13th International Technical Meeting on Air Pollution Modeling and its Application. Sept. 14-17, 1982, Ile D'Embiez (Toulon), France.



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# A NEW MONTE-CARLO SCHEME FOR SIMULATING LAGRANGIAN PARTICLE DIFFUSION WITH WIND SHEAR EFFECTS

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## INTRODUCTION

Simulation modeling is a problem of numerical discretization of a physical system. Such discretization, performed through computer experiments, is particularly important in those cases where physical theories need to be investigated or verified but laboratory experiments are unable to reproduce the complexities of the real world (e.g. stellar evolution).

In the last few decades, under the strong influence of a huge development of computational capabilities, discretization methods have been a major subject of investigation and development. Four major computational techniques have been developed and applied up to now:

- finite difference methods (Richtmyer and Morton, 1967)
- finite element methods (Strang and Fix, 1973)
- boundary element methods (Brebbia, 1978)
- particle methods (Hockney and Eastwood, 1981)

The last technique probably seems today the most advanced available numerical algorithm and, even more important, the most promising tool for numerical simulations with future generations of computer systems.

Using particle models, the temporal evolution of a physical system is described by the dynamics of a finite number of interacting

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particles. Therefore, such models are typically Lagrangian ones, while, for example, finite difference methods are purely Eulerian representations of physical systems.

Three main types of particle models can be derived (Hockney and Eastwood, 1981):

- particle-particle (PP) models, where all interaction forces between particles are computed at each time step
- particle-mesh (PM) models, where forces are computed using a field equation (on a grid) for the potential
- PP-PM (or $P^3M$) models, a hybrid approach where interparticle forces are splitted into a short range component (computed using the PP method) and a slowly varying one (represented in mesh system by the PM method).

Particle models can be purely deterministic or (partially) based on statistical methods. In the first case the simulation of particle time evolution is unique. In the second case, Monte Carlo techniques are used to produce semi-random "perturbations", and, therefore, model outputs represent just a realization from an infinite set of possible solutions.

Length and time scales (as in all discretization systems) play an important role in particle models. In particular, the relation between the actual physical particles (or elements) and the computer model simulation particles is a important factor for the interpretation of the simulation results. In general, three possible cases can be found (Hockney and Eastwood, 1981) :

- a one-to-one correspondence between actual and simulated particles, as, for example, in molecular dynamics simulation
- a description of fluid elements (position, vorticity) as particles, as, for example, in vortex fluid simulations, where the correspondence to physical particles (molecules) is totally lost
- the use of "superparticles", i.e., simulation particles representing a cloud of physical particles having similar characteristics.

Particles models have been mostly applied for simulating (and understanding) the spiral structure of the galaxies, for plasma dynamics simulation and for obtaining realistic representations of turbulence in fluid. Air pollution dispersion by particle methods is at its infancy, even though interesting studies have been published in the last few years (e.g., Watson and Barr, 1976; Hanna, 1979a; Lamb, et al. 1979a; Lange, 1978; Patterson et al. 1981).

This paper, after a description of the discretization problems related to air pollution diffusion simulation by particles, presents a new Monte-Carlo scheme especially designed for handling wind shear effects in the atmospheric boundary layer. Finally, a brief discussion is provided concerning the suitability of new advanced meteorological instrumentation (e.g., the Doppler acoustic sounder) in providing data input for air pollution particle simulation models.

## AIR POLLUTION SIMULATION BY LAGRANGIAN PARTICLES

"The diffusion of a substance released into a turbulent flow cannot be described by any one model or theory" (Hunt, 1981). A short look at all available theories and numerical techniques can easily convince us that the above statement is basically true:

- Gaussian models strongly depend on sigma parameters generally computed through a questionable discretization (stability classes) of atmospheric turbulence status, or by using semi-empirical formulas.
- Grid models have a high operating cost, and moreover, are affected by numerical problems (instabilities, artificial numerical diffusion errors) and physical limitations (e.g., the K-theory is not appropriate for describing large turbulent eddies).
- Particle models are still under development and require meteorological Lagrangian measurements which are generally unavailable and, however, extremely difficult to make.

Nevertheless, Lagrangian particle methods are very appealing. Emitted gaseous material is characterized by particles and each particle is "moved" at each time step by pseudo-velocities, which take into account the three basic dispersion components: 1) the transport due to the mean fluid velocity, 2) the (seemingly) random turbulent fluctuations of wind components (both horizontal and vertical), and 3) the molecular diffusion (if not negligible). With existing computers (the next generation will be even better), enough particles can be stored in memory (say, more than a few thousand) to accurately describe the characteristics of a single plume, or, better, an instantaneous puff release. Particle resolution plays, in fact, an important role. A one-hour simulation of an industrial emission of 1 kg/s of $SO_2$ from a stack emitting 20 $m^3/s$ of gases will require, for example, 3600 "particles", each representing, in reality, a growing puff containing 1 kg of $SO_2$ and having an initial size of 20 $m^3$. The behaviour of this "superparticle" is certainly different from that of a single $SO_2$ molecule. (*)

(*) Puff Modeling (Zannetti, 1981a) is a powerful Lagrangian technique for treating transport and diffusion of such superparticles.

Nevertheless, we must keep in mind that, in air pollution modeling, we do not need to follow precisely each molecule in the atmospheric turbulent flow, but just to define an algorithm for particle displacement computation which gives an accurate particle density distribution. In mathematical notation, if a particle is located in $\underset{\sim}{x}(t_1)$ at $t_1$, its position at $t_2$ will be

$$\underset{\sim}{x}(t_2) = \underset{\sim}{x}(t_1) + \int_{t_1}^{t_2} \underset{\sim}{u}\left[\underset{\sim}{x}(t),\ t\right] dt \qquad (1)$$

where $\underset{\sim}{u}$ is the "instantaneous " wind vector in each point $\underset{\sim}{x}(t)$ of the particle trajectory between $t_1$ and $t_2$.

Atmospheric turbulent properties make $\underset{\sim}{u}$ practically impossible to know, especially due to its semi-random components caused by atmospheric eddies. But the "equivalent" wind rector $\underset{\sim}{u}_e$ can be considered

$$\underset{\sim}{u}_e = \int_{t_1}^{t_2} \underset{\sim}{u}\left[\underset{\sim}{x}(t),\ t\right] dt/(t_2-t_1) \qquad (2)$$

which moves the particle directly from $\underset{\sim}{x}(t_1)$ to $\underset{\sim}{x}(t_2)$ in the interval $(t_1, t_2)$. The problem is then to estimate $\underset{\sim}{u}_e$ from $\underset{\sim}{u}$ measurements, keeping in mind that $\underset{\sim}{u}_e$ must approximate the integral term in Eq. (2) only on a particle ensemble basis. For example, we can define

$$\underset{\sim}{u}_e = \bar{\underset{\sim}{u}}_e + \underset{\sim}{u}_e' \qquad (3)$$

where $\bar{\underset{\sim}{u}}_e$ is our best estimate of the average Eulerian wind vector (transport) at $\underset{\sim}{x}(t_1)$, and $\underset{\sim}{u}_e'$ is a "diffusivity velocity". In other words, $\bar{\underset{\sim}{u}}_e$ (a smoothly variable term) represents our deterministic understanding of the average transport process, based on Eulerian wind measurement interpolation or a meteorological model output, while $\underset{\sim}{u}_e'$ is a single artificial numerical perturbation.

Since, in Eq. (3) $\bar{\underset{\sim}{u}}_e$ is supposed to be known, computing $\underset{\sim}{u}_e'$ is the key problem of Lagrangian particle modeling. Two fundamental approaches can be followed: the deterministic and the statistical ones.

## The deterministic computation of $\underset{\sim}{u}_e'$

A typical example of the deterministic approach is given by the particle-in-cell method of Lange (1978), where, after some

manipulation of the K-theory diffusion equation, we obtain

$$\underset{\sim}{u}'_e = \left(-\frac{K}{C}\right) \nabla C \qquad (4)$$

where K is the usual eddy diffusion coefficient and C the concentration, computed as the number of particles in the cell containing $\underset{\sim}{x}(t_1)$. This method requires partitioning the computational domain into cells and it is able to duplicate K-theory dispersion with the important feature of removing the numerical advection errors associated with finite-difference solutions.

Using this method, the motion of a single particle will be affected by the time-varying concentration field, i.e., by the positions of the other particles (PM model)

The statistical computation of $\underset{\sim}{u}'_e$

The statistical approach (Monte Carlo-type models) certainly seems to be more flexible and appealing. According to the statistical approach, $\underset{\sim}{u}'_e$ is a semi-random component computed by manipulating computer-generated random numbers. To perform this computation, it has been generally assumed that Eulerian measurements of $\underset{\sim}{u}$ can provide statistical information on $\underset{\sim}{u}'_e$. However, these two parameters are not the same and further investigation is required to fully assess this point.

As a first approximation, however, we can accept the above assumption and use, for the diffusivity velocity $\underset{\sim}{u}'_e$ a statistical generation scheme based on our understanding (and Eulerian measurements) of $\underset{\sim}{u}$. In particular, Hanna (1979b) has shown that it is a plausible assumption to describe both Eulerian and Lagrangian wind vector fluctuations by a simple Markov process (autocorrelation process of the first order).

If we extend this assumption to $\underset{\sim}{u}'_e$, we have (*)

$$\underset{\sim}{u}'_e(t_2) = \underset{\sim}{R}_e(t_2-t_1)\ \underset{\sim}{u}'_e(t_1) + \underset{\sim}{u}''_e(t_2) \qquad (5)$$

where $\underset{\sim}{R}_e(t_2-t_1)$ contains the autocorrelations with lag $\Delta t = t_2-t_1$ of the $\underset{\sim}{u}'_e$ components, and $\underset{\sim}{u}''_e$ is a purely random vector.

(*) In this formula (and the following ones) each component of the vector on the left side is computed using only the corresponding component of each vector in the right side (scalar computations).

Equation (5) is the key formula for statistically computing $\underset{\sim}{u}'_c$ which will simply be a recursive sum of two terms---the first function of "previous" $\underset{\sim}{u}'_e$ of the same particle, and the second purely randomly generated. Since Eq. (5) will be computed independently for each particle, two eventually coincident particles at $t_1$ will have, in general, different displacements, even if their past "history" is the same. Using this approach the motion of a particle is not affected by the position of the other particles and, therefore, this numerical algorithm is extremely fast since no interacting forces need to be computed.

To apply Eq. (5) we need the initial $\underset{\sim}{u}'_e(t_0)$ for each particle at its generation time $t_0$ (often assumed to be a zero vector) and the computation of $\underset{\sim}{R}_e$ and $\underset{\sim}{u}''_e$.

Due to the Lagrangian nature of $\underset{\sim}{u}_e$, $\underset{\sim}{R}_e$ has been often identified with $\underset{\sim}{R}_L$, the autocorrelations of the Lagrangian wind vector $\underset{\sim}{u}_L$. $\underset{\sim}{R}_L$ can be related to Lagrangian turbulence time scales, for example, by

$$\underset{\sim}{R}_L = \exp\left[-(t_2-t_1)/\underset{\sim}{T}_L\right] \tag{6}$$

where $\underset{\sim}{T}_L$ contains the two horizontal and the one vertical Lagrangian time scales. Generally, Lagrangian measurements of $\underset{\sim}{T}_L$ (or $\underset{\sim}{R}_L$ directly) are not available, but empirical relations have been proposed (e.g., Hanna, 1981) to estimate $\underset{\sim}{T}_L$ from Eulerian measurement.

Assuming $\underset{\sim}{u}''_e$ a purely random vector with zero-mean, normally-distributed independent components, we have that $\underset{\sim}{u}''_e$ is completely characterized by $\underset{\sim}{\sigma}_{u''}$, i.e., the standard deviations of its components. In this case, taking the variances of Eq. (5), we obtain

$$\underset{\sim}{\sigma}_{u''} = \underset{\sim}{\sigma}_{u'}\left[1 - \underset{\sim}{R}_e^2(t_2-t_1)\right]^{1/2} \tag{7}$$

requiring the knowledge of $\underset{\sim}{\sigma}_{u'}$, the standard deviations of $\underset{\sim}{u}'_e$ which, again, can be approximated by the standard deviations of available Eulerian wind measurements.

From the standard deviations $\underset{\sim}{\sigma}_{u''}$ of Eq. (7) it is easy, using commonly available computer programs, to generate each particle's $\underset{\sim}{u}''_e$ term to be used in Eq. (5).

$\underset{\sim}{R}_e$ and $\underset{\sim}{\sigma}_{u''}$ are, in general, time-dependent (but constant between $t_1$ and $t_2$) and space-dependent. Therefore, they can fully

utilize a three-dimensional meteorological input (Eulerian values) and can, at least theoretically, simulate extremely complex atmospheric diffusion conditions, otherwise impossible to treat with other numerical schemes.

## Conclusion

Dispersion simulation by Lagrangian particles has been called "natural" modeling. These models do not need inputs of artificial stability classes, empirical sigma curves, or diffusion coefficients that are practically impossible to measure. Instead, diffusion characteristics are simulated by attributing a certain degree of "fluctuation" to each particle, using, for example, the computer's capability to generate semi-random numbers.

The basic advantages of this approach (e.g., see Lamb et al., 1979a; Lange, 1978) are:

- Compared with grid models, this method avoids the artificial initial diffusion of a point source in the corresponding cell and the advection numerical errors.
- This method is practically free of restricting physical assumptions, since all uncertainties are combined into the correct determination of pseudo-velocities.
- Each particle can be tagged with its coordinates, source indicator, mass, activity, species and size, allowing computation of wet and dry deposition, decay, and particle size distribution.
- If chemistry is required, a grid can be superimposed and concentrations in each cell computed by counting the particles of each species, allowing the use of any reaction scheme at each time step (*).
- The meteorological input required should be very close to actual measured data. The primary information needed seems to be (Lamb et al., 1979a) the variance of wind velocity fluctuations and the Lagrangian autocorrelation function, which can be related to Eulerian measurements (e.g., Hanna, 1981).

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(*) A rigorous concentration computation should not just add up the number of particles in a given cell at a given time. In fact, concentrations should be computed using the total time spent by each particle in the receptor volume during each time step (as in Lamb et al., 1979b). Moreover, nonlinear chemistry computations (at least for fast reactions) should take into account the effects on the reaction rates of concentration turbulent fluctuations, which seems extremely complicated using Lagrangian methods.

Potentially, the method is superior in both numerical accuracy and physical representativeness. However, much research is still needed to extract, from meteorological measurements and our limited theoretical understanding of turbulence processes, the meteorological input required to run this model (i.e., the pseudo-velocities to move each particle at each time step).

## THE TREATMENT OF WIND SHEAR EFFECTS

Shear flow effects in the atmospheric boundary layer are characterized by the following three factors:

- Vertical variation of the average wind vector (changes in both speed and direction).
- Vertical variation of the intensity of wind fluctuations (especially vertical fluctuations).
- Zero correlation between the along wind and the cross-wind fluctuations.
- Negative correlation between the along wind and the vertical wind fluctuations.

According to the above considerations, derived from the analysis of Eulerian wind measurements, we can expect that a correct computation of $\underset{\sim}{u}_e$ in Eq. (3) will incorporate the first factor in $\bar{\underset{\sim}{u}}_e$ and the other three in $\underset{\sim}{u}'_e$. Therefore, a need exists to generate cross correlated random velocity components for $\underset{\sim}{u}'_e$, and not just independent components as in Eq. (5). To this end, a new Monte-Carlo method has been anticipated in Zannetti (1981b) which is fully discussed below.

Let us consider a special reference system (SRS) where the x axis, for each specified altitude z, is chosen to coincide with the horizontal component of $\bar{\underset{\sim}{u}}_e$. Then, with the notation

$$\underset{\sim}{u}'_e(t) = \left[u'(t),\ v'(t),\ w'(t)\right] \tag{8}$$

$$\underset{\sim}{u}''_e(t) = \left[u''(t),\ v''(t),\ w''(t)\right] \tag{9}$$

the following scheme can be used for $\underset{\sim}{u}'_e$

$$u'(t_2) = \phi_1\, u'(t_1) + u''(t_2) \tag{10}$$

$$v'(t_2) = \phi_2\, v'(t_1) + v''(t_2) \tag{11}$$

$$w'(t_2) = \phi_3\, w'(t_1) + \phi_4\, u'(t_2) + w''(t_2) \tag{12}$$

which is similar to Eq. (5), but with the new Eq. (12) for handling the correlation $r_{u'w'}$ between u' and w'.

If we multiply Eq. (10) by $u'(t_1)$ and then take the average <> we obtain (u" is a purely random component)

$$\phi_1 = \frac{\langle u'(t_1)\, u'(t_2)\rangle}{\langle u'^2(t_1)\rangle} = \frac{\langle u'(t_1)\, u'(t_2)\rangle}{\sigma^2_{u'}} = r_{u'}(\Delta t) \tag{13}$$

where $r_{u'}(\Delta t)$ is the autocorrelation of u' with time lag $\Delta t = t_2 - t_1$.

In an analogous way, working on Eq. (11), we obtain

$$\phi_2 = \frac{\langle v'(t_1)\, v'(t_2)\rangle}{\sigma^2_{v'}} = r_{v'}(\Delta t) \tag{14}$$

where $r_{v'}$ is the autocorrelation of v'.

Multiplying Eq. (12) by $w'(t_1)$ and taking the average <> we have

$$r_{w'}(\Delta t)\, \sigma^2_{w'} = \phi_3\, \sigma^2_{w'} + \phi_1\, \phi_4\, r_{u'w'}(0)\, \sigma_{u'}\, \sigma_{w'} \tag{15}$$

where $r_{w'}$ is the autocorrelation of w' and $r_{u'w'}(0)$ is the cross correlation (with no time lag) between u' and w'.

Multiplying the corresponding members of Eqs. (10) and (12) and taking the average <> we have

$$r_{u'w'}(0)\, \sigma_{u'}\, \sigma_{w'} = \phi_1\, \phi_3\, r_{u'w'}(0)\, \sigma_{u'}\, \sigma_{w'} + \phi_4\, \sigma^2_{u'} \tag{16}$$

Eqs. (15) and (16) represent a system of two equations in two unknowns, which gives the solution

$$\phi_3 = \frac{r_{w'}(\Delta t) - \phi_1 r^2_{u'w'}(0)}{1 - \phi_1^2 r^2_{u'w'}(0)} \tag{17}$$

$$\phi_4 = \frac{r_{u'w'}(0)\,\sigma_{w'}\left[1 - \phi_1 r_{w'}(\Delta t)\right]}{\sigma_{u'}\left[1 - \phi_1^2 r^2_{u'w'}(0)\right]} \tag{18}$$

Finally, taking the variances of Eqs. (10) - (12) we obtain the variances of the purely random fluctuations to be generated at each time step

$$\sigma^2_{u''} = \sigma^2_{u'}(1 - \phi_1^2) \tag{19}$$

$$\sigma^2_{v''} = \sigma^2_{v'}(1 - \phi_2^2) \tag{20}$$

$$\sigma^2_{w''} = \sigma^2_{w'}(1 - \phi_3^2) - \phi_4^2\,\sigma^2_{u'} - 2\,\phi_1\,\phi_3\,\phi_4\,r_{u'w'}(0)\sigma_{u'}\,\sigma_{w'} \tag{21}$$

Eqs. (10)-(12) can then be applied using Eqs. (13), (14), (17)-(21) if the proper meteorological input $r_{u'}$, $r_{v'}$, $r_{w'}$, $r_{u'w'}$, $\sigma_{u'}$, $\sigma_{v'}$, $\sigma_{w'}$ is available at each altitude. In such case, where the scheme of Eqs. (10)-(12) is used instead of Eq. (5), $r_{u'w'}$ is the only additional input required.

The entire scheme above has been numerically tested and it has been verified its capability of correctly producing $u'$ components with any acceptable degree of autocorrelation $\underset{\sim}{R}_e$

$$\underset{\sim}{R}_e = (r_{u'}, r_{v'}, r_{w'}) \tag{22}$$

and cross correlation $r_{u'w'}$.

## METEOROLOGICAL INPUT

As previously discussed, Monte-Carlo techniques require a suitable meteorological input. Meteorological tower and Doppler acoustic sounder instrumentations are the best sources of such data. They provide, at different altitudes and during a selected time interval (e.g., 20 minutes), the average wind vector and the standard deviations of the wind fluctuations with respect to a fixed orthogonal system (x, y, z). Therefore, in such coordinate system, at a certain altitude z, the average measured wind vector will be

$$\bar{\underset{\sim}{u}} = (\bar{u}_x, \bar{u}_y, \bar{u}_z) \tag{23}$$

and $\sigma_{u_x}$, $\sigma_{u_y}$, $\sigma_{u_z}$ will be the measured standard deviations of the wind fluctuations. If we assume that such Eulerian measurements are a good representation of the statistical properties of $\underset{\sim}{u}_e$, then we can firstly say that

$$\bar{\underset{\sim}{u}}_e = \bar{\underset{\sim}{u}} \tag{24}$$

$$\sigma_{w'} = \sigma_{u_z} \tag{25}$$

However, as introduced in the previous chapter, we often need the horizontal wind fluctuations in a special reference system (SRS). Therefore, wind fluctuations in (x, y, z) must be projected into such system through a horizontal rotation of an angle $\theta$

$$\theta = \text{arctg} \frac{\bar{u}_y}{\bar{u}_x} \tag{26}$$

Taking the variances of such projected wind fluctuations and remembering the important property that, in the SRS, the two horizontal wind fluctuations are non-correlated, we obtain

$$\sigma^2_{u'} = \frac{\bar{u}^{-2}_x \sigma^2_{u_x} - \bar{u}^{-2}_y \sigma^2_{u_y}}{\bar{u}^{-2}_x - \bar{u}^{-2}_y} \tag{27}$$

$$\sigma_{v'}^2 = \frac{\bar{u}_x^{-2}\,\sigma_{u_y}^2 - \bar{u}_y^{-2}\,\sigma_{u_x}^2}{\bar{u}_x^{-2} - \bar{u}_y^{-2}} \qquad (28)$$

that together with Eq. (25) can be used in Eqs. (19)-(21) to provide the random fluctuations of each particle at each altitude.

In flat terrain conditions, Doppler or tower measurements can be horizontally extrapolated, therefore providing an appropriate, fully three-dimensional input for particle modelling using statistical Monte-Carlo techniques.

## CONCLUSIONS AND POSSIBLE DEVELOPMENTS

Many aspects of the above described techniques need further investigation. As already discussed, a major problem is the utilization of available Eulerian measurements for inferring $\mu_e$ properties.

Moreover, the assumption of no correlation between the two horizontal components in the SRS, is acceptable only for small time intervals not affected by systematic horizontal wind direction meandering across the average value $\bar{u}_e$. If these conditions are not met, persistent, highly correlated, values between the two components are often measured, unless the meandering factor is preliminary removed from wind measurement data.

To solve all these problems, ad-hoc tracer experiments should be designed specifically for evaluating and validating particle diffusion theories.

It is true, nevertheless, that particle models can easily reproduce, under specific simplifying assumptions, the diffusion results obtainable by other modeling techniques, as the Gaussian model and the K-theory. Particle modeling "natural" approach to air pollution simulation seems, therefore, the most suitable technique for future air pollution modeling research and development.

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