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Original Research Paper

A Finite Difference Model on Atmospheric Pollution and its Application

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ABSTRACT

In view of near-ground atmospheric problem, near-ground atmospheric pollution model was established. Because the applicability of analytical solutions is extremely limited for such conditions, and the distribution and transport of pollutants in air are controlled by geographical conditions, numerical techniques are essential for air pollution modelling. In this paper, finite differential method is used to establish plane two-dimensional numerical model of near-ground atmospheric pollution belt, and truncation errors associated with finite-difference solution of atmospheric pollution were corrected based on the Taylor analysis. The results indicate that this method provides the references for the forecast of pollutants and the management and evaluation of air resources.

INTRODUCTION

With the development of industry, construction and transportation, many pollutants occur in higher quantities causing several environmental problems. Many studies on air pollution modelling and forecasting have been developed at home and abroad, and different air environment prediction models were built, such as Model 3, MM5, CAMX, multi-dimension multi-box model and so on. Byun & Ching (1999) developed EPA Models-3. In the models, two-dimensional, multi-direction model only considers the vertical diffusion, not plane diffusion. Meng et al. (2006) simulated the atmospheric pollution in Beijing and Li et al. (2005) and Li & Shi Jianwu (2007) studied near-ground atmospheric pollution.

In this paper, on the basis of other scholars, near-groundwater atmospheric pollution model is established. And truncation errors associated with finite-difference solution of atmospheric pollution were corrected based on the Taylor analysis.

ESTABLISHMENT OF THE FINITE DIFFERENTIAL EQUATION OF ATMOSPHERIC POLLUTION

Assuming air pollutant particles, air environment particles have the same hydromechanics characteristics. On the basis of discussing parameters and variables, the finite differential equation of air pollution is deduced according to the principles of mass conservation and energy conservation. The process is as follows.

As shown in Fig. 1, pollutant inputting of each volume element in X direction at unit time is:

$$[u_x \cdot c + (-E_x \cdot \frac{\partial(c)}{\partial x})]\Delta y \Delta z$$

Pollutant outputting of each volume element in X direction at unit time is:

$$u_x \cdot c + \frac{\partial u_x \cdot c}{\partial x}\Delta x + (-E_x \frac{\partial c}{\partial x}) + \frac{\partial}{\partial x}(-E_x \cdot \frac{\partial c}{\partial x})\Delta x]\Delta y \Delta z$$

So the pollutant change quantity in X direction at unit time is:

$$[u_x \cdot c + (-E_x \cdot \frac{\partial c}{\partial x})]\Delta y\Delta z - u_x \cdot c + \frac{\partial u_x \cdot c}{\partial x}\Delta x + (-E_x \frac{\partial c}{\partial x}) + \frac{\partial}{\partial x}(-E_x \cdot \frac{\partial c}{\partial x})\Delta x]\Delta y\Delta z =$$

$$-[\frac{\partial(u_x \cdot c)}{\partial x} + \frac{\partial}{\partial x}(-E_x \cdot \frac{\partial(c)}{\partial x})]\Delta x\Delta y\Delta z$$

Similarly, the pollutant change quantities in Y, Z direction at unit time respectively are:

$$\ddot{y} -[\frac{\partial(u_y \cdot c)}{\partial y} + \frac{\partial}{\partial y}(-E_y \cdot \frac{\partial(c)}{\partial y})]\Delta x\Delta y\Delta z - [\frac{\partial(u_z \cdot c)}{\partial z} + \frac{\partial}{\partial z}(-E_z \cdot \frac{\partial(c)}{\partial z})]\Delta x\Delta y\Delta z$$

If air pollution takes place, attenuation reactions and contains sources and sinks in the volume element, corresponding pollutant change quantity will be $(\otimes s - \otimes k \cdot \otimes c)\Delta x \Delta y \Delta z$. Thereupon, in the unit time pollutant change quantity of the volume element is:

$$\frac{\partial(c)}{\partial t}\Delta x\Delta y\Delta z = -[\frac{\partial(u_x \cdot c)}{\partial x} + \frac{\partial}{\partial x}(-E_x \cdot \frac{\partial c}{\partial x})]\Delta x\Delta y\Delta z - [\frac{\partial(u_y \cdot c)}{\partial y} + \frac{\partial}{\partial y}(-E_y \cdot \frac{\partial(c)}{\partial y})]$$

$$\Delta x\Delta y\Delta z - [\frac{\partial(u_z \cdot c)}{\partial z} + \frac{\partial}{\partial z}(-E_z \cdot \frac{\partial c}{\partial z})]\Delta x\Delta y\Delta z - (s - k \cdot c)\Delta x\Delta y\Delta z$$

In a homogeneous flow field, u_x and E_y are the non-dynamic volumes, which can be taken as constants. Order the volume element $\Delta x \Delta y \Delta z = 1$, then the following equation can be obtained:

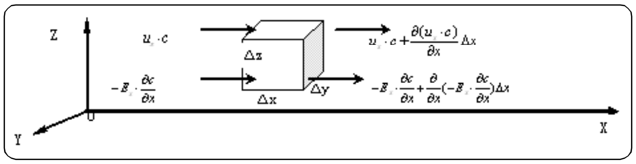

Fig.1: Mass balance in a volume element.

$$\frac{\partial c}{\partial t} = E_x \cdot \frac{\partial^2 c}{\partial x^2} + E_y \cdot \frac{\partial^2 c}{\partial y^2} + E_z \cdot \frac{\partial^2 c}{\partial z^2} - u_x \cdot \frac{\partial c}{\partial x} - u_y \cdot \frac{\partial c}{\partial y} - u_z \cdot \frac{\partial c}{\partial z} + s - k \cdot c \quad ...(1)$$

Where,

c - the concentrations of pollutants, *mg/m³*

E_y - the grey diffusion coefficients in the landscape orientation, *m²/s*

u_x - the grey wind speed in the predominant direction (vertical), *m/s*

s - the sources and sinks of air pollutants, *mg/m³.s*

k - the attenuation coefficient of air pollutants, *s⁻¹*

t - the migration time of air pollutants, *s*

In a homogeneous flow field, assuming the X direction is leading wind direction, we can write $u_y = 0$、$u_z = 0$, If only two-dimensional convection diffusion problems of air pollution is considered, then $u_x \cdot \frac{\partial c}{\partial x} >> E_x \cdot \frac{\partial^2 (c)}{\partial x^2}$ ÿ and $E_z = 0$. After a series of predigestion, two-dimensional finite differential equations of air pollutants can be written as:

$$\frac{\partial c}{\partial t} = E_y \cdot \frac{\partial^2 (c)}{\partial y^2} - \frac{\partial (c \cdot u_x)}{\partial x} + s - k \cdot c \quad ...(2)$$

DIFFERENTIAL NUMERICAL MODEL OF AIR POLLUTION

The governing equation of atmospheric pollution is:

$$\frac{\partial (c)}{\partial t} = E_y \frac{\partial^2 (c)}{\partial y^2} - \frac{\partial (c \bullet u_x)}{\partial x} + S - k \bullet c \quad ...(3)$$

Using finite difference equation to replace differential equation as following:

$$\frac{\partial (c)}{\partial t} = \frac{(c)_i^{n+1} - (c)_i^n}{\Delta t} \quad ...(4)$$

$$\frac{\partial^2 (c)}{\partial x^2} = \frac{(c)_{i+1} - 2(c)_i + (c)_{i-1}}{(\Delta x)^2} \quad ...(5)$$

$$\frac{\partial (c)}{\partial x} = \frac{(c)_{i+1} - (c)_i}{\Delta x} \quad ...(6)$$

Because the finite difference approach uses limited developments of derivatives, it is only an approximation of partial differential equations leading to truncation errors. Truncation errors affect the accuracy of numerical simulations. A Taylor series expansion of c about any grid point is used to determine the form of truncation errors by Ataie-Ashtiani et al. (1999) and Ataie-Ashtiani & Hosseini (2005). If terms of third and higher orders are neglected, then:

$$(c)_{i,j}^{n+1} \approx (c)_{i,j}^n + \Delta t \frac{\partial (c)}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 (c)}{\partial t^2} \quad ...(7)$$

$$(c)_{i\pm1,j}^n \approx (c)_{i,j}^n \pm \Delta x \frac{\partial (c)}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 (c)}{\partial x^2} + 0(\Delta x^3) \quad ...(8)$$

$$(c)_{i,j\pm1}^n \approx (c)_{i,j}^n \pm \Delta y \frac{\partial (c)}{\partial y} + \frac{\Delta y^2}{2} \frac{\partial^2 (c)}{\partial y^2} + 0(\Delta y^3) \quad ...(9)$$

The second-order temporal derivative of c is written in terms of spatial derivatives using the differentiated form. The transport parameters are assumed to be constant within each combination of time and space increments in the finite difference calculations. Thus to second order accuracy:

$$\frac{\partial^2 (C)}{\partial t^2} = [-2(k)(E_y)] \frac{\partial^2 (C)}{\partial y^2} - 2(k)(u_x) \frac{\partial (C)}{\partial x} - (k)(S) + (k)^2 (C) \quad ...(10)$$

Equation 3 may then be written as:

$$\frac{\partial (c)}{\partial t} = [E_y - (k)(E_y)\Delta t] \frac{\partial^2 (c)}{\partial y^2} - [u_x - (u_x)(k)\Delta t] \frac{\partial (C)}{\partial x} + [1 - \frac{\Delta t}{2} k] S - [k + \frac{\Delta t}{2} (k)^2] \bullet c \quad ...(11)$$

$$E_y - (k)(E_y)\Delta t = (E_y)^*,\ u_x - (u_x)(k)\Delta t = (u_x)^*,\ k + \frac{\Delta t}{2}(k)^2 = (k)^*$$

To remove the induced truncation errors from the finite difference model, the model can be rewritten as:

$$\frac{(c)_{i,j}^{n+1} - (c)_{i,j}^n}{\Delta t} = (E_y)^* \frac{(c)_{i,j+1} - 2(c)_{i,j} + (c)_{i,j-1}}{\Delta y^2} - \frac{(u_x)^*}{\Delta x}((c)_{i+1,j} - (c)_{i,j}) + (1 - \frac{\Delta t}{2} k)(s)_{i,j} - [k + \frac{\Delta t}{2}(k)^2] C_i^n \quad ...(12)$$

Namely: $\frac{(E_y) \cdot \Delta t}{\Delta y^2} = a$, $\frac{(u_x) \cdot \Delta t}{\Delta x} = b$ ÿ

$$\{1 + b + 2a + \Delta t \cdot (k)\} \cdot c_{i,j,k+1} - a \cdot c_{i,j-1,k+1} - b \cdot c_{i,j+1,k+1} - b \cdot c_{i-1,j,k+1} - \Delta t \cdot S_{i,j,k+1} = c_{i,j,k}$$

According to the finite differential equation, Matlab program is written.

APPLICATION

Study area

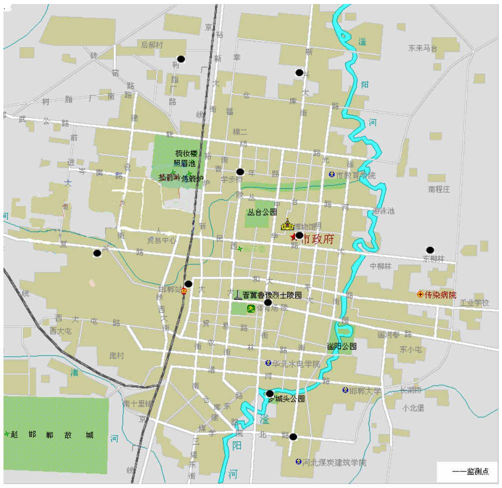

Fig. 2: Sketch of study area.

80	81	51	53	52	54	55	56	57
79	1	2	3	4	5	6	7	58
78	8	9	10	11	12	13	14	59
77	15	16	17	18	19	20	21	60
50	22	23	24	25	26	27	28	61
76	29	30	31	32	33	34	35	62
75	36	37	38	39	40	41	42	63
74	43	44	45	46	47	48	49	64
73	72	71	70	69	68	67	66	65

Fig.3: Number given to grids in simulated region.

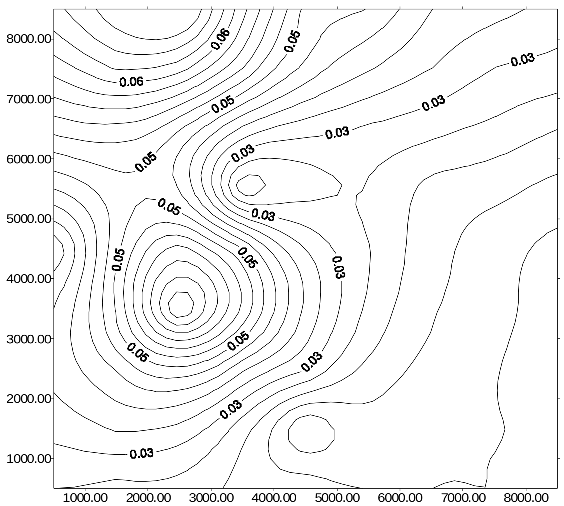

Fig. 4: Simulated result in first time interval.

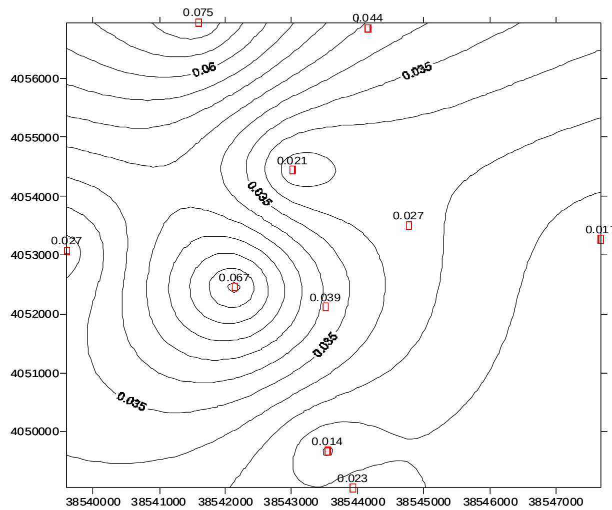

Fig. 5: Observed result in first time interval

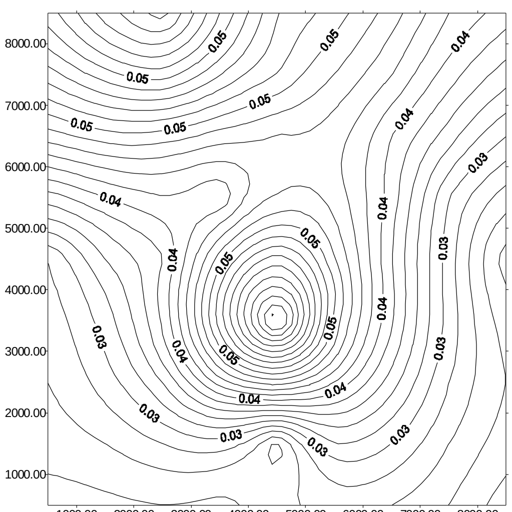

Fig. 6: Simulated result in third time interval.

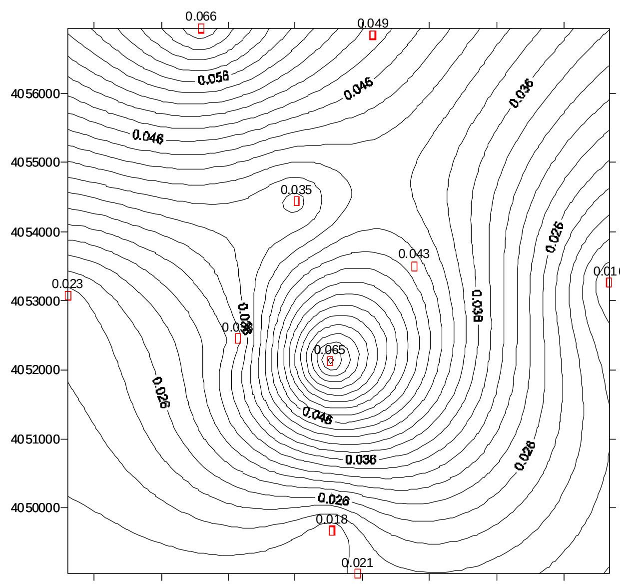

Fig. 7: Observed result in third time interval.

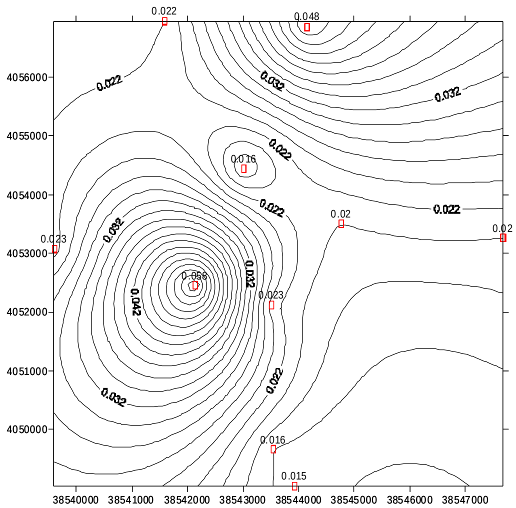

Fig.8: Simulated result in fifth time interval.

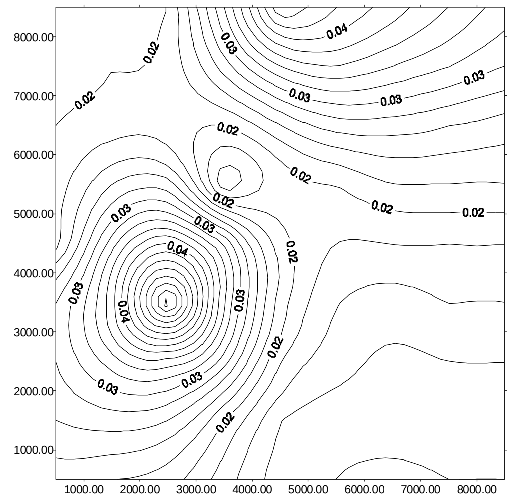

Fig. 9: Observed result in fifth time interval.

Handan is a city located in the south of Hebei Province (Fig. 2). The air quality in Handan is very poor. Air contaminants include TSP, SO_2 and nitrogen oxides. Atmospheric pollution index is 0.84 which belongs the semi-healthy city. A 9×9 rectangle gridding system is founded, the border length of each rectangle gridding is 0.5km × 0.5km. So there are 49 inner nodes and 52 outer nodes. The same initial conditions and boundary conditions are supposed in the two models when the numerical results are compared.

Specific parameters can be expressed as:

$$c = 0, t = 0, x > 0, y > 0\,;$$

$$c = 0, t \geq 0, x \to \infty, y \to \infty$$

In order to simulate the air pollution in Handan city, the region is subdivided into 9 × 9 grids. The side of every grid is 1000m. Among them, there are 49 inner nodes and 52 outer nodes. According to the certain sequence, the grid is given a number, which is shown in Fig. 3.

RESULTS

In the heating period, the initial time is 13th in November, 2004. The monitoring concentration of air contaminant in the day time is considered the initial concentration. The data of source and assemble are determined by the certain model. The simulated time is 105 days and divided as 22days, 38days and 45days. In unheating period, the initial time is 2004.03.31, the simulated time is 207days and divided as 8, 36, 19, 36, 37, 36, 35 days.

The distribution of NOx in Handan city can be seen in Figs. 4-9. The results indicate that this kind of numerical model can simulate the NOx near-ground atmospheric belt. In heating period, the concentration is higher than other periods. Seen from the simulated results, it is reliable and suitable for the observed data which indicate that the numerical method can be adopted.

CONCLUSIONS

1. Fnite difference model is an attempt to simulate atmospheric pollution, which is proved feasible.
2. The case analysis indicates that the finite differential numerical model of atmospheric pollution can simulate and predict the pollution in this area, and its results provide the references for the forecast of pollutants and the management and evaluation of air resources.
3. The results, which are calculated from corrected model, are precise.

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