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SOME ASPECTS OF MONTE CARLO TYPE MODELING OF ATMOSPHERIC TURBULENT DIFFUSION

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1. INTRODUCTION

Monte Carlo-type models or, more generally, Lagrangian particle models represent an advanced and promising technique in simulating air pollution dispersion. A short look at other modeling methodologies will clarify the advantages of this relatively new approach. In the past, most models for simulating air quality dispersion have been Gaussian models or grid models. Both have physical and numerical deficiencies, however. Gaussian models strongly depend on plume sigma parameters generally computed by characterizing atmospheric diffusion using a series of "stability" classes -- a questionable discretization of the continuous turbulent properties of the atmosphere. Grid models are more complex and require significant computer storage and CPU time. Often, however, the increased computations of grid models provide only marginal and qualitative improvements in dispersion simulation. Even though, theoretically, many physical conditions can be handled quite well by grid model techniques (e.g., finite difference methods), they 1) suffer from the practical problem of spatial and temporal resolution limitations, a consequence of their high operating cost, 2) sometimes show numerical instabilities, and 3) above all, always have numerical errors in the form of artificial numerical diffusion due to the discretization of the advective terms of the dispersion equations.

In this context, 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.

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., 1979; Lange, 1978) are:

- This method requires no grid network, thus avoiding the artificial initial diffusion of a point source in the corresponding cell and the advection numerical errors.
- Lagrangian particle modeling 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., 1979) the variance of wind velocity fluctuations and the Lagrangian autocorrelation function, which can be related to Eulerian measurements (e.g., Hanna, 1981).

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 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).

2. LAGRANGIAN PARTICLE DISPLACEMENT

In mathematical notation we can say that 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.

If $\underset{\sim}{u}$ were exactly known at each point and each instant, an emission release (puff or plume) could be correctly simulated by using Eq. (1) with a sufficient number of particles. Then, concentrations in a specified volume of air could be computed by simply counting the number of particles in that volume.

Unfortunately, atmospheric turbulence makes $\underset{\sim}{u}$ practically impossible to know, especially due to its semi-random components caused by atmospheric eddies. Moreover, even with highly accurate information on $\underset{\sim}{u}$, the method would be extremely expensive, due to the numerical computation for each particle of the integral in Eq. (1), with dt sufficiently small.

To overcome these problems we propose to consider the "equivalent" wind vector, $\underset{\sim}{u}_e$

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

which moves the particle directly from $\underset{\sim}{x}(t_1)$ to $\underset{\sim}{x}(t_2)$ in the time interval (t_1, t_2). The problem is then to estimate, from $\underset{\sim}{u}$ measurements, an approximate value $\hat{\underset{\sim}{u}}_e$ of $\underset{\sim}{u}_e$.

We know that, along the particle trajectory in the interval (t_1, t_2), $\underset{\sim}{u}$ can be expressed as the sum of a constant value $\bar{\underset{\sim}{u}}_L$ plus a fluctuation $\underset{\sim}{u}'_L(t)$, where the subscript L indicates that these are Lagrangian values. Therefore,

$$\underset{\sim}{u}_e = \bar{\underset{\sim}{u}}_L + \int_{t_1}^{t_2} \underset{\sim}{u}'_L(t)\, dt \Big/ (t_2 - t_1) \qquad (3)$$

But if we have a sufficient number of particles (e.g., a puff of 1000), we do not need to correctly follow each particle but just to define an algorithm for particle displacement computation which gives an accurate particle density distribution. Therefore, for example, we can define

$$\hat{\underset{\sim}{u}}_e = \bar{\underset{\sim}{u}}_e + \underset{\sim}{u}'_e \qquad (4)$$

where $\bar{\underset{\sim}{u}}_e$ is our best estimate of $\bar{u}_L$, e.g., the average Eulerian wind vector 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 (different for each particle) which approximates, only on a particle ensemble basis, the integral term in Eq. (3).

2.1 Determining $\underset{\sim}{u}'_e$

As discussed above, computing $\underset{\sim}{u}'_e$ for each particle during each interval (t_1, t_2) is the key problem of Lagrangian particle modeling. To this end, two fundamental approaches can be followed: the deterministic and the statistical.

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

$$\underset{\sim}{u}'_e = \left(-\frac{K}{C}\right) \nabla C \qquad (5)$$

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.

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 (e.g., Hanna, 1979a, 1981; Lamb et al., 1979) that Eulerian measurements of $\underset{\sim}{u}$ can provide statistical information on $\underset{\sim}{u}'_e$. As we have tried to show, 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 both Eulerian and Lagrangian wind vector fluctuations $\underset{\sim}{u}'$ can be described by a simple Markov process (autocorrelation process of the first order)*

$$\underset{\sim}{u}'(t + \Delta t) = \underset{\sim}{R}(\Delta t)\, \underset{\sim}{u}'(t) + \underset{\sim}{u}''(t + \Delta t)^{**}, \qquad (6)$$

where $\underset{\sim}{R}$ contains the three wind speed autocorrelation coefficients with lag Δt (one for each space dimension), and $\underset{\sim}{u}''$ is a purely random vector.

If we extend the form of Eq. (6) to $\underset{\sim}{u}'_e$, we have

$$\underset{\sim}{u}'_e(t_2) = \underset{\sim}{R}_e(t_2 - t_1)\, \underset{\sim}{u}'_e(t_1) + \underset{\sim}{u}''_e(t_2) \qquad (7)$$

where $\underset{\sim}{R}_e(t_2 - t_1)$ contains the autocorrelations with lag $t_2 - t_1$ of the $\underset{\sim}{u}'_e$ components, and $\underset{\sim}{u}''_e$ is a random vector.

Equation (7) is the key formula for statistically computing $\underset{\sim}{u}'_e$ 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. (7) will be computed independently for each particle, two eventually coincident particles at t_1 will have, in general,

*Actually, some authors (Watson and Barr, 1976; Lamb, in press) have proposed an autocorrelation process of the second order.

**In this formula (and the following ones in Sections 2 and 3) 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).

different displacements even if their past "history" is the same -- something that cannot be obtained with any purely deterministic computation such as Eq. (5).

To apply Eq. (7) 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 $\underset{\sim}{u}''$.

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

$$\underset{\sim}{R}_L = \exp\left[-(t_2 - t_1)/\underset{\sim}{T}_L\right] \qquad (8)$$

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 $\underset{\sim}{u}''$ a purely random vector with zero-mean, normally-distributed independent components, we have that $\underset{\sim}{u}''$ is completely characterized by $\underset{\sim}{\sigma}_{u''}$, i.e., the standard deviations of its components. In this case, taking the variances of Eq. (7), we obtain

$$\underset{\sim}{\sigma}_{u''} = \underset{\sim}{\sigma}_{u'}\left[1 - \underset{\sim}{R}_e^2(t_2 - t_1)\right]^{1/2} \qquad (9)$$

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

From the standard deviations $\underset{\sim}{\sigma}_{u''}$ of Eq. (9) it is easy, using commonly available computer programs, to generate each particle's $\underset{\sim}{u}''$ term to be used in Eq. (7).

$\underset{\sim}{R}_e$ 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.

3. NUMERICAL SIMULATIONS

A computer program has been written to simulate atmospheric diffusion with the statistical approach described in the previous section by Eqs. (7) and (9). Figure 1 shows the dispersion rate ($\sigma = \sigma_x = \sigma_y = \sigma_z$) as a function of downwind distance, d, of an elevated puff of 330 particles during homogeneous, stationary conditions, with $\underset{\sim}{u}_L = (3, 0, 0)$ m/s, $\underset{\sim}{R}_e = (r, r, r)$, $\underset{\sim}{\sigma}_{u'} = (\sigma_u, \sigma_u, \sigma_u)$, and $\Delta t = t_2 - t_1 = 60$ sec. Solid lines show the variation of $\sigma(d)$ with r (and fixed $\sigma_u^2 = 0.2\ m^2 s^{-2}$), while dotted lines show that with σ_u (and fixed r = 0.7).

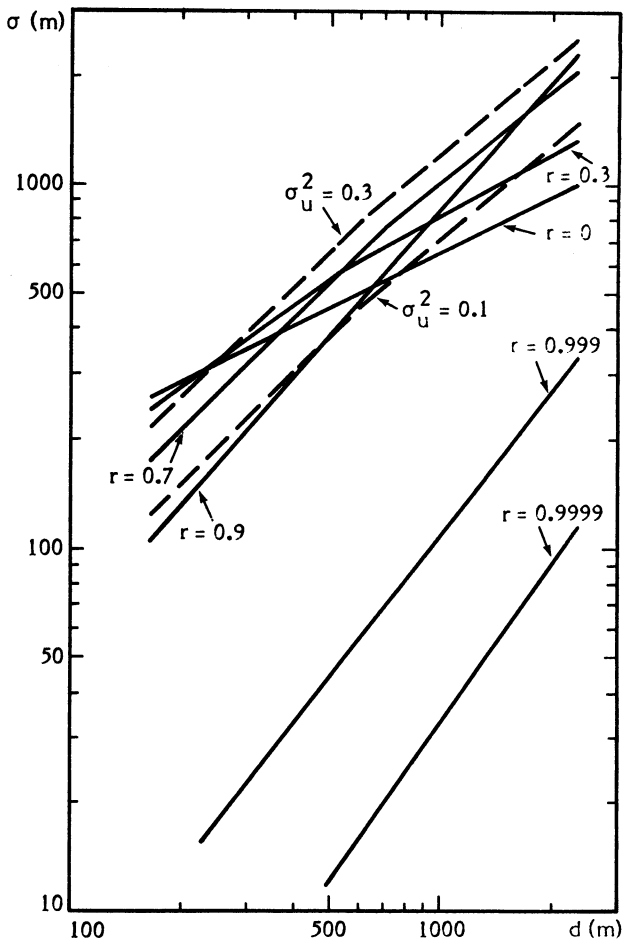

Fig. 1 - Rates of increase of the standard deviation of a puff as a function of the autocorrelation r and standard deviation σ_u of particles pseudo-velocities.

Since we simulate an instantaneous puff from a point source, the initial $\underset{\sim}{u}'_e(t_0)$ have been assumed to be the same (a zero vector) for each particle, which causes the low initial σ values for high r. Other authors (e.g., Hanna, 1979) have suggested generating $\underset{\sim}{u}'_e(t_0)$ with a random distribution so that the diffusion rate is not conditioned by their values.

The following important considerations derive from the analysis of our preliminary numerical simulations:

- with stationary and homogeneous turbulence, σ increase can be approximately expressed as a power law of d($\sigma = ad^b$), even though we sometimes have a small decrease of b after a certain d (see Figure 1).
- different r values (from 0 to 1) give b values in the range from 0.5 to 1.5, which characterize dispersion regimes previously identified in puff diffusion theoretical and experimental studies (Pasquill, 1974).
- σ_u values do not affect b.
- Δt variations seem to affect both a and b (not shown in Figure 1).

These considerations seem to indicate (but further numerical simulations are required) that, if we want to reproduce exactly the same dispersion conditions with a different $\Delta t = t_2 - t_1$, we have to modify σ_u (lower for higher Δt and vice-versa). This is inconsistent with both Eulerian or Lagrangian formulations, where r should depend upon Δt, as in Eq. (8), and σ_u should not. This inconsistency seems to provide the numerical confirmation that $\underset{\sim}{u}'_e$ has different statistical characteristics from $\underset{\sim}{u}'$ measurements and the problem of inferring $\underset{\sim}{u}'_e$ from $\underset{\sim}{u}$ is still open.

4. A NEW STATISTICAL SCHEME FOR CONSIDERING WIND SHEAR EFFECTS

Eulerian measurements have shown that wind shear effects cause a non-zero (negative) correla tion between vertical and along-wind fluctuations. A correct statistical representation of $\underset{\sim}{u}'_e$ should take this phenomenon into account.

With the notation $\underset{\sim}{u}'_e(t) = \left(u'(t),\ v'(t),\ w'(t)\right)$ and $\underset{\sim}{u}''_e(t) = \left(u''(t),\ v''(t),\ w''(t)\right)$, the following scheme can be used

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

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

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

which is similar to Eq. (7), but with the new Eq. (12) for handling the correlation r_{uw} between u' and w'. After some analytical manipulations of Eqs. (10) through (12), and using the notations $\underset{\sim}{R}_e(t_2 - t_1) = (r_u,\ r_v,\ r_w)$, $\underset{\sim}{\sigma}_{u'} = (\sigma_{u'},\ \sigma_{v'},\ \sigma_{w'})$, and $\underset{\sim}{\sigma}_{u''} = (\sigma_{u''},\ \sigma_{v''},\ \sigma_{w''})$, we obtain

$$\phi_1 = r_u \tag{13}$$

$$\phi_2 = r_v \tag{14}$$

$$\phi_3 = \frac{r_w - \phi_1 r_{uw}^2}{1 - \phi_1^2 r_{uw}^2} \tag{15}$$

$$\phi_4 = \frac{r_{uw} \cdot \sigma_{w'} (1 - \phi_1 r_w)}{\sigma_{u'} (1 - \phi_1^2 r_{uw}^2)} \tag{16}$$

$$\sigma_{u''}^2 = \sigma_{u'}^2 (1 - \phi_1^2) \tag{17}$$

$$\sigma_{v''}^2 = \sigma_{v'}^2 (1 - \phi_2^2) \tag{18}$$

$$\sigma_{w''}^2 = \sigma_{w'}^2 (1 - \phi_3^2) - \phi_4^2\, \sigma_{u'}^2 - 2\, \phi_1\, \phi_3\, \phi_4\, r_{uw}\, \sigma_{u'}\, \sigma_{w'} \tag{19}$$

which allow the application of the statistical scheme of Eqs. (10) through (12) if the additional input r_{uw} is available. Vertical profiles of Eulerian r_{uw} values are now available from advanced meteorological towers. We also expect advanced Doppler instrumentation to soon provide this important parameter on a regular basis.

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

5. CONCLUSIONS

This study clarifies the difference between wind measurements and pseudo-velocities to be used for Lagrangian particle modeling techniques. A new Monte Carlo scheme is also proposed for taking into account wind shear effects in the atmospheric boundary layer.

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