollutants decay within the volumetric element and there is a source-sink term, the variable quantity in atmospheric pollutants resulted from this is,

$$\left(\otimes s-\otimes k\cdot\otimes c\right)\Delta x\Delta y\Delta z \tag{6}$$

Then the variable quantity of pollutant in the volumetric element per unit time is as follows:

$$\begin{aligned}\frac{\partial\left(\otimes c\right)}{\partial t}\Delta x\Delta y\Delta z = &- \left[\frac{\partial\left(\otimes u_x\cdot\otimes c\right)}{\partial x}+\frac{\partial}{\partial x}\left(-\otimes E_x\cdot\frac{\partial\left(\otimes c\right)}{\partial x}\right)\right]\Delta x\Delta y\Delta z\\ &- \left[\frac{\partial\left(\otimes u_y\cdot\otimes c\right)}{\partial y}+\frac{\partial}{\partial y}\left(-\otimes E_y\cdot\frac{\partial\left(\otimes c\right)}{\partial y}\right)\right]\Delta x\Delta y\Delta z\\ &-\left[\frac{\partial\left(\otimes u_z\cdot\otimes c\right)}{\partial z}+\frac{\partial}{\partial z}\left(-\otimes E_z\cdot\frac{\partial\left(\otimes c\right)}{\partial z}\right)\right]\Delta x\Delta y\Delta z-\left(\otimes s-\otimes k\cdot\otimes c\right)\Delta x\Delta y\Delta z\end{aligned} \tag{7}$$

In a uniform flow field, $\otimes \mathrm{u}$and $\otimes E_y$are non-dynamic variables, which can be regarded as constants.
Let the micro volume element

$$\Delta x\Delta y\Delta z=1 \tag{8}$$

Then:

$$\begin{aligned}\frac{\partial\left(\otimes c\right)}{\partial t}=&\otimes E_x\cdot\frac{\partial^2\left(\otimes c\right)}{\partial x^2}+\otimes E_y\cdot\frac{\partial^2\left(\otimes c\right)}{\partial y^2}+\otimes E_z\cdot\frac{\partial^2\left(\otimes c\right)}{\partial z^2}-\otimes u_x\cdot\frac{\partial\left(\otimes c\right)}{\partial x}\\ &-\otimes u_y\cdot\frac{\partial\left(\otimes c\right)}{\partial y}-\otimes u_z\cdot\frac{\partial\left(\otimes c\right)}{\partial z}+\otimes s-\otimes k\cdot\otimes c\end{aligned} \tag{9}$$

Where: $\otimes \mathrm{c}$------ grey concentration of pollutant, mg/m^3; $\otimes E_y$------ dispersion coeffective in lateral direction, m^2/s; $\otimes u_x$------ gray wind speed in the predominant wind direction (longitudinal) of the atmosphere, m/s; $\otimes s$ ------ source sink item of atmospheric pollutants, mg/m^3; $\otimes \mathrm{k}$ ------ attenuation coefficient of atmospheric pollutants,s^{-1}; t------ the transport time of atmospheric pollutant, s;
In the uniform flow field, assume the x-axis is the dominant wind direction, then

$$\otimes u_y=0、\otimes u_z=0 \tag{10}$$

If only the 2D diffusion of atmospheric pollution dominated by convection is considered, then

$$\otimes u_x\cdot\frac{\partial\left(\otimes c\right)}{\partial x} \gg \otimes E_x\cdot\frac{\partial^2\left(\otimes c\right)}{\partial x^2}\text{, and }\otimes E_z=0 \tag{11}$$

After a series of simplifications as described above, a 2D gray differential equation for the diffusion of atmospheric pollution can be obtained:

$$\frac{\partial\left(\otimes c\right)}{\partial t}=\left(\otimes E_y\right)\cdot\frac{\partial^2\left(\otimes c\right)}{\partial y^2}-\left(\otimes u_x\right)\cdot\frac{\partial\left(\otimes c\right)}{\partial x}+\left(\otimes s\right)-\left(\otimes k\right)\cdot\left(\otimes c\right) \tag{12}$$

3. Analysis of solution method of grey numerical model

The above basic gray numerical model contains a lot of interval gray numbers, so that the solution to the basic gray numerical model should be based on the gray theory to obtain the "grey" result. Here two types of different solutions are discussed below. The first algorithm is to map the upper and lower limits of the gray parameter, the gray variable and the gray concentration function in the model to each other in order to form two independent whitening linear equations, by which the corresponding upper and lower limits of the gray

concentration function are evaluated. This algorithm is a "bottom-to-bottom, top-to-top" mode (Tu et al.,, 2017). The second algorithm is a set of calculation formulas established based on the operation properties of gray sets and gray numbers. Compare the two methods and choose a better one for solving the basic gray numerical model.
Lower limits of gray parameters, gray variables and the gray concentration function in the model are mapped to constitute a whitened linear equation by which the lower limit of the gray concentration is available,

$$[C_a]_{i,j}, i=1,2,...m; j=1,2,...,n \tag{13}$$

Then the upper limits of gray parameters, gray variables and the gray concentration function in the model are mapped to get a whitened linear equation, thereby obtaining the upper limit of the gray concentration,

$$[C_b]_{i,j}, i=1,2,...m; j=1,2,...,n \tag{14}$$

In short, this algorithm is a "bottom-to-bottom, top-to-top" mode. It gets the upper and lower limits of the gray concentration function by solving two independent linear equations, as given in equations (9) and (10).

$$\begin{aligned}&\left[1+\frac{\Delta t\cdot u_a}{\Delta x}+2\frac{\Delta t\cdot E_a}{(\Delta y)^2}+\Delta t\cdot k_a\right]\cdot[c_a]_{i,j,k+1}-\frac{\Delta t\cdot E_a}{(\Delta y)^2}\cdot[c_a]_{i,j\text{-}1,k+1}\\&-\frac{\Delta t\cdot E_b}{(\Delta y)^2}\cdot[c_a]_{i,j+1,k+1}-\frac{\Delta t\cdot u_a}{\Delta x}\cdot[c_a]_{i-1,j,k+1}-\Delta t\cdot[s_a]_{i,j,k+1}=[c_a]_{i,j,k}\end{aligned} \tag{15}$$

$$\begin{aligned}&\left[1+\frac{\Delta t\cdot u_b}{\Delta x}+2\frac{\Delta t\cdot E_b}{(\Delta y)^2}+\Delta t\cdot k_b\right]\cdot[c_a]_{i,j,k+1}-\frac{\Delta t\cdot E_b}{(\Delta y)^2}\cdot[c_b]_{i,j\text{-}1,k+1}\\&-\frac{\Delta t\cdot E_b}{(\Delta y)^2}\cdot[c_b]_{i,j+1,k+1}-\frac{\Delta t\cdot u_b}{\Delta x}\cdot[c_b]_{i-1,j,k+1}-\Delta t\cdot[s_b]_{i,j,k+1}=[c_b]_{i,j,k}\end{aligned} \tag{16}$$

Assume a certain range of atmospheric ground pollution zone is dissected into 30 rectangular nets, totaling 30 nodes, as shown in Fig. 2. The calculation time interval (i.e. Δt) is divided into three, namely 1h, 2h, 3h. When comparing the numerical results, the results from the two numerical methods of the grey numerical model is considered. The calculation results of classical numerical models are given to compare the two models. In terms of input information, in order to facilitate the explanation of the problem, it is assumed that the physical conditions are given, and only the relationship between the wind speed u, [u_a,u_b] and the output concentration c, [C_a, C_b] is analyzed.

25	26	27	28	29	30
1	2	3	4	5	6
7	8	9	10	11	12
13	14	15	16	17	18
19	20	21	22	23	24

Figure 2: Numerical example section diagram

4. Model verification and analysis

The test is conducted on the above well-established gray numerical model. We calculate it using the "indirect method". For the gray concentration, the upper bound of the concentration "grey band" should be higher than the classical numerical solution, the lower bound lower the classical numerical solution, then the classical numerical solutions must all fall within its "grey band". It may be said that, therefore, the gray numerical model has practicality. According to the calculated results from the gray numerical model, the state comparison curve of NO2 in the heating period is plotted, as shown in Fig. 3 and Fig. 4, in conjunction with the comparison curve of the typical node NOx process variables in the non-heating period, as shown in Fig. 5.

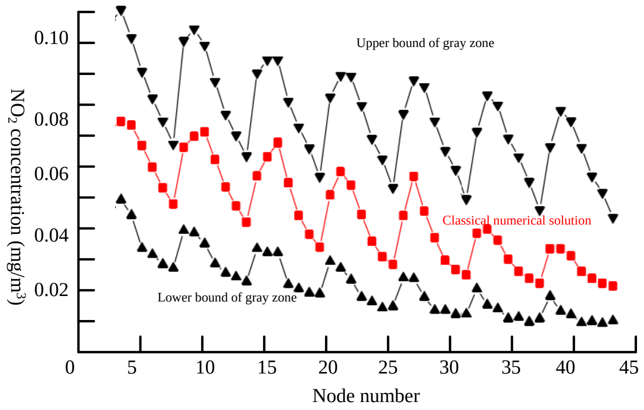

Figure 3: Comparison curve of NO2 calculation results in the first heating period

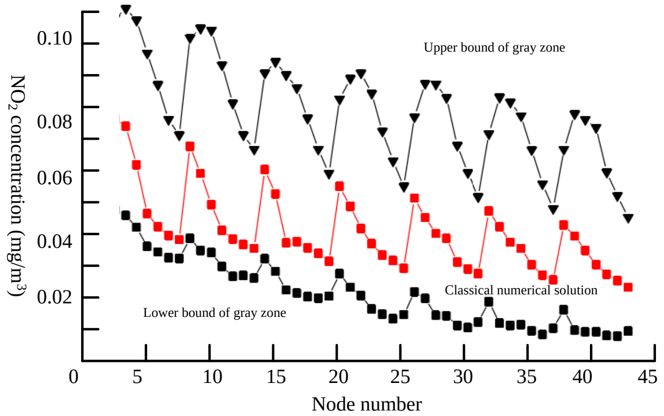

Figure 4: Comparison curve of NO2 calculation results in the second heating period

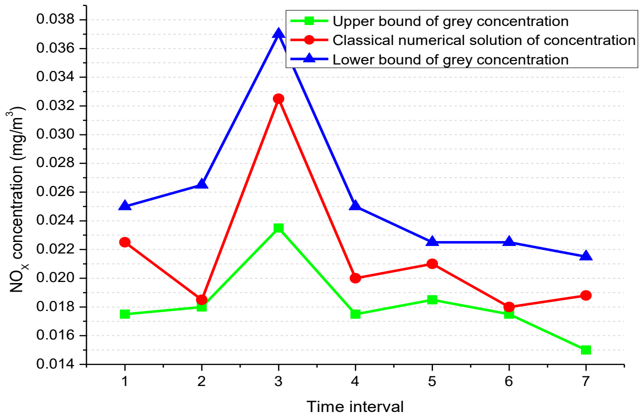

Figure 5: Comparison curve of NOx calculation results of No.27 node in non-heating period

It is known from the above state curves in various time periods and processes that the verification of the gray numerical model has achieved the expected effect, and the classical numerical solutions are included in the "grey band" of the gray model. It is suggested that the model can reflect the real problems. Therefore, the gray numerical model is built for atmospheric pollution to predict the state of change in given pollutants. It is also possible that the model can also be used for scientific management of environmental pollution. Currently, there are lack of information about migration and conversion pathways of atmospheric pollutants and trace gas monitoring data, and more of them are inaccurate. This study provides the clues to the application of gray system theory in this field.

5. Conclusion

There are two main characteristics of the Grey Numerical Model: first, the known information in the atmospheric diffusion system is fully utilized. The model framework and modeling ideas are based on the pre-test knowledge of hydrodynamics and meteorology, and the two is to fully consider the unknown information in the atmospheric diffusion system. Generally speaking, the behavior of the system can be divided into two parts: the deterministic behavior and the accidental behavior, and the grey system theory holds that the deterministic behavior can be divided into the ascertained behavior and the unascertained behavior. As the input and output of the model is gray, the range of the change of the grey process is emphasized, so that the model not only describes the true knowledge of the system, but also describes the uncertain behavior and the accidental behavior in the grey process. The classical model only describes the true behavior of the system, and the stochastic model takes the deterministic behavior as the ascertained behavior, emphasizing only the analysis of the accidental behavior. Obviously, the grey numerical model is more in-depth than the classical deterministic model and stochastic model in describing the atmospheric diffusion system.

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