THE CELL-MOVE-EXPANSION MODEL FOR THE EVALUATION OF GROUND LEVEL POLLUTANT CONCENTRATION

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ABSTRACT

A model for evaluating pollutant concentrations near the ground is developed. The main advantages of the model are its ability to estimate the distribution and variation of ground concentration under non-uniform or unsteady wind field with minimal computations and the elimination of numerical pesudo-diffusion.

I. INTRODUCTION

Many numerical grid models for the evaluation of pollutant concentrations under the influence of non-uniform or unsteady wind fields have been proposed. But due to computational pseudo-diffusion, obvious errors often appear in the models mentioned above. During the last two decades, under the influence of significant developments in computer capabilities, discretization methods have become a major subject of investigation and development. The particle method is probably the most advanced numerical algorithm available. The Particle-In-Cell model of Sklarew et al. (1970) is an effective method for elimination of spurious short waves or pseudo-diffusion. However it requires a large amount of computation which cannot be completed with a microcomputer. Statistical approach seems to be more flexible and appealing. Hanna (1979) has shown that both Eulerian and Lagrangian wind vector fluctuations can be described by a simple Markov process. Zannetti (1983) developed a new diffusion simulative scheme and suggested that the diffusion-velocity can be treated as a semi-random number and obtained by statistical procedure. Sheih (1978) in his puff-on-cell model suggests that generally a puff or a "grid cell" be regarded as an expansion with time and down wind distance. In fact, the volume of a puff emitted from a source often varies with time while it is moving. In this paper, a more convenient model with efficient computations for evaluation of ground pollutant concentration is developed. Since a hybrid Eulerian-Lagrangian coordinate system has been used, pseudo-diffusion can be eliminated. In this model, the following factors are considered: the advection of pollutant; the expansion or contraction of puffs due to the effects of diffusion velocities, and the manipulation of the source term and removal term.

II. THE MEAN WIND FIELD AND ADVECTION

Assuming that the velocity vector of turbulent diffusion is given by:

$$V'_d = -(K \cdot \nabla C)\frac{1}{C}, \tag{1}$$

where C is the concentration, K is the eddy viscosity and it is assumed that the advective effects are mainly caused by the mean wind. Thus the advection-diffusion equation in an incompressible fluid can be approximately written as

$$\frac{\partial C}{\partial t} = -V\cdot\nabla C - V\cdot(V'_d C) + S + R, \tag{2}$$

where C is the pollutant concentration and V is the mean wind vector. Here we mainly discuss the distribution of ground concentration. Since the vertical component of the mean wind near the surface is approximately equal to zero, the first term of the right-hand side of the equation expresses the horizontal advection of pollutant concentration caused by the horizontal wind vector near the surface; the second term on the right-hand side of the equation is the flux-divergence of concentration resulting from the effects of diffusivity as parameterized by the velocity V'_d; S is the source parameter, and R is the removal term.

In order to evaluate the advection of ground pollutant concentration, a two-dimensional mean wind field must be first determined. There are many schemes which can be used to obtain the two-dimensional wind field or the mean wind input at each grid-point; one of the scheme is based on observational results at some locations, such as the distance-weighting method or the objective analysis scheme. Sherman (1978) developed a mass-consistent model for complex terrain conditions, with which the non-uniform wind field over uneven surface can be well determined. Even though under these conditions the vertical velocity near the surface is not yet equal to zero, assumption is tenable that the streamlines are nearly parallel to the contours of ground. Thus the advective variations of ground concentration can be approximately computed on the basis of the two-dimensional wind field.

Now we discuss the computation of the advection term in a hybrid Eulerian-Lagrangian coordinate system, in order to minimize the pseudo-diffusion. We assume the concentrations are vertically uniform within a mixed layer and divide the horizontal area concerned into many grids and let the concentration value at each grid-point represent the central concentration of a corresponding "puff" or "cell". For each time step, in the Eulerian coordinate system, the pollutants in a grid will move with the wind, a distance $u\Delta t$ in the X direction and $v\Delta t$ in the Y direction, respectively. We assume that, at the beginning, the origin of the Lagrangian coordinate system is located at grid-point (i, j) and then moves with the wind speed at this point. Thus, from time t to $t+\Delta t$, in the Lagrangian coordinate system the Eulerian grid-point (i, j) has moved to point $(i-u\Delta t,$ $j-v\Delta t)$; i. e. the pollutant concentration at Eulerian grid-point (i, j) will be replaced by the pollutant concentration at point $(i-u\Delta t,\ j-v\Delta t)$, after time Δt. Thus we have

$$C_{ij}^{t+\Delta t} = C_{i-u\Delta t, j-v\Delta t}^{t}, \tag{3}$$

where $C_{ij}^{t+\Delta t}$ is the concentration at Eulerian grid-point (i, j) and at time $t+\Delta t$; $C_{i-u\Delta t, j-v\Delta t}^{t}$ is the concentration at point $(i-u\Delta t,\ j-v\Delta t)$ and time t. Clearly here only the advective variation of pollutant concentration is taken into account. We will discuss the diffusive variation in the next section. In order to evaluate the value of the above-mentioned concentration, a function of concentration distribution needs to be established. Many experimental results prove that most puffs or plumes approximately show a normal distribution. It is proposed that the concentration $C_{i-u\Delta t, j-v\Delta t}^{t}$ can be regarded as the superposition of four puffs (or cells) whose centre is located at its surrounding grid-points, each with a two-dimensional quasi-normal distribution of concentration. The following equations are assumed:

$$C^{t^2}_{i-u\Delta t,\ j-v\Delta t}=\sum_{k=1}^{4}\frac{C^{t^2}_k}{2\pi\sigma^2_k}\exp\left[-\frac{A^2r^2_k}{2\sigma^2_k}\right] \tag{4}$$

or

$$C^{t+\Delta t}_{ij}=\left(\sum_{k=1}^{4}\frac{C^{t^2}_k}{2\pi\sigma^2_k}\exp\left[-\frac{A^2r^2_k}{2\sigma^2_k}\right]\right)^{1/2}, \tag{5}$$

where C^t_k are the corresponding concentrations at surrounding grid-points at time t. If $u\geqslant 0$ and $v\geqslant 0$, then

$$C^t_1=C^t_{i,j};\ C^t_2=C^t_{i-1,j};\ C^t_3=C^t_{i-1,j-1};\ C^t_4=C^t_{i,j-1}, \tag{6}$$

r_k are the distances from point $(i-u\Delta t,\ j-v\Delta t)$ to surrounding grid-points, respectively; i. e.

$$r_1=(u^2+v^2)^{1/2}\Delta t \qquad (k=1) \tag{7}$$

$$r_2=[(d-u\Delta t)^2+v^2\Delta t^2]^{1/2} \qquad (k=2) \tag{8}$$

$$r_3=[(d-u\Delta t)^2+(d-v\Delta t)^2]^{1/2} \qquad (k=3) \tag{9}$$

$$r_4=[u^2\Delta t^2+(d-v\Delta t)^2]^{1/2} \qquad (k=4). \tag{10}$$

Obviously, if $u<0$ and $v<0$ or in other condition, the "surrounding grid-points" will be changed. σ_k is the standard deviation of relative concentrations (or C^2/C^2_k), $d=\Delta x=\Delta y$ is the horizontal grid length, and A is a distance factor.

The following restricted condition is also necessary for computational stability.

$$(u^2+v^2)^{1/2}\Delta t\leqslant d \tag{11}$$

III. THE DIFFUSION COMPONENT

There are two basic effect factors in the air pollution: (a) the transport due to the mean wind speed which has been taken into account and discussed in the above sections; (b) the random turbulent fluctuations which lead to turbulent fluxes and dispersion of pollutants. The second term in right-hand side of Eq. (2) is the turbulent flux-divergence of pollutants.

Zannetti (1983) has suggested that the diffusivity velocity V'_d be not only regarded as a semi-random variable but also easily computed with a Monte-Carlo-type model. To perform this computation, it has been generally considered that the Eulerian measurements of wind can provide the statistical information about V'_d. Though these two parameters are not the same, as a first approximation it seems to be suitable to accept this assumption and use it to evaluate the diffusivity velocity with a statistical scheme based on measurements of wind. Hanna (1979) has described both Eulerian and Lagrangian wind vector fluctuations by a simple Markov process (an auto-correlation process of the first order). If we extend this result to V'_d, we have

$$V'_d(t+\Delta t)=R_d(\Delta t)\cdot V'_d(t)+V''_d(t+\Delta t), \tag{12}$$

where $V'_d(t)$ is the scalar value of diffusive velocity at time t. The initial value $V'_d(t_0)$ can be obtained by taking $V'_d(t_0)=V'_{t_0}$, where V'_{t_0} is the fluctuation of the Eulerian wind speed at initial time (t_0). $V''_d(t+\Delta t)$ is a purely random number with normal distribution and zero mean which is characterized by the standard deviations of the random variable. To estimate the above-mentioned standard deviations, we need to take the variance of equation (12); thus we can obtain

$$\sigma_{V_d^*} = \sigma_{V'_d}[1-R_d^2(\Delta t)]^{1/2}. \qquad (13)$$

R_d in Eq. (12) and Eq. (13) is the auto-correlation factor of V'_d with lag $\Delta t = t_2 - t_1$; $\sigma_{V'_d}$ is the standard deviation of V'_d.

In general, the Lagrangian variables $\sigma_{V'_d}$ and R_d can be approximated by the standard deviation and the auto-correlation of Eulerian wind measurements, i. e.

$$\sigma^2_{V'_d} = \frac{1}{N}\sum_{i=1}^{N}(v(t_i)-\bar{V})^2 = \frac{1}{N}\sum_{i=1}^{N}V'(t_i)^2 \qquad (14)$$

and

$$R_d(\Delta t) = \frac{\langle V'(t_i)V'(t_i+\Delta t)\rangle}{\sigma^2_{V'_d}}, \qquad (15)$$

where $V'(t_i)$ is the velocity perturbation of the Eulerian wind measurement at time t_i and $V'(t_i+\Delta t)$ is that at $t_i+\Delta t$. $\langle V'(t_i)V'(t_i+\Delta t)\rangle$ expresses the auto-covariance of $V'(t_i+\Delta t)$ with lag Δt.

Usually $\sigma_{V'_d}$ and $R_d(\Delta t)$ vary with space and with atmospheric stability. Each grid-value of $\sigma_{V'_d}$ and $R_d(\Delta t)$ can be obtained by means of interpolation, form Eulerian wind measurements at several sites.

Eq. (12) is the key formula for computing V'_d and is seen to be a recursive sum of two terms: the first is the previous value of V'_d and the second is a purely random component generated by computer. Generally in the same puff, σ_k and $\nabla \cdot (V'_d\ C)$ have positive correlation. Thus diffusive action can also be taken into account by readjusting σ_k. Since $C^l_{i-u\Delta t, j-v\Delta t}$ should be equal to C^r_1 when $r_1 = 0$ before diffusion, it follows that

$$\sigma_k^2 = 1/2\pi \quad (\text{when } u=0, v=0, V'_d=0)$$

and

$$\exp\left[-\frac{A^2r_k^2}{2\sigma_k^2}\right]=1 \qquad (\text{when } r_k=0)$$

and

$$\exp\left[-\frac{A^2r_k^2}{2\sigma_k^2}\right]\to 0 \qquad (\text{when } r_k\to d).$$

The latter is easy to satisfy, as long as d is great enough. Considering the effects of diffusion, we take

$$\sigma_k^2 = \frac{1}{2\pi}(1+\xi_k)^2, \qquad (16)$$

ξ_k is related to the diffusivity velocity V'_d. To determine the relation between ξ_k and V'_d, we have to use the following analysis and discussion.

It is assumed that around each grid point there has a "puff" or "cell" whose centre is at the corresponding grid-point and whose radius equals L. As mentioned above, before diffusion begins $\xi_k = 0$ and $\sigma_k^2 = 1/2\pi$; thus, the pollutant mass in the "puff" (or cell) can be written as

$$M_1=\frac{C_k^2}{2\pi\sigma_k}\int_0^2\int_0^L \exp(-A^2r^2/2\sigma_k^2)rdrd\theta$$

$$=C_k^2\int_0^2\int_0^L \exp(-\pi A^2r^2)rdrd\theta$$

$$=\frac{C_k^2}{A^2}[1-\exp(-\pi A^2L^2)]. \tag{17}$$

After a time step Δt, L would be extended by ΔL due to the diffusive velocity:

$$\Delta L=V'_d\Delta t, \tag{18}$$

where V'_d is the value of the diffusive velocity, which depends on the coordinates of the grid-point and is considered isotropic.

At time $t+\Delta t$, the radius of the cell mentioned above becomes

$$\text{radius}=L+V'_d\Delta t. \tag{19}$$

Note that equation (19) has significance only if L and V'_d are within the same turbulent eddy. Thus we take the initial radius L as equivalent to the scale of the turbulent eddy, i. e.

$$L=\int_0^\infty R_d(x)dx, \tag{20}$$

where $R_d(x)$ is the spatial auto-correlation coefficient of the Eulerian wind.

Using Eqs. (16) and (19), the mass of the same puff after expansion (or contraction) caused by the diffusive velocity V'_d in a time Δt, can be written approximately as

$$M_2=\frac{C_k^2}{A^2}\left\{1-\exp\left[-\frac{\pi A^2(L+V'_d\Delta t)^2}{(1+\xi_k)^2}\right]\right\}. \tag{21}$$

According to the mass-conservation law, $M_1=M_2$ and comparing Eq. (21) with Eq. (17), we have

$$(1+\xi_k)^2\doteq\frac{(L+V'_d\Delta t)^2}{L^2}, \tag{22}$$

and Eq. (12) becomes

$$\sigma_k^2\doteq\frac{1}{2\pi}\,\frac{(L+V'_d\Delta t)^2}{L^2}. \tag{23}$$

Because of the advective variation mentioned above and referred to equation (4), the concentration at grid-point (i,j) and time $t+\Delta t$ is

$$C_{i,j}^{t+\Delta t}=\left\{\sum_{k=1}^{4}\frac{L^2C_k^{t2}}{(L+V'_d\Delta t)^2}\exp\left[-\frac{\pi A^2r_k^2L^2}{(L+V'_d\Delta t)^2}\right]\right\}^{1/2}. \tag{24}$$

The influence of flux-divergence on pollutant concentrations has been embodied in σ_k with Eqs. (23) and (24).

IV. PARAMETERIZATION OF SOURCE TERM AND REMOVAL TERM

Since we are mainly concerned with the evaluation of ground concentration for a specified source with an effective height of emission $H>0$, parameterization of the source term must be made in order to carry out the above-mentioned computation. Noting that in a time step Δt, the pollutant emitted from a source is not a point-source, but has expanded and become a puff with a certain volume. When the puff falls down to the ground, it will cover a finite area. With reference to the analytical solution of the diffusion equation and taking $K_X=K_Y=\mu K$; $K_z=K$, the source term can be expressed as

$$S\Delta t \doteq Q\Delta t\cdot\mu^{-1}\cdot(4\pi K\Delta t)^{-3/2}\exp\left\{-\frac{1}{4K\Delta t}\left[\mu^{-1}(X-X_0-u\Delta t)^2 + \mu^{-1}(Y-Y_0-v\Delta t)^2+H^2\right]\right\}, \tag{25}$$

where Q is the emission rate; (X_0,Y_0) is the coordinates of the source site. H is the effective height of the source and u, v are the components of wind speed at the source. $K_z(=K)$ is the vertical diffusive coefficient which can be determined by way of analysis of the wind speed profile and K_X, K_Y are the horizontal-diffusive coefficients in the X and Y direction respectively, and μ is an experimental factor.

As for removal term, it is usually written as the following form:

$$C^{t+\Delta t}=C^t e^{-\lambda\Delta t} \tag{26}$$

or

$$R\Delta t=C^{t+\Delta t}-C^t=-(1-e^{-\lambda\Delta t})C^t, \tag{27}$$

where $R\Delta t$ is the variation of pollutant concentration affected by removal actions in the time interval Δt. If we let

$$P=1-e^{-\lambda\Delta t}, \tag{28}$$

then

$$R\Delta t=-PC^t \tag{29}$$

or

$$C^{t+\Delta t}=(1-P)C^t, \tag{30}$$

namely the removal effects are equivalent to multiplying Eq. (24) by a factor $(1-P)$. Referring to Eq. (2) and taking its finite-difference form, and using Eq. (24) and Eq. (30), we have

$$C_{ij}^{t+\Delta t} = (1-P)\cdot\left\{\frac{L^2C_k^{t\,2}}{(L+V'_d\Delta t)^2}\exp\left[-\frac{\pi A^2r_k^2L^2}{(L+V'_d\Delta t)^2}\right]\right\}^{1/2}+S\Delta t. \tag{31}$$

The P value in the equation is estimated on the basis of the half-attenuation-period of the pollutants. (If the half-attenuation-period of SO_2, is nearly 3 h.; and $\Delta t=5$ min., thus $P=0.02$.)

Equations (12), (25), (31) as well as the condition (11) are the basic set of the model.

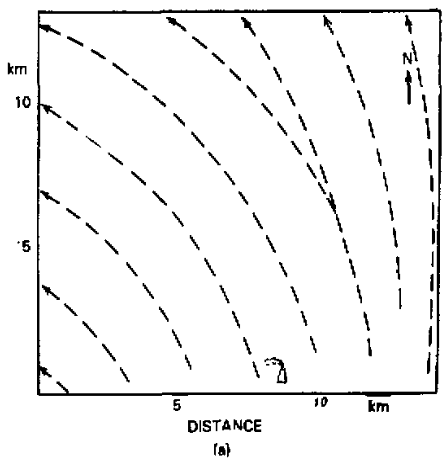
V. EXAMPLES OF COMPUTATION

Based on data from the Zhanjiang Chemical Engineering Factory which is the only source several kilometers long, we have made an example computation using the model and compared the output with the monitoring results.

In the period of simulation, the wind records were taken every hour, proving that the meteorological condition was essentially steady-state in this period. Since wind speeds are generally less than 3 m/s, in order to satisfy the condition (11), we take $d=\Delta x=\Delta y=$ 1 km and $\Delta t=5$ min, the emission rate of SO_2 at the ZCE factory is 183 kg/h or 50.8 g/s and the effective emissive height, evaluated by Briggs formula, is neary 100 m. According to analysis of the wind profile in Zhanjiang, in terms of the theory of the logarithmic wind profile (Holton, 1979) and taking $K = ku^*H$, we obtain $K = 10.8\ m^2/s$; experimentally assume $A = 1.4 \times 10^{-3} m^{-1}$ and $\mu = 10$; background value $\sim$ 0.005 mg/m^3. The two-dimensional wind fields were simulated on the basis of actual observations using interpolation (refer to Fig. 1a). The model output at each time has been shown in Fig. 1 b–c by solid lines. The dashed lines in Fig. 1d are the monitoring results. Comparing these curves each other proves that the model is able to describe the distribution and variation of ground level air pollution under the effects on non-uniform flows or unsteady wind field.

Fig. 2 expresses the situation of transport and dispersion in a shear flow pattern, which shows that with changing wind, the distribution of pollutant concentrations changes.

A comparison between CME Model and Gaussian Plume Model as well as monitoring results is shown in Table 1 which proves that the outputs of CME Model basically correspond to actual monitoring results; the average absolute error is 0.018 mg/m^3 and the average relative error is 35%, better than Gaussian Model.



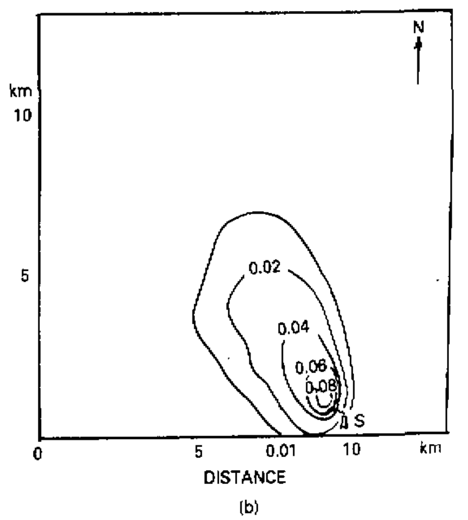
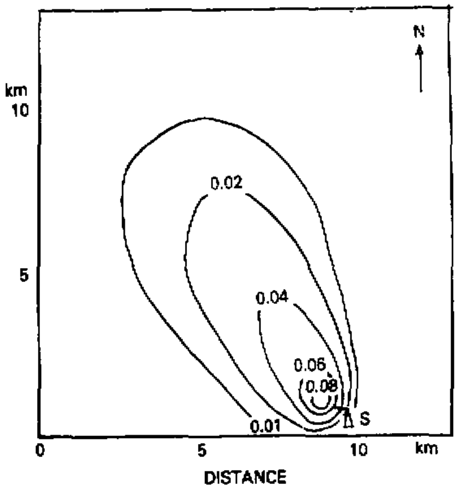


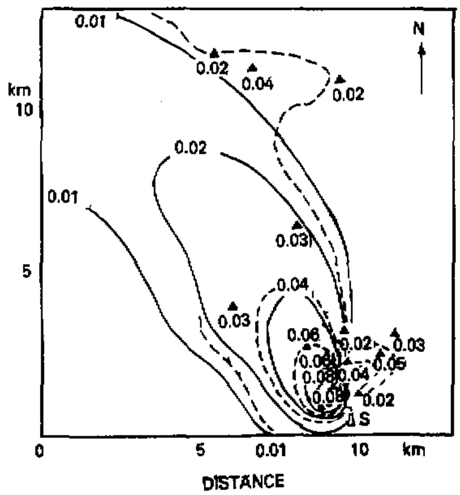
Fig. 1a. July 15, 1982, 1000–1200. A two-dimensional wind field represented by streamlines, simulated on the basis of actual observational data. 1000 is the initial time of SE wind in Zhanjiang.

Fig. 1b. The model output of SO_2 concentration (mg/m^3) at 1030, July 15, 1982, in Zhanjiang, around the C.E. factory.



(c)

Fig. 1c. The model output of SO_2 concentration (mg/m^3) near the ground at 1100.



(d)

Fig. 1d. The model output of SO_2 concentration at 1200, dashed lines and digits (▲) are monitoring results (mg/m^3).

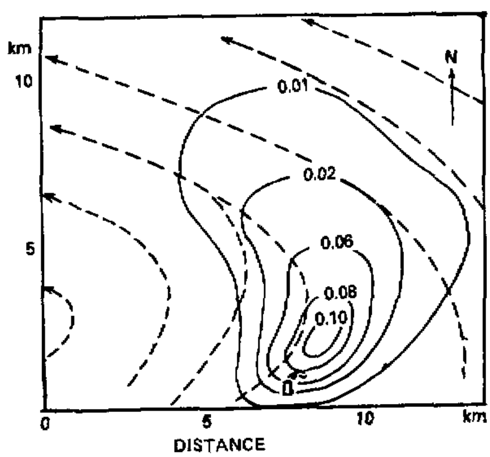


Fig. 2. Predicted SO_2 ground concentration in a shear flow pattern; output of the model at the time of its coming to steady state. Streamlines are shown as dashed lines.

Table 1. A Comparison between Two Models and Monitoring Results. (SO_2). C: CME Model; G: Gaussian Plume Model; M: Monitoring Results (mg/m³)

Location	Date	Time	Model	Monitoring Sites (S-N) 1	2	3	4	5	6	7	8	9	10	11	12	Average absolute error	Average relative error
Z.C. Factory	15th July 1982	1200	C	.07	.01	.01	.03	.06	.01	.02	.03	.02	.01	.01	.01	.0125	34%
			G	.12	.08	.03	.05	.05	.01	.03	.02	.01	.01	.01	.01	.021	57%
			M	.08	.02	.05	.04	.06	.03	.02	.03	.03	.02	.04	.02		
Z.C. Factory	21th July 1982	1100	C	.08	.04	.02	.04	.05	.02	.02	.02	.02	.01	.01	.01	.010	27%
			G	.13	.09	.04	.06	.03	.02	.03	.02	.01	.01	.01	.01	.020	55%
			M	.09	.04	.05	.03	.06	.03	.02	.04	.03	.02	.01	.02		
Meixian Power-station	9th June 1985	0200	C	.04	.03	.11	.05	.06	.24	.009	.009					.031	39%
			G	.02	.03	.10	.12	.15	.21	.01	.01					.041	51%
			M	.07	.04	.15	.06	.09	.16	.04	.03						
Meixian Power-station	12th Jan. 1986	1400	C	.009	.02	.11	.04	.012	.04	.02	.03					.020	38%
			G	.009	.01	.17	.12	.07	.02	.01	.01					.028	53%
			M	.02	.06	.15	.06	.04	.04	.03	.02						

VI. SUMMARY

We have developed a new model for the computation of air pollution near surface, under the influence of a non-uniform or unsteady wind field. The complex variations of pollutant concentrations near the ground are simulated with a minimum amount of computation. The pseudo-diffusion error has been eliminated using a hybrid Eulerian-Lagrangian coordinate system to evaluate non-linear terms. The flux-divergence of pollutants is determined utilizing the diffusivity velocity which can be regarded as semirandom amount and computed with a Monte-Carlo-type model. Using theoretical analysis, parameterizations of the source term and the removal term are made. The main advantage of the model is that it can solve, with a minimum of computation, complicated problems concerning variations of ground level concentration, even under the condition of non-uniform or unsteady wind fields.

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