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SIMULATION OF TRANSFORMATION, BUOYANCY AND REMOVAL PROCESSES BY LAGRANGIAN PARTICLE METHODS

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INTRODUCTION AND SUMMARY

Particle methods (Hockney and Eastwood, 1981) are the most recent and advanced numerical tools for computer modeling of dynamic systems. They seem particularly successful in simulating turbulent fluid dynamics, due to their capability of incorporating semi-random components. Particle modeling of air pollution diffusion phenomena has recently become the subject of a great deal of investigation (e.g., Diehl et al., 1982; Legg and Raupach, 1982; Ley, 1982, Zannetti and Al-Madani, 1983). The promising results of these studies are, however, accompanied by the persisting difficulty of properly evaluating Lagrangian velocity statistics from Eulerian measurements (see Davis, 1982). Nevertheless, particle methods provide outstanding advantages over other air pollution diffusion modeling techniques, such as Gaussian models and grid models, as discussed below.

Atmospheric diffusion processes are characterized by turbulent eddies in which the motion of different air parcels is strongly auto-and cross-correlated. With simulation particles, the computer modeling of these eddies would, therefore, require the expensive computation of the interactions between each particle and its surrounding ones. A different approach can be followed if only ensemble averages need to be computed. In this case, in fact, each simulation particle can move independently from the others and its motion can be very realistically simulated by semi-random

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fluctuations generated by computer Monte-Carlo techniques. These Lagrangian simulations with stochastic components seem extremely useful for at least reproducing such phenomena, as atmospheric turbulent diffusion, whose physical mechanism is too complex to be simulated by deterministic techniques.

A need exists to incorporate suitable numerical tools for the simulation of atmospheric phenomena besides turbulence into the Lagrangian particle methods. Therefore, this paper, after a few introductory remarks, discusses the definition and the computer implementation of special algorithms for the simulation of dynamic plume rise, chemical decay, and deposition-resuspension effects by particle methods. These algorithms have been incorporated into a prototype computer diffusion code (MC-LAGPAR, written in APL language) whose simulation results for a few test cases are presented and discussed.

THE MODEL

In the atmospheric boundary layer, the dispersion of emitted gaseous material can be described by a suitable number of fictitious particles moving, at each time step, according to pseudo-velocities simulating (1) transport, (2) turbulent fluctuations, and (3) molecular diffusion (if not negligible). These pseudo-velocities do not intend to simulate the real trajectory of a specific pollutant parcel, but to provide realistic dynamics of the pollutant motion on an ensemble basis.

The pseudo-velocities are decomposed into two terms: the space-dependent average values $\bar{u}_x$, $\bar{u}_y$, $\bar{u}_z$ (which must be provided by a meteorological model or by an interpolation-extrapolation of meteorological measurements), plus the particle-dependent fluctuations. Different Monte-Carlo schemes have been proposed to calculate the fluctuations u', v', and w' of the pseudo-velocities (e.g., Watson and Barr, 1976; Hanna, 1981). To properly simulate the wind shear effects, Zannetti (1981) developed a scheme in which the pseudo-velocity fluctuations are auto-correlated (for all three components) and cross-correlated (between the vertical and along-wind fluctuations):

$$u'(t_2) = \phi_1 u'(t_1) + u''(t_2) \tag{1a}$$

$$v'(t_2) = \phi_2 v'(t_1) + v''(t_2) \tag{1b}$$

$$w'(t_2) = \phi_3 w'(t_1) + \phi_4 u'(t_2) + w''(t_2) \tag{1c}$$

In this scheme, the ϕ parameters and the intensities of the purely random components u", v", w" can be inferred from algebraical manipulations of known meteorological input parameters (intensities and correlations of the wind fluctuations).

In addition to transport and diffusion, particle methods can be used in a particularly effective way for providing a realistic treatment of buoyancy, chemical decay and ground deposition-resuspension effects. In the following sections, specific algorithms are proposed for the treatment of these special effects.

Dynamic Plume Rise

Particle methods provide a straightforward treatment of the dynamic plume rise. In fact, each emitted particle, tagged with its emission characteristics, can consume an increment of its initially supplied buoyancy F at each time step Δt:

$$\Delta F = \frac{\partial F}{\partial t} \Delta t \qquad (2)$$

where $\partial F/\partial t$ is a function of meteorology (e.g., wind speed, temperature, stability). Each ΔF can then provide an additional vertical velocity

$$w_{pr} = f(\Delta F) \qquad (3)$$

that moves each particle $w_{pr}\, \Delta t$ in the vertical direction, effectively simulating a dynamic plume rise.

Alternatively, a simpler computation can be performed rearranging existing semi-empirical plume rise formulas, as shown in the example below.

After the transformation $x = ut$, the TVA plume rise formula (Stern, 1976) can be written

$$\Delta h(t) = cF^{1/3}u^{-1/3}t^{2/3} \qquad (4)$$

in which the constant c is

$$c(z) = 1.58 - 0.414 \frac{\partial \theta}{\partial z} \qquad (5)$$

$\partial\theta/\partial z$ is the potential temperature gradient ($^{o}C/100$ m), F is the buoyancy (m^4s^{-3}) and u is the wind speed (ms^{-1}).

Both c and u vary with z. This suggests an empirical dynamic two-step computation in which the trajectory

$$z(t) = H + \Delta h(t) \tag{6}$$

of each particle is computed by (2nd step)

$$z(t+\Delta t) \simeq z(t) + w_{pr} \Delta t \tag{7}$$

where

$$w_{pr} = \left(\frac{dz}{dt}\right)_{t+\Delta t/2} = \left(\frac{d\Delta h}{dt}\right)_{t+\Delta t/2}$$

$$\simeq c\left[z(t+\Delta t/2)\right]F^{1/3} \quad u\left[z(t+\Delta t/2)\right]^{-1/3} \frac{2}{3} (t+\Delta t/2)^{-1/3} \tag{8}$$

and (1st step)

$$z(t+\Delta t/2) \simeq z(t) + \left(\frac{dz}{dt}\right)_t \Delta t/2 \tag{9}$$

where

$$\left(\frac{dz}{dt}\right)_t = \left(\frac{d\Delta h}{dt}\right)_t \simeq c\left[z(t)\right]F^{1/3} \quad u\left[z(t)\right]^{-1/3} \frac{2}{3} t^{-1/3} \tag{10}$$

Emitted particles do not need to be provided with the same buoyancy. Actually, the extra vertical diffusion produced during plume rise will be realistically simulated by releasing particles with a buoyancy defined by

$$F = \bar{F} + F' \tag{11}$$

where $\bar{F}$ is the average value and F' is a random component (particle-dependent) of suitable intensity.

Chemical Decay

An exponential decay, taking into account all removal factors except ground deposition, can be performed at each time step. If the time scale of the phenomenon is T_c (where T_c can be a function of the type of pollutant and of the meteorology) the probability of removal for each particle at each time step is

$$p_c = 1 - \exp(-\Delta t/T_c) \tag{12}$$

Consequently, $p_c n_p$ particles must be randomly cancelled from the computational domain, where n_p is the current number of active (i.e., not cancelled or deposited) particles.

Ground Deposition-Resuspension

At the end of each time step, all active particle locations need to be tested to single out those particles (say n_b) that have been moved below terrain ($z<0$). Some of these n_b particles will be reflected and the rest of them will be deposited on the ground. If T_d is the time constant of this partial deposition process, each of the n_b particles currently below the terrain has a probability of

$$p_d = 1 - \exp(-\Delta t/T_d) \tag{13}$$

to be deposited. Therefore, $p_d n_b$ randomly selected particles (among the previously identified n_b) will be deposited and the rest of them ($n_b - p_d n_b$) will be reflected.

Particles deposited on the ground can be resuspended back to the computational domain or permanently absorbed by the ground. If n_d is the current number of deposited particles and T_s is the time scale of the resuspension process, each of the n_b particles has a probability of

$$p_s = 1 - \exp(-\Delta t/T_s) \tag{14}$$

to be resuspended. Therefore, at each time step, $p_s n_d$ particles will be resuspended; but, at the same time, if a particle remains deposited on the ground for a period of time greater than a critical value T_{dmax}, the particle will be permanently absorbed.

T_d, T_s and T_{dmax} are functions of the meteorology (especially the surface wind speed) and the characteristics of both the pollutant and the ground surface. The proper inference of these values allows realistic diffusion simulations very difficult to obtain using other modeling techniques.

THE MC-LAGPAR CODE

A prototype computer code written in APL has been developed that incorporates, among other things, the algorithms previously described. The code simulates the diffusion of a single puff in flat terrain with non-homogeneous non-stationary meteorological conditions. The code is fully grid-free, since the meteorological variables are inputted at selected altitudes and then linearly interpolated at each particle's elevation. In this way, abrupt variations of the meteorological input parameters (causing artificial shear effects) are avoided. Moreover, since the selected altitudes do not need to be equally spaced, any degree of resolution in inputting the meteorological values can be obtained.

The meteorological variables required at each altitude at each time step are:

- the average wind components $\bar{u}_x$, $\bar{u}_y$, $\bar{u}_z$
- the standard deviations $\sigma_{u'}$, $\sigma_{v'}$, and $\sigma_{w'}$ of the pseudo-velocities (u' and v' are the along-wind and the cross-wind components; w' is along z)
- the auto-correlations $r_{u'}$, $r_{v'}$, $r_{w'}$ of the pseudo-velocities
- the cross-correlation $r_{u'w'}$
- the potential temperature gradient $\partial\theta/\partial z$.

In addition to these, T_c, T_d, T_s, T_{dmax} need to be inputted (a single value for the entire domain).

The time increment Δt must be carefully chosen. All model parametrizations are independent from Δt, but nevertheless, abrupt variations of particle elevations should be avoided and $w' \, \Delta t$ values should be less than the length scale of the vertical variation of the meteorological input. Ten seconds is probably a reasonable upper limit value for Δt.

COMPUTER SIMULATIONS

The MC-LAGPAR code has been applied for the simulation of a few test cases to provide a qualitative demonstration of the flexibility and the high degree of resolution of this numerical approach. Each simulation (150 steps of 10 seconds each) generates a puff of 100 particles at the source location. Particle locations (x,z) are plotted every three time steps thus generating a continuous plume up to a few kilometers downwind of the source. The vertical dimension chosen was twice the horizontal one.

Fig. 1 shows a slightly buoyant plume released at an altitude of 100 m during dispersion conditions of moderate vertical turbulence. The wind speed is 1 ms^{-1} at the ground and 4 ms^{-1} at the top of the domain. The $\sigma_{u'}$ and $\sigma_{v'}$ parameters start with 0.5 ms^{-1} at the ground to 1.0 ms^{-1} at 100m, remaining constant above that level. The $\sigma_{w'}$ parameter has the same behaviour, i.e., from 0.2 ms^{-1} at the ground to 0.5 ms^{-1} at 100m. The autocorrelations $r_{u'}$, $r_{v'}$, and $r_{w'}$, are constant at 0.7, 0.7, and 0.5, respectively. The cross-correlation $r_{u'w'}$ increases from -0.3 at the ground to -0.1 at the top.

Fig. 2 shows the dynamics of an elevated (150m) hot plume during conditions of low vertical turbulence. Meteorological values are similar to the previous simulation, except $\sigma_{w'}$, which now grows from 0.1 ms^{-1} at the ground to 0.35 ms^{-1} at 100m, then decreasing to 0.15 ms^{-1} at the top.

The simulation in Fig. 3 is very similar to the previous one. Now, however, an elevated inversion layer has been added by forcing $\sigma_{w'}$ equal to 0.1 ms^{-1} and $\partial\theta/\partial z$ equal 2 ^{o}C/100m between 500m and 550m. Most particles have enough buoyancy to penetrate the inversion layer and be trapped inside. Only a few particles perforate the inversion layer reaching the more turbulent region above. This simulation is characterized by a very unusual result, i.e., the decrease of the plume's σ_z with the downwind distance at 2 km from the source.

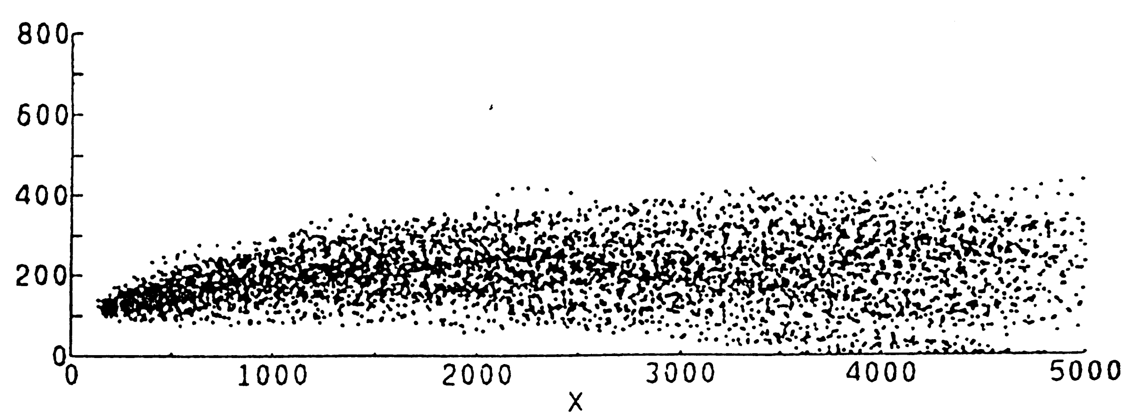

Fig. 1 - Simulation of a slightly buoyant elevated plume with moderate turbulence.

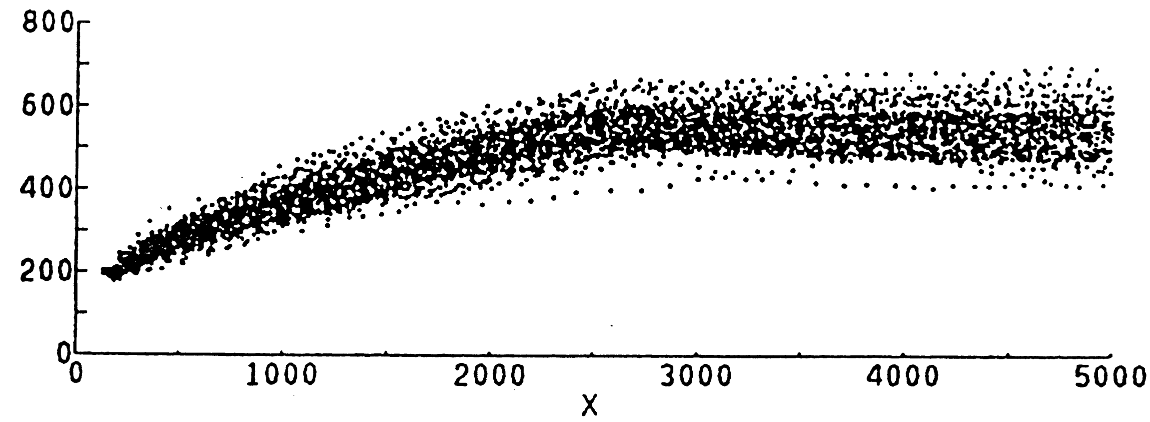

Fig. 2 - Simulation of a hot elevated plume with low turbulence.

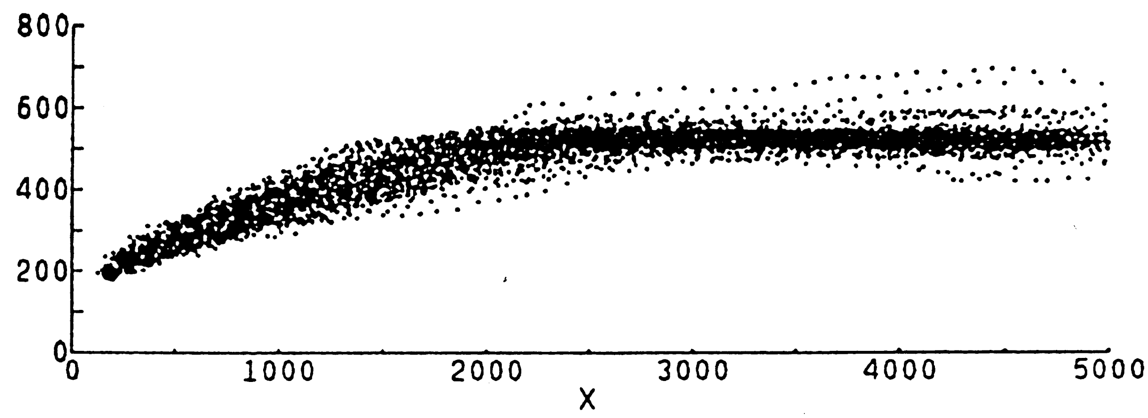

Fig. 3 - Simulation of a hot elevated plume with low turbulence and the presence of an elevated inversion layer between 500 m and 550 m.

Fig. 4 shows the release of a non-buoyant plume in moderate vertical turbulence in which σ_w, reaches its maximum (0.6 ms^{-1}) at 250m, just below an elevated inversion layer between 250 m and 300 m. With a non-buoyant plume, the inversion layer acts more like a reflection barrier for the particles, even though particle trapping effects are still evident.

Finally, Fig. 5 presents a low-level release (at 10 m) with slight buoyancy in moderate vertical turbulence. Deposition-resuspension phenomena are accounted for by T_d = 10 s, T_{dmax} = 50 s and T_s = 1000 s. With these values, 23% of the emitted mass is found permanently deposited on the ground 1500 s from its release.

CONCLUSIONS

Lagrangian particle methods applied to air pollution dispersion simulations can easily provide a degree of resolution and accuracy not obtainable by other simulation techniques. This method can also incorporate a realistic treatment of such phenomena as buoyancy and deposition-resuspension. This technique can be seen as a very "natural" and effective way of simulating atmospheric dispersion processes. In fact, whereas other modeling techniques operate a questionable discretization of the atmospheric turbulence into "stability" classes or require a meteorological input (e.g., the eddy diffusion coefficients K's) not directly measurable, the particle methods require meteorological input parameters (i.e., the pseudo-velocity statistics) that seem very close to the measurable wind statistics. Nevertheless, much investigation is still required to provide a fully acceptable method of relating Eulerian wind measurements to the required pseudo-velocity (Lagrangian) statistics.

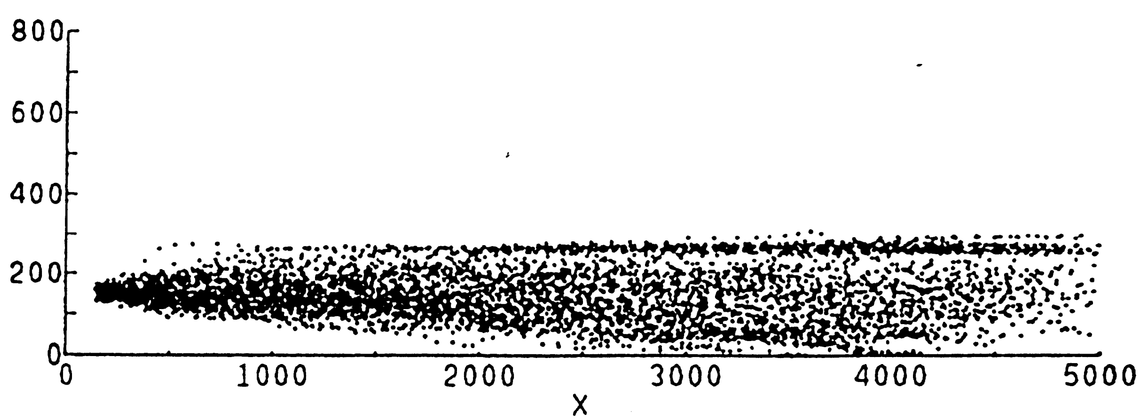

Fig. 4 - Simulation of a non-buoyant plume with moderate turbulence and the presence of an elavated inversion layer between 250 m and 300 m.

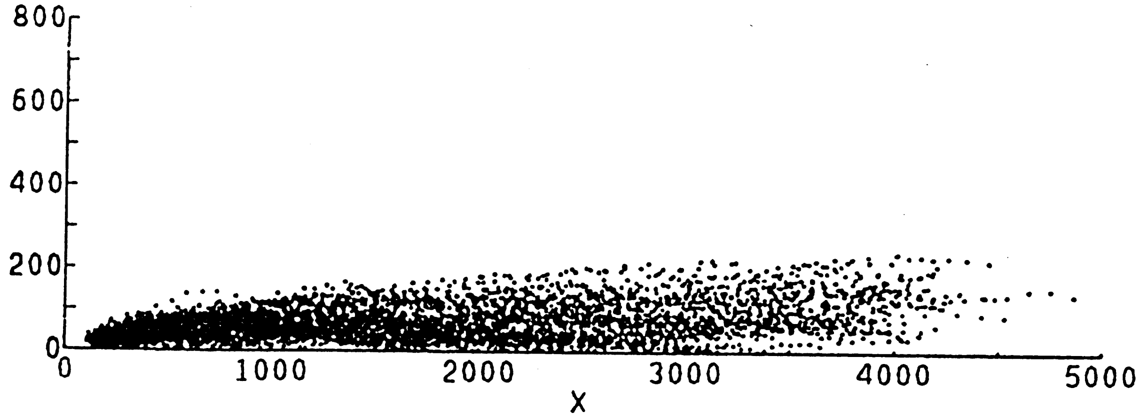

Fig. 5 - Simulation of a low-level release with slight buoyancy, moderate vertical turbulence, and deposition-resuspension effects.

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