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NUMERICAL SIMULATION FOR THE EFFECTS OF PBL AND THE SURFACE ON POLLUTANT CONCENTRATIONS

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ABSTRACT

On the basis of theoretical and experimental results of study of planetary boundary layer (PBL), the physical parameters describing the structure of PBL are calculated by using the data obtained from a meteorological tower and the effects of PBL and the surface on pollutant concentrations are numerically simulated with a time-dependent two-dimensional advection and diffusion equation.

It is shown that the diurnal variation of PBL results in that of concentration. The height of mixing layer is an important factor to determine the ground-level concentration. As for an elevated point source, the height of mixing layer, growing from lower to higher than the releasing height is a necessary condition for the phenomenon of fumigation. It is also shown that the surface may be considered as a boundary with perfect reflection when $V_d \leqslant 0.001$ m s^{-1}, but has an important effect on concentration and must be carefully dealt with when $V_d \geqslant 0.01$ m s^{-1}.

I. INTRODUCTION

In the study of mesoscale air pollution problems, various meteorological factors, such as atmospheric stability, wind (speed and direction), diffusivity, mixing height and features of the surface boundary, which play an important role in air pollution and strongly influence the distributions of pollutants, have been more and more concerned by many researchers in recent years.

Ragland et al.[1] have investigated the effects of profiles of variable wind and diffusivity on pollutant concentrations. Tangermann[2] has conducted a numerical simulation of diffusion of pollutants in a stratified PBL and Carmichal et al.[3] have argued the dynamical response of a step model, describing the development of mixing layer under some ideal conditions. All above works have given some useful results. However, the development of mixing layer is not in step-fashion as a matter of fact, concentration is affected by the structure of the whole PBL, and the underlying surface has important effects on the results of pollutant dispersion.

The purpose of this paper is that by using the data of wind and temperature obtained from a meteorological tower, the calculations of parameters for describing the structure of PBL are conducted based on theoretical and experimental results of PBL, and then, by taking the calculated parameters as an input, the effects of the structure of PBL and the surface on pollutant concentrtions are discussed through a time-dependent two-dimensional advection and diffusion equation.

II. EQUATION AND ITS SOLUTION

A time-dependent two-dimensional advection and diffusion equation with proper initial and boundary conditions is chosen to simulate the effects of the structure of PBL and the surface, i.e.

$$\frac{\partial C(x,z,t)}{\partial t}+u(z,t)\frac{\partial C(x,z,t)}{\partial x}=\frac{\partial}{\partial z}\left[K(z,t)\frac{\partial C(x,z,t)}{\partial z}\right], \qquad (1)$$

where C is the pollutant concentration, $u(z, t)$, the wind speed along the x-direction, $K(z, t)$, the vertical diffusivity, x and z are the Cartesian coordinates, and t is the time.

The initial condition is

$$C(x,z,0)=0. \qquad (2)$$

If the concentration at the source is assumed to be a δ-function, then

$$C(0,z,t)=\frac{Q}{u(h)}\delta(z-h), \quad t>0. \qquad (3)$$

The boundary condition is

$$K(z,t)\frac{\partial C}{\partial z}=V_d C, \quad z=0,\ z_H, \qquad (4)$$

where Q is the source strength, h, the source height, z_H, the height of mixing layer, and V_d the deposition velocity. Eq. (1) may be solved by the method of fractional steps[4]. According to this technique, Eq. (1) can be split into two one-dimensional equations, i. e.

$$\frac{\partial C}{\partial t}+u(z,t)\frac{\partial C}{\partial x}=0, \qquad (5)$$

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial z}\left[K(z,t)\frac{\partial C}{\partial z}\right]. \qquad (6)$$

In a given time step $t+\Delta t$, Eqs. (5) and (6) should be treated interatively to obtain the solution of Eq. (1). In other words, in the first step the advection equation (5) is solved in the whole x–z integration region over the time interval Δt with the concentration at time t as initial condition and Eq. (3) as boundary condition. The diffusion equation (6) is solved, in the second step over the same time interval and here, the initial condition is provided by the concentration field obtained from the first step and boundary condition by Eq. (4). Thus, the concentration at time $t+\Delta t$ is obtained and that is an approximation to the solution of Eq. (1).

In order to avoid the pseudo-diffusion error caused by solving advection equation with a finite-difference scheme, a Lagrangian technique proposed by Runca and Sardei[5] is used for Eq. (5), but Eq. (6) is solved with a conventional Eulerian finite-difference scheme[6]. However, this numerical treatment brings a new problem. Because the Lagrangian technique determines the transporting trajectories of the pollutants, but a fixed grid frame is required for the Eulerian finite-difference scheme and the calculations of concentration are carried out for each grid point at any time. When wind speed is not constant, Eq. (5) could not be satisfied by translation the whole concentration field to the grid points of the Eulerian frame. Therefore the two equations could not be well connected together. This difficulty may be solved by selecting a proper step-function. At any time step n, the step-function for a grid point k is defined as

$$u_k^n = P_k^n / q u_{\max}, \quad P_k^n \leqslant q,$$
$$(k = 1, 2, \cdots, N_z; \quad n = 1, 2, \cdots, T) \tag{7}$$

where N_z denotes the number of vertical grid points T, the travel distance of pollutants, u_{max}, the maximum wind speed at the time of interest, P and q are positive integers, and q should be large enough to give good approximation to the $u(z, t)$ profiles. The horizontal interval Δx is defined as

$$\Delta x = \frac{u_{\max}}{q} \Delta t. \tag{8}$$

Thus, the pollutants with a speed of u_k^n, after a time step Δt is translated to the distance $P_k \Delta x$. In doing so, Eqs. (5) and (6) could be well connected.

The above Lagrangian treatment of advection equation does satisfy the mass conservation and avoid pseudo-diffusion error generated by solving advection equation with the conventional Eulerian finite-difference scheme. For solving diffusion equation, the implicit Crank–Nicholson difference scheme

$$C_{j,k}^{n+1} - \frac{\Delta t}{2(\Delta z)^2}[K_{k+\frac{1}{2}}^n (C_{j,k+1}^{n+1} - C_{j,k}^{n+1}) - K_{k-\frac{1}{2}}^n (C_{j,k}^{n+1} - C_{j,k-1}^{n+1})]$$
$$= C_{j,k}^n + \frac{\Delta t}{2(\Delta z)^2}[K_{k+\frac{1}{2}}^n (C_{j,k+1}^n - C_{j,k}^n) - K_{k-\frac{1}{2}}^n (C_{j,k}^n - C_{j,k-1}^n)] \tag{9}$$

is used, where n denotes time, j and k represent the numbers of grid points in x and z–directions, respectively. Since the implicit Crank–Nicholson difference scheme is numerically non–conditional stable, the selection of step for time or space is arbitrary except that the specific accuracy of calculation is required for certain problems.

III. PHYSICAL PARAMETERS

1. *Stability*

Atmospheric diffusion is related to turbulent intensity. Since the data of wind and temperature are provided, the Richardson number R_i is adopted to classify atmospheric stability and defined as

$$R_i = \frac{g(\partial\theta/\partial z)}{\bar{T}(\partial u/\partial z)^2}, \tag{10}$$

Where $\bar{T}$ is the mean ambient temperature (K), g, the gravitational acceleration (m s^{-2}) and θ, the potential temperature. The data of wind speed and potential temperature at two heights, 9 m and 32 m are utilized for the calculations.

2. *Mixing Height*

Much work has been done on the study of mixing height both at home and abroad. In this paper, a mxing height model developed by USAF[7] is used. It reads

$$Z_H = 20.17(6 - P_L)(\bar{T} - T_d) + 0.00725 P_L (u_* + 0.5) / f \ln \frac{z}{z_0}, \tag{11}$$

where P_L denotes the Pasquill stability, and its values are taken to be 1 for A stability to 6 for F stability, T_d is the dew point temperature (K), f, the Coriolis parameter ($\doteq 1.12 \times 10^{-4} \mathrm{s}^{-1}$), z_0, the surface roughness length, and u_z, the wind speed at z.

3. *Deposition Velocity*

The depletion of diffusion material will be produced due to the existence of the surface boundary. Deposition velocity is a measure of accumulation ability of diffusion material at the surface and it is related to the diameters of particles and features of the ground. The data collected by McMahon[8] from the measurements in laboratories and fields showed that for particle in the range of 0.04—30 μm in diameter, the deposition velocity over grassland normally varies from 0.02 to 4 cm s^{-1}. From the point of view of numerical experiment, several deposition velocities will be chosen and discussed in contrast with the situation where $V_d=0$.

4. *Diffusivity*

The Businger's empirical expression[9] as well as the Dyer and Hicks'[10] is utilized for diffusivity in the surface layer. i. e.

$$K(z)=0.4u_*z(1-5R_i)^{-1} \quad \text{for } R_i \geqslant 0, \tag{12}$$

$$K(z)=0.4u_*z(1-16R_i)^{\frac{1}{2}} \quad \text{for } R_i<0, \tag{13}$$

where u_* is the frictional velocity and can be derived from the measurements of wind and temperature on the basis of similarity theory[11].

Although little information about K-profile in PBL is known due to the limitations of theory and technique, the observational results from Moor and Clarke et al. encourage us to utilize the Kumar's expression[12] with an exception that the term of molecular diffusivity is omitted. The Kumar's expression may be written as

$$K(z)=(K_c-\nu)\left(1-\frac{z-z_c}{z_H-z_c}\right)^R+\nu, \tag{14}$$

where K_c is the diffusivity at z_c (the height of the surface layer), ν is the diffusivity at H and its values are taken as 0.1, 0.6, and 4.0 $\mathrm{m}^2\ \mathrm{s}^{-1}$ for neutral, stable and unstable conditions respectively.

5. *Profiles of Wind Speed*

The power law expression for wind speed changing with height

$$u(z)=u_1(z/z_1)^s \tag{15}$$

is used for th wholee PBL, where exponent s is calculated by the following expression according to Shir[13]

$$s=\ln(u_2/u_1)/\ln(z_2/z_1), \tag{16}$$

where u_1 and u_2 provided from measurements are the wind speeds at z_1 and z_2, respectively.

IV. RESULTS AND ANALYSES

From the point of view of application, meteorological conditions vary from time to time, the features of the ground differ from one site to another, and concentration distributions are the results influenced by all the meteorological factors. By using data of wind speed and temperature obtained from the meteorological tower on October 10, 1981, this paper is to start with the calculations of $R_i(t)$, $z_H(t)$, $u(z, t)$ and $K(z, t)$, then a numerical simulation is carried out with assumptions of $h=400$ m, $Q=1$ g m s^{-1} and $V_d=0.01$ m s^{-1}, through a time-dependent two-dimensional advection and diffusion equation, and finally, the results are analysed.

1. *Effects of the Structure of PBL on Pollutant Concentrations*

The structure of PBL is usually described by stability, wind, diffusivity, mixing height etc., and suitable combinations of the above parameters will lead to considerable diurnal variation of the structure of PBL. The meteorological conditions in the suburbs of Beijing on October 23, 1981, revealed this feature. On the whole, R_i varied from -0.1908 to 0.1854, and its values by day were negative, indicating the atmosphere being in unstable conditions but at night the values of R_i for six hours were positive, showing the atmosphere being in stable conditions. The mixing layer also has obviously diurnal variation, and it was more shallow at night with an average height of 600 m, but thicker in the daytime with an average height of 1100 m. The lowest and highest mixing heights were 255 and 1669 m respectively. The profiles of wind and diffusitivity had obviously diurnal variations too. Generally speaking, wind speeds on October, 23, 1981 were strong, and their values as well as diffusivities were greater in the daytime than at night.

Depicted in Fig. 1 are the variations of the ground-level axial concentrations against times for four distances, 5, 10, 20, and 39 km, from which the effects of the structure of PBL on ground-level axial concentrations are revealed. As expected, the ground-level axial concentrations have obvious response to the changes of the structure of PBL, i. e. concentrations are lower at night, higher by day and the amplitudes decrease with increasing distance from the source.

In order to deeply understand the effects of the structure of PBL on the whole concentration field, cases for several typical times are analysed. Illustrated in Fig. 2 are the curves of the ground-level axial concentrations against distances for four times 04, 10, 15 and 20 LST. It shows that the concentrations at 04 LST are lower than that at any other times. For both times 04 and 20 LST, the concentrations increase monotonously within distance 40 km, and the tendences of variation are nearly the same. And yet, for the times 10 and 15 LST, the concentrations increase at first and then slowly decrease with increase of distance. There exist the maximum concentrations at 10—20 km.

The concentration fields in the x—z plan and vertical profiles of winds and diffusivities are given in Fig. 3. It can be seen that the curves with narrowed-space appear at the time 04 LST, which indicate a stronger vertical concentration gradient. In contrast, the curves with widened-space appear at 10 and 15 LST, which show weaker vertical concentration gradients and the isoline of concentration 10^1 μg m^{-3} is extended to the height of 800 m beyond distance of 15 km. For the time 20 LST, the curves indicate a moderate-vertical concentration gradient. In conjunction with the parameters, i. e. R_i, mixing height wind and diffusivity, etc., whereby the structure of PBL is described, it is not difficult to understand and interpret the above phenomena.

For the time 04 LST, $R_i=0.185$, the maximum of the day, which shows the atmosphere is in a moderate-stable condition. The mixing height is as low as 260 m, approching the minimum value of the day. The value of vertical diffusivity is equal to or smaller than 4

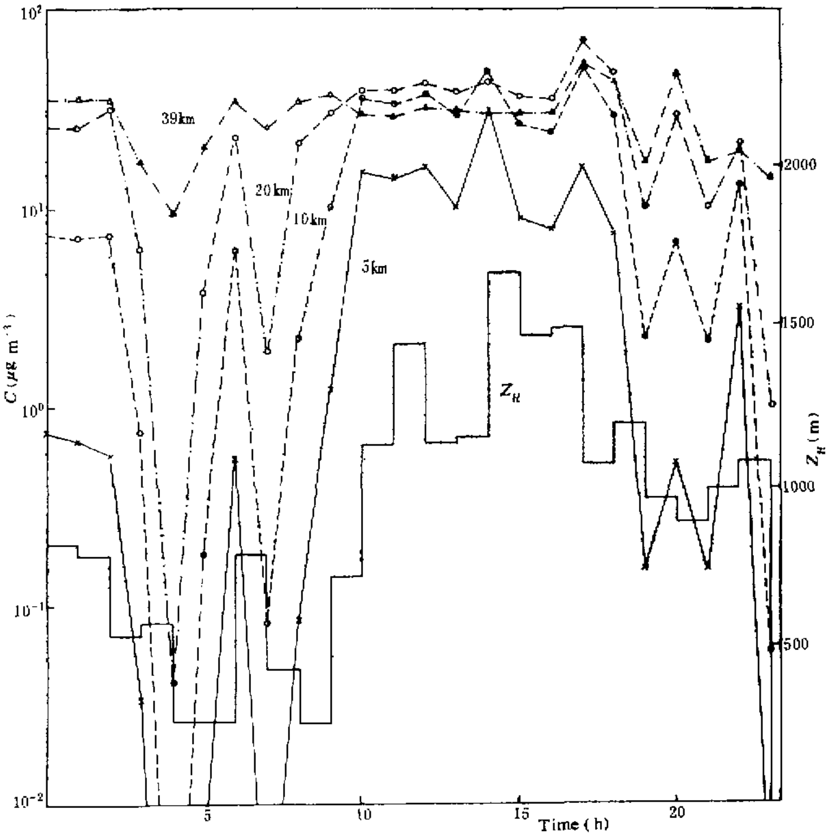

Fig. 1. Variations of mixing layer and ground-level axial concentrations against times.

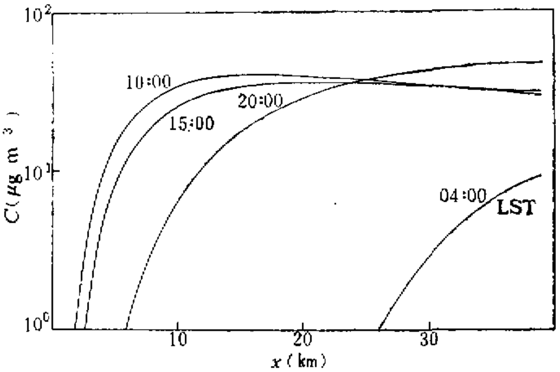

Fig. 2. Variations of the ground-level axial concentrations with distances.

$m^2\ s^{-1}$, also approximating the minimum value. The wind speeds in the whole PBL at this time are lower than the others. Simultaneously, weather shows a very unfavourable meteorological condition for the diffusion of pollutants. Furthermore, pollutants are released at height 400 m, just being above the mixing layer. Therefore, they could hardly reach the ground, resulting in the lower level axial concentrations and the higher vertical concentration gradient. For the time 10 LST, R_i equals -0.0767, which shows that the atmosphere is in a weak-unstable condition; the mixing height goes up to 1130 m, approximating the average height of the day; the K-profile strongly varies with height and reaches 54 $m^2\ s^{-1}$ at the top of the surface layer; and wind speed is faster. All of these show a better mixing ability. Moreover, the releasing height is just in the mixing layer and the pollutants could be quickly diffused in the vertical, so that the concentration gradient in the x—z plan is smaller and the maximum of ground-level axial concentration appears at distance 10—20 km downwind from the source. In comparision with the case at 10 LST, although the z_H at 15 LST is greater than that at 10 LST; R_i is negative and equal to -0.011; and wind speed and diffusivity are nearly the same for both times. Similar situation occurs at this time

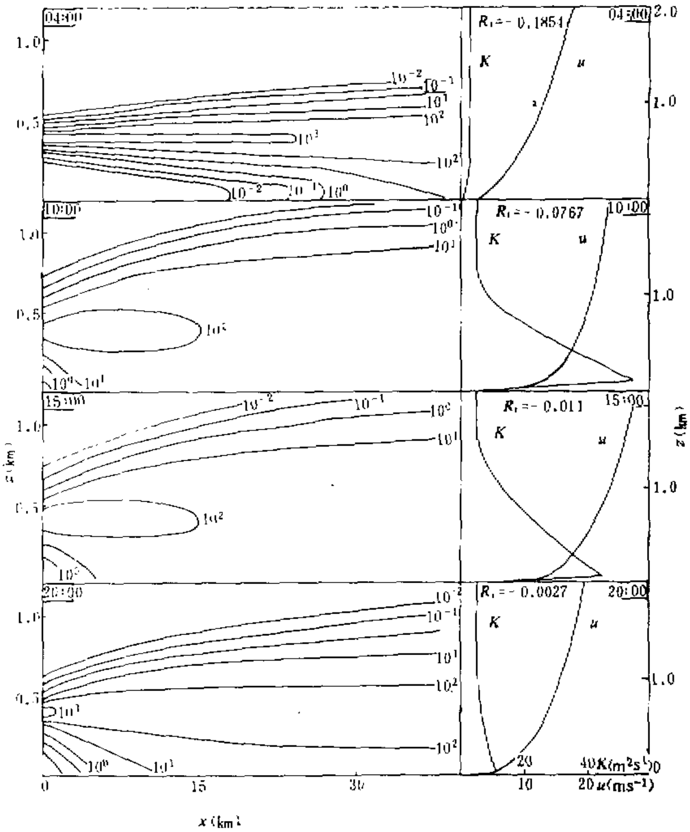

Fig. 3. The concentration fields in the x—z plan and profiles for u and K

due to the fairly alike features of PBL. For the time 20 LST, in spite of the fact that z_H descends to 880 m, the R_i is equal to -0.0027 which shows the atmosphere is in a very weak-unstable condition; the wind speed for the whole PBL is close to that at 10 LST; and the values of diffusivities are smaller than that at 10 and 15 LST and have a much slower variation. Though pollutants are released in the mixing layer, the concentration field in the x—z plan and the ground level axial concentrations are among those at 04, 10 and 15 LST due to the vertical mixing ability which is better than that at 04 LST and worse than that at 10 and 15 LST.

In all cases, the temporal and spatial distributions of concentration for pollutants released from an elevated point source are dominated by the parameters, such as stability, mixing height, wind, diffusivity etc., by which the structure of PBL is described.

In addition, from Fig. 1 one can see twice the sharply increased phenomena in concentration, i. e. the typical fumigation processes. One appears at 06 LST with a shorter persistance, and the other at 09 LST with a longer persistance and is connected with the following higher concentrations. The analyses have shown that before and after fumigation, the stability, wind and diffusivity have no considerable variations except the mixing height. However, before appearance of the fumigation phenomena, the mixing height is lower than the releasing height so that pollutants could not be well diffused and diluted. As the mixing height is developing and getting higher than the releasing height, the pollutants accumulated in the level above could be rapidly diffused to the ground and the higher ground-level concentrations occur. Therefore, the mixing height, developing from lower to higher than the releasing height is a necessary condition for inducing fumigation phenomenon and investigation of this has great significance.

2. *Effects of the Surface Boundary*

As mentioned above, boundary provides a sink for diffused pollutants, and V_d is a measure of accumulative velocity at the surface boundary. Depicted in Fig. 4 are the effects of various deposition velocities. It shows that the curve with $V_d=0.001$ m s^{-1} is not as much different as that with $V_d=0$, but the curve with $V_d=0.01$ m s^{-1} differs greatly in comparison with the same curve $V_d=0$. The former is lower than the latter by a factor of 1.25—1.3. These results indicate that in practice, the surface may be considered

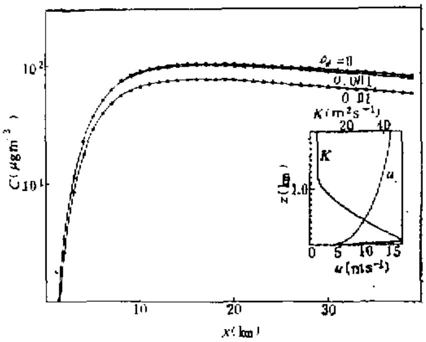

Fig. 4. Changes of the ground-level axial concentrations for various deposition velocities.
(In the figure $O_d=0$ should be corrected a5 $V_d=0$)

as a boundary with perfect reflection and has no important effects on the results of calculations provided $V_d \leqslant 0.001$ m s^{-1}. On the contrary, it does affect the results of calculations when $V_d \geqslant 0.01$ m s^{-1}. Otherwise, greater errors will be made.

V. CONCLUDING REMARKS

Numerical simulation for the effects of the structure of PBL and the surface on pollutant concentrations has shown.

(1) The variation of the structure of PBL leads to diurnal variations of concentration fields, and the concentrations are affected by the parameters describing the structure of PBL. In general, by day, vertical concentration gradient is smaller and ground-level concentration is higher because of the unstable atmosphere, thick mixing height, strong wind and diffusivity. On the contrary, vertical concentration gradient is greater and ground-level concentration is lower at night due to the stable atmosphere and weak diffusivity.

(2) The variation of mixing layer with height considerably influences the ground-level concentrations. For an elevated point source, the mixing layer growing from lower to higher than the releasing height is a necessary condition for inducing fumigation phenomenon and investigation of this has great significance in practice.

(3) The actually existed surface provides a good condition for the dry deposition of pollutants. Numerical simulation has shown that when $V_d \leqslant 0.001$ m s^{-1}, the deposition is neglegibly small and thus the ground may be considered as a boundary with perfect reflection. And yet, deposition is great and the surface should be carefully treated if $V_d \geqslant 0.01$ m s^{-1}. Otherwise, greater errors will be made.

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