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General Research Paper

Analytical Solutions of the $PM_{2.5}$ Diffusion Model and Its Application

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ABSTRACT

Air pollution has no national boundaries, which has caused widespread concern around the world. In order to analyse the diffusion and distribution characteristics of the particulate matter smaller than 2.5 micrometers ($PM_{2.5}$), the $PM_{2.5}$ diffusion model was established. By comparatively analysing the solutions of instantaneous point source equation with and without wind, the solution of continuous point source equation with wind, and the correction solution of an elevated point source model; the conclusion was drawn that the Gauss smoke cloud model adopted can solve the problem of diffusivity of $PM_{2.5}$. The results show that the Gauss smoke model with wind can reliably analyse the actual problem by numerical simulation and the monitoring data in Xi'an of China. Through the analysis of the causes and general rules of $PM_{2.5}$, it was found that the human activities play the leading role for $PM_{2.5}$.

INTRODUCTION

With the rapid development of the economy, the numbers of private cars have increased dramatically in China. The exhaust from automobiles and coal consumption contribute to the particulate matter smaller than 2.5 micrometers ($PM_{2.5}$). The continuous haze occurs so frequently and has become a new type of severe weather (Peng et al. 2005). The haze weather can not only lead to the serious air pollution, but also increases the concentration of fine particulates in the air, which contain a lot of poisonous and harmful chemicals (Li et al. 2013, Chang et al. 2012).

The newly added particle (particle diameter less than or equal to 2.5 microns) in the new assessment standard of air quality, also known as $PM_{2.5}$, is not a single component of air pollutants. It is a complex and variable atmospheric pollutant being composed of a number of different chemical compositions of the man-made or natural sources. In terms of the sources, $PM_{2.5}$ can be directly discharged by the pollution source, and it also can be the source of gaseous pollutants by condensation or a complex chemical reaction. $PM_{2.5}$ has important effects on the visibility and the air quality. The fine particle contains a lot of poisonous and harmful substances. Due to a long stay in the atmosphere and transmission distance, $PM_{2.5}$ has a great influence on human health. The related research shows that the particles can cause damage to the respiratory system, the cardiovascular system, lead to asthma, lung cancer, cardiovascular disease, birth defects and premature death (Zhao et al. 2013, Sun et al. 2009). The smaller the particle is, the greater the damage to human body health is. $PM_{2.5}$ has a strong penetrating power. It may penetrate the bronchial wall and interfere with gas exchange in the lungs (Yang et al. 2013, Rosen et al. 2008).

Now only very few people are studying $PM_{2.5}$. The statistics of $PM_{2.5}$ and the related data are too little. It is not enough to understand the objective laws of $PM_{2.5}$. However, the fine particulate $PM_{2.5}$ leads to serious air pollution and has a great influence on human health. The research of the fine particulate $PM_{2.5}$ is imminent and it is of great significance to protect the environment.

$PM_{2.5}$ DIFFUSION MODEL AND ITS ANALYTICAL SOLUTIONS

The Gaussian model is widely applied in the pollution gas leakage simulation (He et al. 2010, Tanaka et al. 2007). This model is mainly suitable for the light and the neutral gas, which has a simple, quick and accurate advantage. Thus, the $PM_{2.5}$ diffusion problem was mainly researched by using the Gaussian model. Since the $PM_{2.5}$ concentration gradient in space is in all directions, the three-dimension model should be established to predict the atmospheric environmental quality in cities. The three-dimension model of environmental air quality was drawn by using fluid mechanics, as follows (Pan & Jiang 2001).

$$\frac{\partial C}{\partial t} = E_{t,x}\frac{\partial^2 C}{\partial x^2} + E_{t,y}\frac{\partial^2 C}{\partial y^2} + E_{t,z}\frac{\partial^2 C}{\partial z^2} - u_x\frac{\partial C}{\partial x} - u_y\frac{\partial C}{\partial y} - u_z\frac{\partial C}{\partial z} - KC \quad ...(1)$$

In the formula 1, u_x, u_y and u_z are the corresponding velocity component of *x*-, *y*- and *z*- directions. $E_{t,x}$, $E_{t,y}$ and $E_{t,z}$ are the corresponding turbulent diffusion coefficients of *x*, *y*- and *z*- directions. *K* is the attenuation constant of the pollutants. According to the different conditions, the three-dimension diffusion model can be simplified in practice.

The solution of instantaneous point source equation without wind: When there is no wind, u_x=0. For the instantaneous point source, the formula (1) needs satisfy the initial conditions and boundary conditions as follows.

The initial conditions: When $t = 0$, $x = 0$, $C \to \infty$; When $x \neq 0$, $C \to 0$. The boundary condition: When $t \to \infty$ $C \to 0$.

Supposing that $\sigma_x^{\ 2} = 2E_{t,x}t$, $\sigma_y^{\ 2} = 2E_{t,y}t$, $\sigma_z^{\ 2} = 2E_{t,z}t$, the formula (2) was obtained as follows:

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

Where *C* (*x*, *y*, *z*, *t*) is the concentration of a group of smoke which is discharged in the space point (*x*, *y*, *z*) and in the time of *t*; *Q* is the source of emissions, and *x*, *y* and *z* are the forecasts location of the point respectively. σ_x, σ_y and σ_z are the concentration distribution of the standard deviation in the *x*-, *y*- and *z*- directions, which are called diffusion parameters, and of which values are closely related to the atmospheric stability and can be obtained through the related look-up table (Table 1 and Table 2).

The solution of instantaneous point source equation with wind: Assuming that there is a constant average wind speed $\overline{u_x}$ (its direction is in the same direction as the smoke movement) in the origin of coordinates (0, 0, 0). A group of smoke is released when $t = 0$, then the smoke regiment will flap and continuously swell by the diffusion. At the heart of the smoke regiment position the system (u_x, *t*, 0, 0) is relative to a fixed coordinate. For another moving coordinate system, the origin is located in the centre of the mobile smoke group, and formula (2) is the diffusion equation from the centre of the smoke cloud. Then the analytical solution of the instantaneous point source with wind of the fixed coordinates can be obtained as follows (Li et al. 2012):

$$C(x,y,z,t) = \frac{Q}{2\pi^{3/2}\sigma_x\sigma_y\sigma_z}\exp\left[-\left(\frac{\left(x-\overline{u_x}t\right)^2}{2\sigma_x^{\ 2}}+\frac{y^2}{2\sigma_y^{\ 2}}+\frac{z^2}{2\sigma_z^{\ 2}}\right)\right] \quad ...(3)$$

If the direction of the wind speed is different from the smoke regiment, the gas diffusion rate of the observation points is decided jointly by the wind speed and the speed of the gas spreading itself. In a relatively stable atmospheric environment, the wind speed of different observation points is usually influenced by the wind direction under complicated conditions, including with the wind, local wind, no wind, completely against the wind, local against wind, etc. The angle between the line OA and the wind speed *v* is shown in Fig. 1, and the line OA is from the leakage source point O to the observation point A.

The solution of continuous point source equation with wind: The strength of *Q* at the continuous point source can be regarded as a constant. Due to the continuing role of the pollution sources, the diffusion process can be considered as the norm, namely that $\frac{\partial C}{\partial t}=0$. The concentration is only a function of the spatial coordinates.

When $\overline{u_x} \geq 1m/s$, the advective transportation on the material mass in the *x* direction is greater than the diffusion effect, which means $\overline{u_x}\frac{\partial C}{\partial x} \gg E_{t,x}\frac{\partial^2 C}{\partial x^2}, E_{t,x}\frac{\partial^2 C}{\partial x^2}$ can be ignored. The boundary conditions: $x = y = z = 0$, then $C \to \infty$; $x\to\infty$, $y\to\infty$, $z\to\infty$, then $C \to 0$.

Considering the above conditions, the analytical solution of the continuous point source with wind can be obtained as follows (Eq. 4):

$$C(x,y,z,t) = \frac{Q}{2\pi\overline{u_x}\sigma_y\sigma_z}\exp\left[-\left(\frac{y^2}{2\sigma_y^{\ 2}}+\frac{z^2}{2\sigma_z^{\ 2}}\right)\right] \quad ...(4)$$

The correction solution of an elevated point source model: In the process of various pollutants transferring, they are more or less at a certain height (plus the height of the building in the city). Since, it is not accurate to only consider the pollutants spreading on the ground, the effective height of the pollutants transportation should be counted.

For the instantaneous elevated point sources without wind, the formula 2 can be corrected as:

$$C(x,y,z,t) = \frac{Q}{2\pi^3\sigma_x\sigma_y\sigma_z^{3/2}}\exp\left[-\left(\frac{x^2}{2\sigma_x^{\ 2}}+\frac{y^2}{2\sigma_y^{\ 2}}\right)\right]\{\exp[-\frac{(z-H_\varepsilon)^2}{2\sigma_z^{\ 2}}]+\exp[-\frac{(z+H_\varepsilon)^2}{2\sigma_z^{\ 2}}]\} \quad ...(5)$$

For the instantaneous elevated point sources with wind, the formula (3) can be corrected as:

$$C(x,y,z,t)=\frac{Q}{2\pi^3\sigma_x\sigma_y\sigma_z^{3/2}}\exp\left[-\left(\frac{x-\bar{u}_x t^2}{2\sigma_x^2}+\frac{y^2}{2\sigma_y^2}\right)\right]$$

$$\{\exp[-\frac{(z-H_\varepsilon)^2}{2\sigma_z^2}]+\exp[-\frac{(z+H_\varepsilon)^2}{2\sigma_z^2}]\} \quad ...(6)$$

For a continuous elevated point sources with wind, the formula 4 can be corrected as:

$$C(x,y,z,t)=\frac{Q}{2\pi^3\sigma_x\sigma_y\sigma_z^{3/2}}\exp\left(-\frac{y^2}{2\sigma_y^2}\right)$$

$$\{\exp[-\frac{(z-H_\varepsilon)^2}{2\sigma_z^2}]+\exp[-\frac{(z+H_\varepsilon)^2}{2\sigma_z^2}]\} \quad ...(7)$$

Where, H_ε is the effective height.

Formula 5 and formula 6 are the instantaneous transient elevated point sources of Gaussian model without wind and with wind, respectively. Formula 7 is a Gaussian plume model of continuous elevated point sources with wind.

The Gauss smoke cloud model and the Gaussian plume model are classified according to the release time of the leakage source and the continuity and instantaneity of gas diffusion. The instantaneous discharge time is shorter than the leakage diffusion time. The gas diffusion model of instantaneous leakage shows that an air mass is instantly released in a very short period of time. The Gauss smoke cloud model is usually adopted for the mathematical description. The continuous leakage means that a continuous leakage source or the leakage time is greater than or equal to the diffusion time. The continuous leakage of atmospheric diffusion model is a kind of stable discharge. The gas emission in a period of time is relatively stable.

In the homogeneous steady flow field, the simulation results of the two models are similar. In the non-uniform stable flow field, the simulation results of the segmented plume model are discrete, while the smoke model conforms to the actual situation. Therefore, the Gauss smoke cloud model can overcome the limitations of the Gaussian plume model. So the Gauss smoke cloud model is adopted to solve the problem of diffusivity of $PM_{2.5}$.

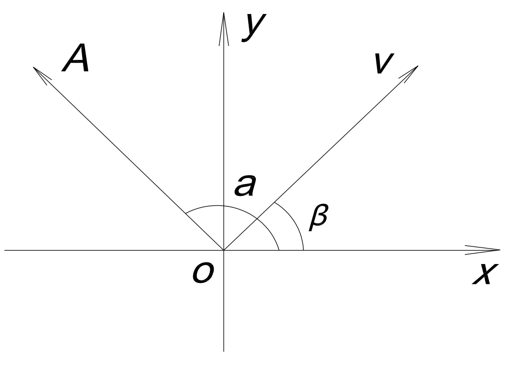


Fig. 1. The relationship graph of the line OA and the wind speed in the x-y coordinate system.

NUMERICAL ANALYSIS OF GAUSSIAN SMOKE CLOUD MODEL

According to the above analysis of the models, we can only use the Gauss smoke cloud model to solve the problem of the diffusivity of $PM_{2.5}$. And comparing the conditions of with wind and without wind, a better model was chosen.

Take the $PM_{2.5}$ monitoring values of Jingkai District in Xi'an city on January 1, 2013 as an example, and supposing that the wind direction and the $PM_{2.5}$ diffusion direction are not in the same line, then formula 6 can be described as follows:

$$C(x,y,z,t)=\frac{Q}{2\pi^3\sigma_x\sigma_y\sigma_z^{3/2}}\exp\left[-\left(\frac{\left(x-\mu|\cos\alpha|t\right)^2}{2\sigma_x^2}+\frac{\left(y-\mu|\sin\alpha|t\right)^2}{2\sigma_y^2}\right)\right]$$

$$\{\exp[-\frac{(z-H_\varepsilon)^2}{2\sigma_z^2}]+\exp[-\frac{(z+H_\varepsilon)^2}{2\sigma_z^2}]\} \quad ...(8)$$

For the solution of the model, the diffusion parameter σ can be obtained by using Pasquale grade (Table 1) and Briggs diffusion parameters (Table 2) (Robins 2003).

The wind in Xi'an is not very strong, in which the speed of 4 m/s is common. Also the illumination in Xi'an is not generally strong. The atmospheric stability in Xi'an is the level B in Pasquale grade table. In the Briggs diffusion parameters, one can get the atmospheric diffusion parameters as follows:

$$\sigma_y=0.32x(1+0.0004x)^{-1/2}, \sigma_z=0.24x(1+0.001x)^{-1/2}$$

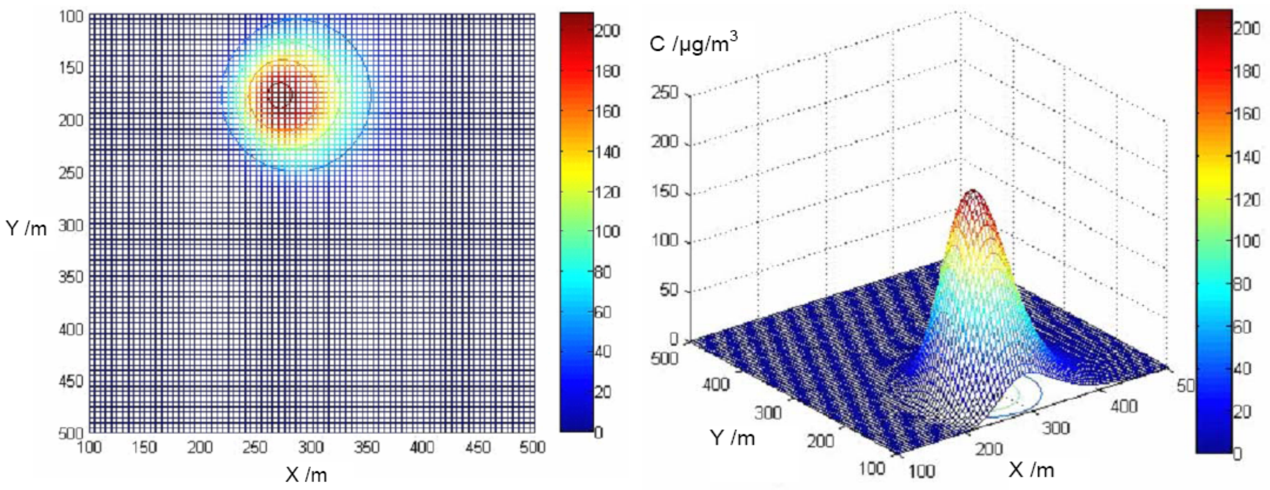
Based on the above parameters given, the 2d and 3d stereogram of $PM_{2.5}$ diffusion in Jinkai District in Xi'an on January 1, 2013 can be drawn through MATLAB (Fig. 2). And the spread stereogram of $PM_{2.5}$ can be drawn through MATLAB (Fig. 3).

From Fig. 2, one can see that the density of the source coordinates (280,180) is 215. However, this value is not consistent with the actual measured data. From Fig. 3, one can see that the density of the source point coordinates (418,192) is 65. Within the permit scope, the value is similar with the monitoring value where the density of the source coordinates (420,170) is 70. Thus, it is practical to consider

Table 1: Pasquale grade.

The ground wind speed at height of 10 m (m/s)	Daytime sunlight			A cloudy day or at night	Night	
	Strong	Medium	Weak		Cloud cover or low clouds > 4 m/s	< 4 m/s
< 1.9	A	A-B	B	D		
2-2.9	A-B	B	C	D	E	F
3-4.9	B	B-C	C	D	D	E
5-5.9	C	C-D	D	D	D	D
>6	C	D	D	D	D	D

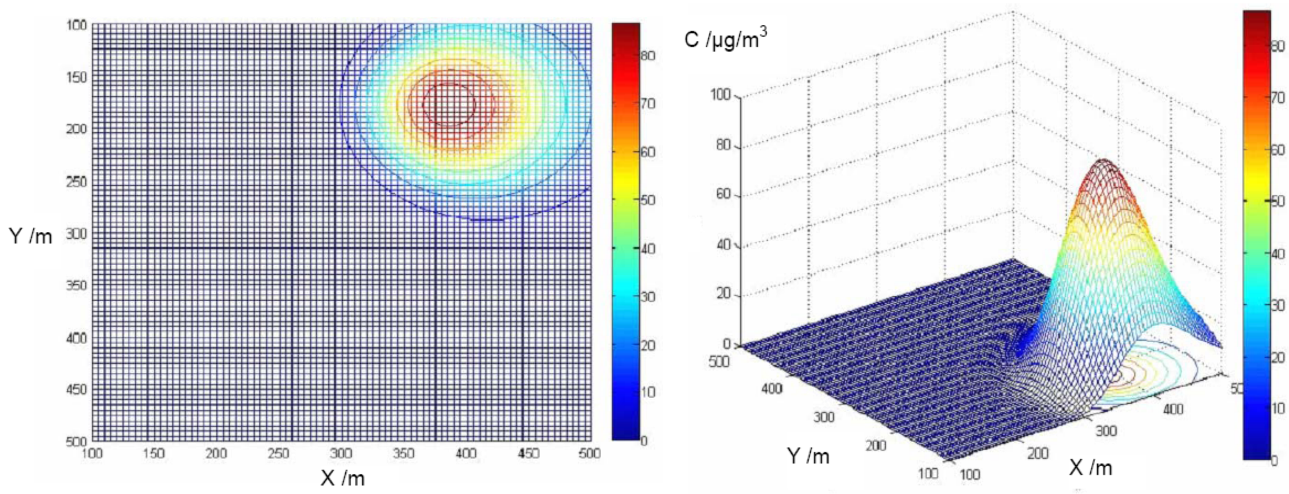
Notes: A-especially unstable, B-unstable, C-little unstable, D-normal, E-little stable, F-stable



(a) 2d

(b) 3d

Fig. 2: The pollution distribution diagram of Jingkai district's $PM_{2.5}$ on January 1, 2013.



(a) 2d

(b) 3d

Fig. 3: The prediction distribution diagram of Jingkai District's $PM_{2.5}$ on January 2, 2013.

Table 2: Briggs parameters.

Stability	Cities (100m ≤x≤ 10000m)	
	σ_y (m)	σ_z (m)
A	$0.32x(1+0.0004x)^{-1/2}$	$0.24x(1+0.001x)^{-1/2}$
B	$0.32x(1+0.0004x)^{-1/2}$	$0.24x(1+0.001x)^{-1/2}$
C	$0.22x(1+0.0004x)^{-1/2}$	$0.20x$
D	$0.16x(1+0.0004x)^{-1/2}$	$0.14x(1+0.001x)^{-1/2}$
E	$0.11x(1+0.0004x)^{-1/2}$	$0.08x(1+0.001x)^{-1/2}$
F	$0.11x(1+0.0004x)^{-1/2}$	$0.08x(1+0.001x)^{-1/2}$

the status of the wind. From the above analysis, the Gauss smoke model with wind, is of representative significance, which can reliably analyse the actual problem.

CAUSES AND GENERAL RULES OF $PM_{2.5}$

According to the existing research results, one can find that the $PM_{2.5}$ formation is related with a number of factors in Xi'an. Firstly, a large amount of industrial waste gas and the population of food consumption will increase the $PM_{2.5}$ concentrations; the intensive industrial and residential areas are the origins of $PM_{2.5}$. Secondly, setting off firecrackers during the traditional Spring Festival and Lantern Festival can also increase $PM_{2.5}$ concentrations significantly. Thirdly, the exhaust from automobiles and the coal consumption contribute to the $PM_{2.5}$ pollution together. So human activities have become the leading contributors to $PM_{2.5}$.

In general, there are three kinds of the $PM_{2.5}$ formations: (1) Direct discharge in solid forms of a particle; (2) The discharge gas with the high temperature that can be condensed into a solid condensation particles in the process of dilution and cooling of a plume; and (3) The gaseous pollutants that are generated by atmospheric chemical reactions of the secondary particles.

The main particles of $PM_{2.5}$ are generated by fossil fuels (mainly oil and coal) and biomass fuel combustion. But some areas of the industrial processes can also produce a large number of $PM_{2.5}$ at a time. Another particle source is from top-dress and top-dress raising unorganized emissions in the mineral processing and refining process and so on. Other sources such as construction, farms and wind erosion of the surface dust can also make a little contribution to the environmental $PM_{2.5}$. The condensed particles mainly consist of the semi volatile organic compounds, and the common gaseous pollutants through the heterogeneous chemical reaction can be converted into tiny particles. In most places, sulphur and nitrogen observed is the main composition of $PM_{2.5}$, and the secondary organic aerosols may also be important components in some areas.

There are many factors that influence the evolution of $PM_{2.5}$. These factors include four aspects. The first is the discharge conditions of the pollution sources, such as emission height and emission distance of the pollution sources. The second is the meteorological factors, such as temperature, gas pressure and wind speed. The third is the topography factors, such as hills and valleys, beach and land, or the urban heat island. The fourth is the characteristics of $PM_{2.5}$, which have lots of connection with other major air pollutants.

CONCLUSION

The current situation of China's air pollution is still very serious, especially concerning the smoke cloud pollution. So the Gaussian smoke cloud model is established to describe the distribution of $PM_{2.5}$. By the space-time image and a large amount of data, the distribution characteristics of $PM_{2.5}$ are summarized and the main causes and the evolution of the $PM_{2.5}$ are also analysed.

The accuracy of the model is verified by the practical monitoring data. There are three kinds of the $PM_{2.5}$ formation. The evolution characteristics and many influential factors of $PM_{2.5}$ are analysed. The results show that the human activities play the leading role for $PM_{2.5}$. Since human existence cannot be lacking of air, let us start now to work together to protect the atmospheric environment.

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