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A PUFF MODEL REVISED BY MONTE-CARLO METHOD ON MESOSCALE RANGE

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ABSTRACT

A puff model is developed in this study, which simultaneously considers the Monte-Carlo technique, the time and space changes of atmospheric parameters, multiple continuity pollutant sources, linear chemical transformation and removal of pollutants, and the effect of complex terrain. The continuously observed turbulent statistical quantities, Lagrangian time scales, mesoscale flow field, and mixing layer depth in the PBL in the Dianchi area in China are directly put into the model, and the diurnal variations of air pollution are forecasted, which are dominated by such mesoscale local circulations as mountain and valley breeze, land and lake breeze, and city heat island (Kunming City). The results show that in the case of inputting the same data, they are in good agreement with the experimental data, as well as with the results of the three-dimensional advection-diffusion model (TD-ADM); the diurnal variation of mesoscale local circulation results in the obvious diurnal variation of mesoscale concentration distribution patterns; the Dianchi lake (appr. 300 km^2) has a considerable effect on the distribution of air pollution in the area.

I. INTRODUCTION

Because the Monte-Carlo method is simple and applicable, there is no difficulty in calculation as compared with the use of the diffusion equation. It has been widely used in the study of turbulence and diffusion since the mid-1970's. By using this method, much progress and lots of useful results have been obtained in the research on simulating the effect of inhomogeneous turbulence in the surface layer on feature of the diffusion, on simulating pollutant behavior under convectional condition, on the relation between Lagrangian and Eulerian time scales, and on analysing the effect of inhomogeneous terrain (Hanna, 1978; Rwnca, 1981; Reid, 1979; Durbin, 1980; Lamb, 1982; Ley, 1982; Wileon, 1981; Alsmiller, 1979). Recently, the characteristics of atmospheric turbulence and diffusion, and the distribution laws of three-dimensional concentration in the mesoscale range have been numerically simulated by Lei and Den (1986), Den and Lei (1986) with the Monte-Carlo method and some valuable results have been obtained. These numerical simulating methods and programs have provided a basis for establishing the model, but such numerical simulating work has entirely been carried out under the condition of given parameterization of PBL turbulent construction, which differs from the actual atmosphere and specific terrain to some degree. Therefore, how to apply the Monte-Carlo method to practical questions is the critical step that decides whether the method can be widely put into practice. Real application of the Monte-Carlo method to practical air pollution forecast, especially application of the technique to complex terrain, is just beginning.

The puff model (Ren and Lei et al., 1981) is widely used both at home and abroad, but a disadvantage of this kind of model is that the turbulent construction in PBL is not involved, which is very important when we put emphasis on studying practical problems in the mesoscale range.

A central problem is that the puff model designed is well combined with the Monte-Carlo method pointed out by Lei and Den (1986) and the effect of turbulent quantities must be included. *In doing so, the model can be tested using data of turbulence and mean wind in* the PBL, and data of concentrations obtained from field observations in the Dianchi area. Its function and the probability of practical utilization are also analysed.

II. ESTABLISHMENT OF THE MODEL

The plume from a continuous pollutant source is approximately simulated by a series of puffs. The concentration at a point (x, y, z) of interest is computed by summing all the contributions of the puffs to that point (Ren and Lei et al., 1981)

$$c(x,y,z,t)=\sum_{i_0=1}^{M}\sum_{j=1}^{N}Q_{i,j}P_h(x-\bar{X}_j,y-\bar{Y}_j)P_z(z,t), \tag{1}$$

where M is the total number of the pollution sources; N is the total number of puffs; P_h and P_z are the horizontal and vertical distribution functions of pollutant concentration, respectively; $Q_{i,j}$ is the source emission rate in the j-th puff emitted from the i-th source.

$$P_h(x-\bar{X}_j,y-\bar{Y}_j)=\frac{1}{2\pi\sigma_x\sigma_y}\exp\left\{-\frac{1}{2}\left[\left(\frac{x-\bar{X}_j}{\sigma_x}\right)^2+\left(\frac{y-\bar{Y}_j}{\sigma_y}\right)^2\right]\right\}, \tag{2}$$

where $\bar{X}_j$ and $\bar{Y}_j$ are the mean trajectory coordinates for the plume, σ_x and σ_y are the standard deviations of the puff trajectory. P_z is written as (Ren and Lei et al., 1981; Sheih, 1977)

$$P_z(z,t)=(4\pi K_z t)^{-1/2}\exp\left\{\frac{(z-z_s)^2}{4K_z t}-\frac{2V_{d_1}t^{1/2}}{(\pi K_z)^{1/2}}-A_1 t\right\}, \tag{3}$$

where A_1 is the chemical conversion rate of pollutant (2×10^{-5} s^{-1}, Ren and Lei et al., 1981), V_{d_1} is the dry deposition velocity (3.1 cm/s, Israel, 1974), Z_s is the plume effective emissive height. The height of plume is computed by Briggs formula (Lei et al., 1984). k_z is the vertical eddy diffusion coefficient, and takes the following form according to Pasquill (1975), Lei and Ren (1983):

$$k_z=T_L^w\sigma_w^2, \tag{4}$$

where T_L^w is the vertical Lagrangian time scale, and σ_w is the standard deviation of the vertical velocity fluctuations.

To calculate the concentration, firstly the parameters σ_x, σ_y, $\bar{X}_j$ and $\bar{Y}_j$ must be determined. These turbulent diffusion characters are calculated by the Monte-Carlo method in *this paper. The main point is that all the trajectories of the particles simultaneously released* from the source point at time $t=t_0$ are tracked; then the ensemble statistical characters of the trajectories are deduced from thousands of the trajectories. Therefore, how to construct a total velocity field is the key problem. The total velocity of the particle in the i direction can be written as

$$v_i=\bar{v}_i+v_i', \tag{5}$$

$$v_i'(t+t)=v_i'(t)\rho_L^{i\Delta t}+\rho_i, \tag{6}$$

where $i=1,2,3$, represents the u, v, and w components of the velocity in x,y and z directions, respectively; Δt is the time step; $\rho_L^{i\Delta t}$ is the Lagrangian autocorrelation coefficient for component i and time step Δt; $\bar{v}_i$ is the mean component of the wind. The turbulent fluctuation velocity v_i' has two components—correlated component and a random component. The random walk or Monte-Carlo component ρ_i is picked randomly from a Gaussian distribution with zero mean and standard deviation $\sigma_{\rho i}$. It reads

$$\sigma_{pi}=\sigma_i\{1-[\rho_L^{i\Delta t}]^2\}^{1/2}, \tag{7}$$

in which

$$\rho_L^{i\Delta t}=\exp(-\Delta t/T_L^i). \tag{8}$$

The trajectory for each particle is given by

$$X_{ai}=X_{0ai}+\sum_{n=1}^{N_0}V_{nai}\Delta t, \tag{9}$$

where N_0 is the tracked step number, a is the label for emitted particles. The mean trajectory centre of the particles is

$$\bar{X}_i(t)=\frac{1}{K}\sum_{a=1}^{K}X_{ai}, \tag{10}$$

where K is the total number of emitted particles. The variance of the particle trajectory is

$$\sigma_i^2(t)=\frac{1}{K}\sum_{a=1}^{K}(X_{ai}-\bar{X}_i)^2. \tag{11}$$

Thus, the required parameters of the model are deduced conveniently by the Monte-Carlo technique, and the continuously observed turbulent quantities in the PBL are also put into the model.

III. DATA INPUTTING INTO THE MODEL

For finishing calculation of the whole model, the following basic data must be input into the model:

a. the emissions inventories of pollution sources and background concentrations;
b. the horizontal wind field in the mesoscale range;
c. the upper wind fields in the mesoscale range;
d. the distributions of surface temperature;
e. the time and space distributions of the turbulent statistical quantities;
f. the time and space distributions of the mixing layer depths or boundary layer heights;
g. the parameters in the surface layer;
h. the data of the geography elevations;
i. the measured surface concentrations.

In order to obtain the above data, we have carried out a comprehensive field research project in the Dianchi area with 50 × 70 km^2.

For the mesoscale circulations, 17 electrical wind-direction and wind-speed apparatus are at our disposal, and a set of data for every 10 minutes can be obtained. In order to determine the laws of variation of wind speed with height in the PBL and the characters of the boundary layer depths (or mixing layer depths), we have five low-level radiosounding, and pilot-balloon observation points at our disposal observations are carried out every two hours, the measured height being 1.5 km. In order to measure the variations of inversion layer and mixing depth, a single-point soundar of Model HKS-1 is used and observations are continuously carried out for 24 h. At the same time, for analysing the characters of land and lake breeze, observations of water temperature are also carried out. The distribution of all observation points are given in Fig. 1. The time and space distribution for the mean wind and temperature in the area can well be represented by the above observational projects. For the inhomogeneity and unsteady consideration, the density and interval of the data are enough.

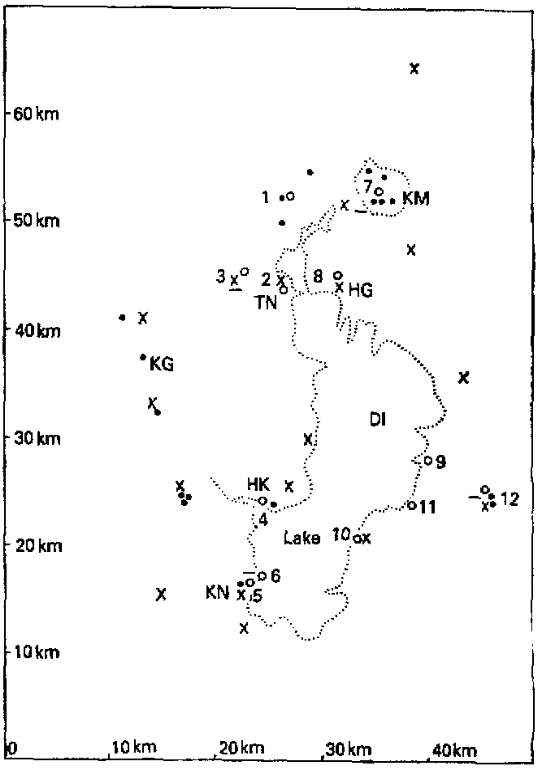

Fig. 1. Distribution of all field determining points.

○ Monitor Point	DI Dianchi	KN Kunlin
● Pollutant Source	KM Kunming	KG Kungang
× *Surface Observation*	*HG Haigeng*	*TN Taihuashan*
— Radiosounding Point	HK Haikou	

In order to obtain the laws of variation of turbulent statistical quantities with height in the PBL, continuous observational data for 24 hours are first obtained by Model M-2000 Doppler sounder; the highest measured can reach 1.5 km. The hourly average data of variations of σ_u, σ_v and σ_w with height and time can be directly provided for the model. Multi-point 24 hour continuous observations have been carried out by fully automatic ultrasonic wind speed and temperature apparatus, and three components of the fluctuation velocity can be automatically recorded every two seconds. The characters of continuous variation of σ_u, σ_v and σ_w with time can be provided for the model under different terrains. The Eulerian time scale T_E^u, T_E^v and T_E^w can be obtained by the following expression (Hanna, 1980, Yang and Lei, 1983):

$$T_L/T_E=\beta=\frac{0.6}{i}=0.6\,\frac{\bar{u}}{\sigma_u}, \tag{12}$$

where T_L^u, T_L^v and T_L^w can be deduced conveniently; i is the intensity of turbulence. In order to obtain parameters in the surface layer, gradient observations of turbulence, wind and temperature are simultaneously carried out at a height of more than twenty meters above the ground, and all data can be automatically sampled during 24 hours. This provides the parameters of surface layer velocity scale u_*, Monin-Obukhov length L and local roughness length z_0 for the model.

All the data which represent inhomogeneity in the horizontal have been obtained except for the variation of turbulent quantities with height. Of course, to obtain good data of turbulence a multipoint sounder system is needed, which, unfortunately, is not yet available in this country. Nevertheless, there are five measured points with z_0, u_* and G (geostrophic wind) in our studied area, and these quantities also represent to some degree the effect of horizontal inhomogeneity of terrain on turbulence. Thus, the internal relationships between the data of variation of σ_u, σ_v and σ_w with height that are obtained by the Doppler sounder and z_0, u_* and G of the measured point can be found (Hanna, 1980). For other points where variations of turbulent statistical quantities with height are not measured, the profile form is the same as the measured one; only the local values of z_0, u_* and G are used at different points. The horizontal inhomogeneity of variation of turbulent quantities with height can be approximately represented by the above method.

A continuous plume is approached by 10 puffs emitted hourly, $\Delta t=120$ s. The longest tracking time is 10 hours in the studying range. A total of 100 random walk particles are emitted within each puff. The four parameters which have to be put into the model can be deduced at the time through the 100 random numbers, as well as the mean wind fields and the turbulent fields at corresponding times.

As for the problem of effect of emitted particle numbers on statistical characters, comparison has been made, which shows that, if distributions of the concentration are deduced directly from the Monte-Carlo method, the 100 random numbers are excessively little, and that would arouse inconsecutive concentration distribution, and the inconsecutive degrees would increase with the studying range becoming larger. For this reason, Den and Lei (1986) had to emit thousands of particles to study the distributions of pollution concentration in the mesoscale range. But to obtain the four statistical character quantities that are necessary in the model calculation, there is not much difference between emitted 100 particles and 1000 particles (Lei and Den, 1986). So 100 particles are selected in order to save computer time and memory.

The concentration distribution at any time can be calculated from the model, but only the 3-hour average concentrations are analysed to compare with the measured concentrations.

IV. TEST OF THE MODEL

In order to test the reliability of the application of the model to the Dianchi area which is dominated by mountain and valley breeze, land and lake breeze, and city heat island, we have compared simulated results and monitor concentrations at the same time (Clear day data of 12 monitor stations are used). The ratios of calculation to measured concentrations for three-hour ensemble average and daily means of 12 monitor stations and three-hour instantaneous values for both Haikou and Kunming are given in Tables 1 and 2, respectively. In order to compare, in the case of inputting the same data, the ratios of calculating values with the TDADM to measured values are also given in the last row of Table 1 (Lü and Lei et al., 1986)

Table 1. Ratios of Calculated to Measured Concentrations

Stations NO	1	2	3	4	5	6	7	8	9	10	11	12	Mean Value
3 h mean	1.18	0.51	0.52	0.96	0.75	1.15	0.60	0.63	0.54	1.04	0.83	0.79	0.79±0.243
Daily mean	0.82	0.51	0.51	0.90	0.67	1.01	0.56	0.63	0.52	0.85	0.83	0.66	0.71±0.171
TDADM	0.56	0.45	0.43	0.73	1.49	1.32	0.53	0.43	0.52	1.26	0.67	0.39	0.73±0.393

Table 2. Ratios of Calculated to Measured Concentrations for 3h Instantaneous

Monitor stations	Time (LST) 1—4	5—8	9—12	13—16	17—20	21—24	Mean Value
Haikou	0.75	1.19	0.57	1.00	1.50	0.76	0.96±0.312
Kunming	0.52	0.53	0.57	0.86	0.67	0.47	0.6±0.143

Regarding Tables 1 and 2, the following points should be noted: (1) The values are less than one. One of the reasons is that only the larger pollutant sources are inputted into the model; the other reason is that the calculated results represent an average value in an area of 4 km^2, but the measured results only represent values at a fixed point; therefore, the calculated value is smaller than the measured value. Both the TDADM and our model is smaller than measured values, indicating that the forecasting tendency of both the models is consistent. (2) The average ratios of calculated values to measured values for both the models are in the range of 0.7 to 0.8, which shows that calculation results are in good agreement. (3) The values of ratios for daily average concentration are smaller than those for 3-hour average, and scattering degree is also less, which is consistent with general law. (4) Table 2 shows that, even if the diurnal variation of atmospheric parameters is very violent, the results

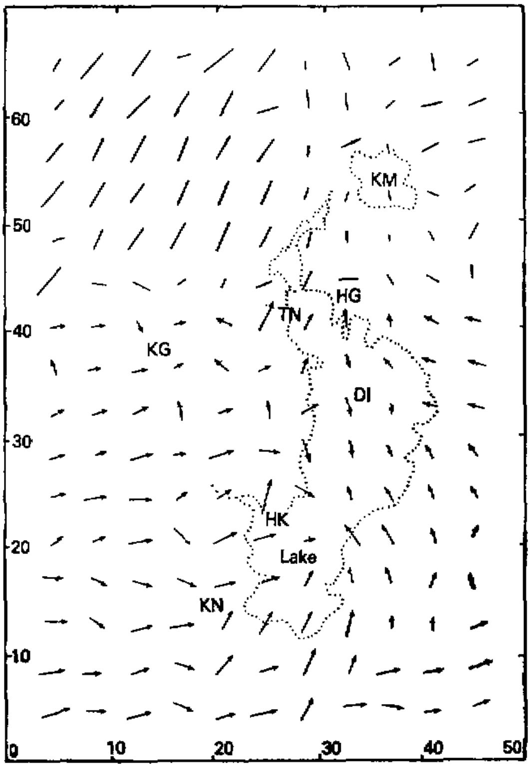

Fig. 2. The mesoscale circulation pattern at 4 LST.

simulated by the model are still fairly good. For example, the lowest value of ratio for Kunming city is 0.47, showing that the model possesses stronger adaptive powers. (5) In a word, in the Dianchi area under such a complex mesoscale circulation (Fig. 2), it is encouraging that there is good agreement between measured and predicted results for studies of atmospheric environmental impact, and the model is dependable.

V. ANALYSIS OF DIAGNOSTIC RESULTS

The distribution laws of concentration that are dominated by typical mesoscale local circulation in the Dianchi area are simulated by the model; diurnal variation laws of concentration distribution are especially revealed. Figure 3 is the daily mean surface concentration under the condition of local circulation.

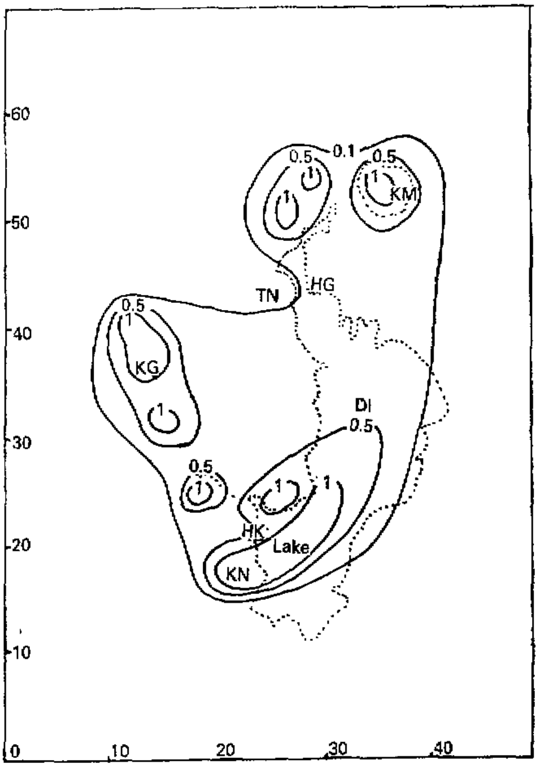

Fig. 3. Distribution of daily mean surface concentration (μg/m^3).

From the horizontal distribution of concentration one can see that there are three obvious pollution centres in the studied area. The first one is at Kunming city and the west industrial area; the second one is an industrial area where phosphate fertilizers are produced to the west of Taihuashan; the third one is in the west shore area of the lake, in which the Kunlin plant is centred (including Haikou). These centres coincide with large pollution sources, but Fig. 3 also shows that the region which contains the three centres enveloped by the 0.1 μg/m^3 equiscalar line is very large, and has a pollution area of 30 × 40 km^3. This result clearly tells us that now pollution in the Dianchi area is not limited to an area of a few kilometres but has become a regional pollution problem. This conclusion is supported by both qualitative analysis of monitor results and results simulated with TDADM.

Taihuashan and the area to its west is a relative low concentration belt. This is due to the fact that the area west of Taihuashan is hilly, the wind velocity is small and it is controlled by local mountain and valley breezes. In addition, the local land and lake breezes themselves caused by the large Dianchi Lake waters form a new system. So the pollutants travel only in the lower diffusion layer, and can not affect the west of the mountain. The pollutants at the east and west sides of the mountain in the surface layer do not connect with each other. Therefore, a relatively low concentration belt is formed in the mountain and its west area. The pollution at the SW side of Dianchi Lake is heavier than at the north and the east side of it lighter than the west.

Owing to existing mountain, waters and city in the area, local mesoscale circulations formed by differences of surface heat effect possess obvious diurnal variation. Therefore, the concentration distribution patterns also possess considerable diurnal variation. Figures 4–6 clearly show the diurnal variation process.

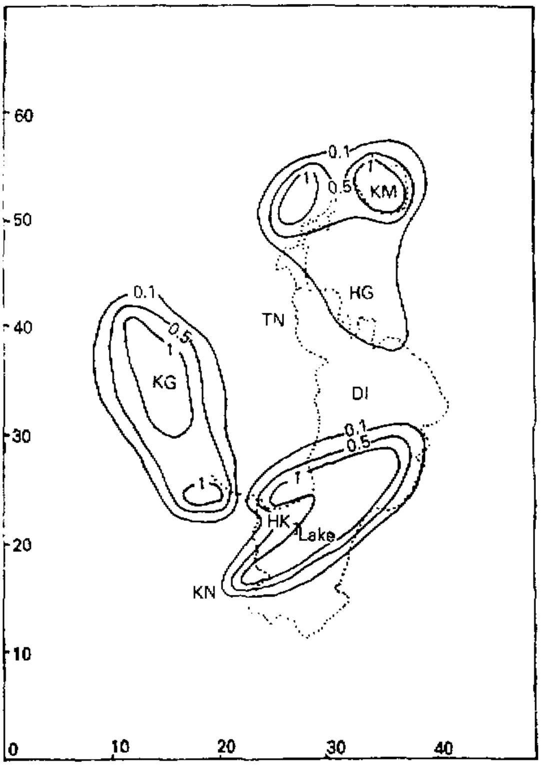

Fig. 4. Distribution of surface concentration ($\mu g/m^3$) at 1–4 LST.

Figure 4 represents typical clear nocturnal conditions. Owing to the effect of Kunming city, a thin flow blows toward the lake surface, the pollutants emitted from industries and city residential areas slowly travel south and affect the Haigeng area, but because of light wind in the night, the pollutants can not be transported to the south to mix with pollutants emitted by Kunlin. The pollutants whose centre is situated in Kungang are dominated mainly by local mountain breeze, and slowly travel from NW to SE, so that a pollution belt is formed. The pollutants emitted from Kunlin are dominated by land breeze at this time, and are transported from SW to NE along the shores of the lake, then merge with the Haikou pollution source. But due to light wind and stable atmospheric conditions at night, the effects of pollutant sources are basically local. The 0.1 $\mu g/m^3$ equiscalar lines isolate three pollution centres.

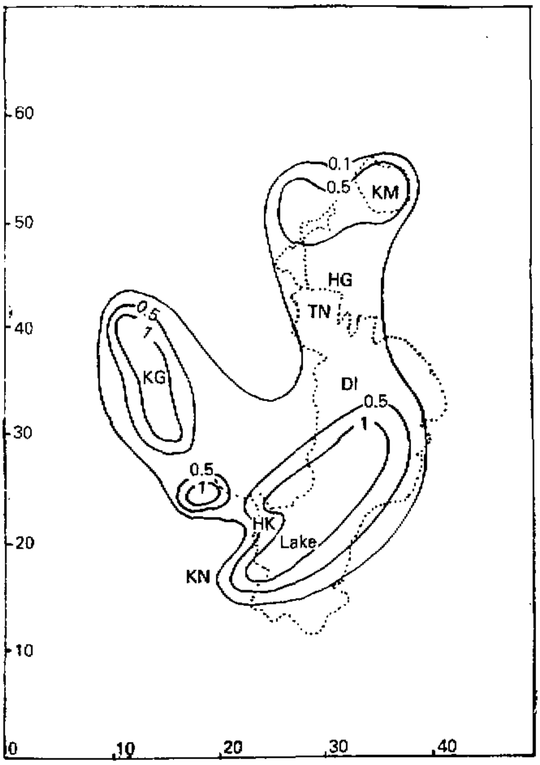

Fig. 5. Distribution of surface concentration ($\mu g/m^3$) at 5–8 LST.

Figure 5 gives the conversion period from land breeze to lake breeze or from mountain breeze to valley breeze. The wind directions are variable, but the wind velocity becomes stronger than at night. The three pollution centres begin to connect into a whole body, but the pollutants of the west of Taihuashan still do not merge with the east.

Figure 6 represents 9–12 LST condition. At this time, land breeze has already converted to lake breeze, and mountain breeze has already converted to valley breeze, but the wind speed is not strong. The ranges of effect of the pollutants have greatly expanded at this time, the range involved by the 0.1 $\mu g/m^3$ equiscalar line is the largest in the day. Due to lake breeze strengthening, the 0.5 $\mu g/m^3$ equiscalar line near Kunlin which is shown in Fig. 5 has obviously shrunk towards the SW at this time. Due to the effect of daytime upslope wind, the pollutants of Kungang have obviously expanded towards the NE.

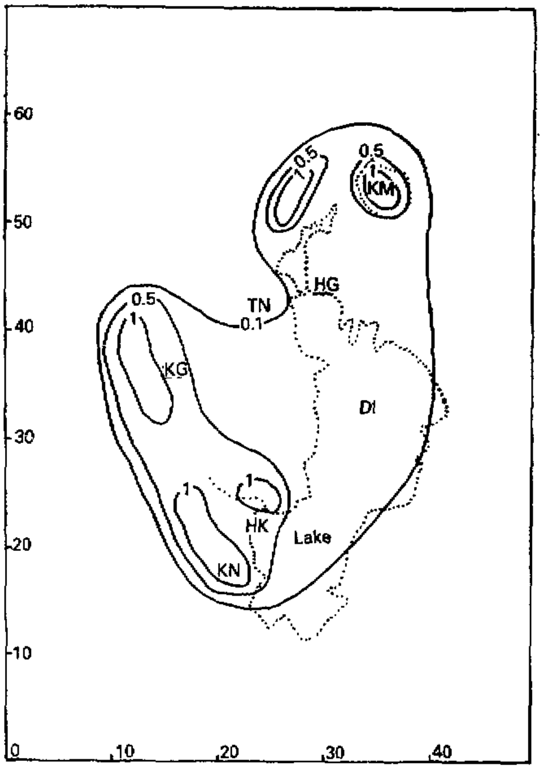

Fig. 6. Distribution of surface concentration ($\mu g/m^3$) at 9–12 LST

VI. CONCLUSION

As mentioned above, the diurnal and space variations of concentration distribution are well described by our model that uses measured data and the effects of mesoscale circulation owing to ground inhomogeneous heating. They are in good agreement with the results of the TDADM in the case of inputting the same data (Lü and Lei et al., 1986). It shows that the model using the Monte-Carlo technique can be applied successfully in such complex terrain as the Dianchi area.

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