Monte-Carlo Simulation of Auto- and Cross-Correlated Turbulent Velocity Fluctuations (MC-LAGPAR II MODEL)

Paolo Zannetti

AeroVironment Inc., 825 Myrtle Avenue, Monrovia, CA 91107, USA

Abstract

This paper discusses the application of Monte-Carlo Lagrangian particle models for the simulation of turbulent dispersion phenomena in the atmosphere. This type of modeling approach requires a numerical scheme for the stochastic generation of wind fluctuations. A new, fully three-dimensional, Monte-Carlo scheme is proposed here which is able to generate wind fluctuations with a specified degree of auto- and cross-correlation. All three spatial cross-correlations are included in the numerical scheme.

This numerical method has been programmed using the APL language (MC-LAGPAR II model) and successfully tested. The listing of the key APL computational routine is presented and provides an example of the flexibility and computational power of the APL compact notation.

Key Words: Air pollution, Lagrangian modeling, Monte-Carlo, Particle models, APL

1. INTRODUCTION AND OVERVIEW

Particle modeling is the most recent and powerful computational tool for the numerical simulation of the dynamics of a physical system. It has been particularly successful in a wide spectrum of applications[1], which range from the atomic scale (e.g., electron flow in semiconductors, and molecular dynamics) to the astronomical scale (e.g., galaxy dynamics), with other important applications to plasma and turbulent fluid dynamics.

Particle models can be purely deterministic or possess stochastic components. In the first case, particle motion is generated from particle interactions and/or potential fields. The simulation of particle trajectories is, in this case, uniquely determined. But particle methods can also possess stochastic characteristics that can be numerically simulated by Monte-Carlo techniques, generating semi-random "perturbations" of particle velocities. In this second case, each simulation of particle dynamics is just a realization from an infinite set of possible solutions.

Particle models have been applied to air pollution dispersion simulations[2,3,4,5,6] but they have not been used as extensively as other dispersion techniques, such as Gaussian models and K-theory grid methods. In particular, Monte-Carlo techniques have provided a straightforward and computationally fast method for simulating, with semi-random particle velocities, the actual stochastic fluctuations (i.e., the effects of turbulent eddies) in the atmosphere. The basic algorithm of this Monte-Carlo Lagrangian particle approach is given by the two equations

$$\mathbf{x}_p(t + \Delta t) = \mathbf{x}_p(t) + \mathbf{V}[\mathbf{x}_p(t), t]\,\Delta t \tag{1}$$

$$\mathbf{V}[\mathbf{x}_p(t),t] = \bar{\mathbf{V}}[\mathbf{x}_p(t)] + \mathbf{V}'[\mathbf{x}_p(t), t, p, \Delta t] \tag{2}$$

which represent the motion $\mathbf{x}_p(t) = [x(t), y(t), z(t)]_p$ of a <u>computer</u> particle p tracing the atmospheric motion described by a space- and time-dependent velocity field $\mathbf{V} = [u_x, u_y, u_z]$. Eq. (1) is rigorously correct only for $\Delta t \to 0$, while Eq. (2) uses the common approximation of splitting the velocity field $\mathbf{V}$ into an "average" term $\bar{\mathbf{V}}$ (which is assumed to vary only with space) and a fluctuating component $\mathbf{V}'$ that needs to be computed at each time step Δt.

The objective of each simulation is to provide dispersion computations in which the motion and spread of the computer particles approximate, on an <u>ensemble</u> basis, atmospheric dispersion properties. The term $\bar{\mathbf{V}}$ is assumed known from average wind measurements or meteorological analyses, while the term $\mathbf{V}'$ needs to be generated by an appropriate Monte-Carlo scheme. Eq. (2) points out that the fluctuation $\mathbf{V}'$ is generally assumed to be particle-dependent (i.e., it depends upon the previous fluctuations $\mathbf{V}'$ of the same particle p) and affected by the length of the time interval Δt.

In the air quality applications of Monte-Carlo dispersion methods, several problems have been encountered; mainly

1. Monte-Carlo models (as all Lagrangian models) require a Lagrangian meteorological input which is not available. However, this input can somehow be derived from Eulerian measurements under certain simplifying assumptions[7,8,9].

2. Eulerian meteorological measurements show that, especially in the surface layer, the along-wind velocity fluctuations u' are negatively correlated with the vertical wind components w' (i.e., $\overline{u'w'} < 0$). Numerical schemes which take this effect into account have been proposed[10,11,12].

3. Eulerian meteorological measurements show that the vertical wind velocity fluctuations w' have a skewed distribution in which a negative w' is more frequent than a positive w', but possesses a lower average intensity $\overline{|w'|}$. Methods have been proposed for incorporating a skewed representation of w'[12,13,14].

0266-9838/86/010025 - 05 $2.00

Paper received September 1, 1985. Referee: Professor John H. Seinfeld

4. Eulerian meteorological measurements show considerable variation with altitude of the vertical turbulent fluctuation intensity, which is characterized by the standard deviation σ_w of the vertical wind fluctuations w'. The incorporation of a σ_w dependent upon z in Monte-Carlo models has created numerical simulation problems, with seemingly inaccurate mass accumulation effects in layers with lower σ_w. In order to avoid this phenomenon, semi-empirical correction factors have been proposed[13,15,16]. Moreover, some contradictions among these semi-empirical approaches have been investigated and clarified[17].

Most of the currently available Monte-Carlo models are limited by the common assumption that the components of the velocity fluctuations **V'** are statistically independent from each other. Schemes have been proposed which include the negative correlation between the along-wind u' and the vertical-wind w' velocity fluctuations[10,11,12]. These schemes assume the x-axis along the main wind direction, so that

$$\bar{\mathbf{V}} = (\bar{u}, 0, 0) \tag{3}$$

$$\mathbf{V'} = (u', v', w') \tag{4}$$

$$\overline{u'v'} = \overline{v'w'} = 0 \tag{5}$$

$$\overline{u'w'} < 0. \tag{6}$$

The main wind direction, however, varies with the position $x_p(t)$ (especially the altitude z), thus requiring the x-axis to vary along the particle trajectory, as performed in a proposed particle-dependent Special Reference (SR) system[18].

Another complication derives from the fact that most Eulerian measurements of the statistical properties of the fluctuation **V'** are performed with respect to a fixed reference system (e.g., an east-north system) in which the x-axis is not aligned with the average wind direction. Algorithms have been developed for estimating the along-wind and cross-wind fluctuation intensities $\sigma_{u'}$ and $\sigma_{v'}$ as a function of the average wind components, $\bar{u}_x$ and $\bar{u}_y$, and the fluctuation intensities $\sigma_{u'_x}$, $\sigma_{u'_y}$ measured in a fixed orthogonal system (x, y)[18]:

$$\sigma^2_{u'} = \frac{\bar{u}_x^2 \, \sigma^2_{u_x} - \bar{u}_y^2 \, \sigma^2_{u_y}}{\bar{u}_x^2 - \bar{u}_y^2} \tag{7}$$

$$\sigma^2_{v'} = \frac{\bar{u}_x^2 \, \sigma^2_{u_y} - \bar{u}_y^2 \, \sigma^2_{u_x}}{\bar{u}_x^2 - \bar{u}_y^2} \tag{8}$$

These equations are not valid, however, when $|\bar{u}_x| \simeq |\bar{u}_y|$; i.e., when the wind direction is close to a multiple of 45° in the (x, y) system.

It is clear that, when a full set of measurements (or inferences) of wind fluctuation variances $\sigma^2_{u'_x}$, $\sigma^2_{u'_y}$ and $\sigma^2_{u'_z}$, autocorrelations $\overline{u'_x(t)\, u'_x(t+\Delta t)}$, $\overline{u'_y(t)\, u'_y(t+\Delta t)}$, $\overline{u'_z(t)\, u'_z(t+\Delta t)}$, and cross correlations $\overline{u'_x(t)\, u'_y(t)}$, $\overline{u'_x(t)\, u'_z(t)}$, $\overline{u'_y(t)\, u'_z(t)}$, is available with respect to any fixed orthogonal reference system, a need exists for incorporating this information into an appropriate Monte-Carlo scheme which makes use of this input. This paper does not address the difficulties and uncertainties still present in the measurement (or inference) of the statistical properties of **V'**. Instead, our objective here is to present a new Monte-Carlo scheme which is able to account for this additional meteorological input, when available.

In the rest of this paper, the new Monte-Carlo scheme is described in Section 2, while Section 3 discusses the APL-coded computer implementation of this method (MC-LAGPAR II model).

2. THE NEW MONTE-CARLO SCHEME

Let us consider the $\mathbf{V'} = [u'_x, u'_y, u'_z]$ wind velocity fluctuations in a fixed orthogonal reference system. In this system, u'_x, u'_y and u'_z can be generated by the Monte-Carlo scheme

$$u'_x(t_2) = f_1\, u'_x(t_1) + u''_x(t_2) \tag{9a}$$

$$u'_y(t_2) = f_2\, u'_y(t_1) + f_3\, u'_x(t_2) + u''_y(t_2) \tag{9b}$$

$$u'_z(t_2) = f_4\, u'_z(t_1) + f_5\, u'_y(t_2) + f_6\, u'_x(t_2) + u''_z(t_2) \tag{9c}$$

where u''_x, u''_y, u''_z are uncorrelated zero-averaged Gaussian "noises" (i.e., random numbers) with standard deviation $\sigma_{u''_x}$, $\sigma_{u''_y}$ and $\sigma_{u''_z}$. The system (9) provides a recursive computation of u'_x, u'_y, and u'_z if the parameters f_1, f_2, f_3, f_4, f_5, and f_6 are known, together with the standard deviations $\sigma_{u''_x}$, $\sigma_{u''_y}$, and $\sigma_{u''_z}$. (Initial values of u'_x, u'_y, and u'_z also need to be provided; however, they can be generally assumed equal to zero.) The objective of the following analytical manipulations is to estimate the nine input parameters (six f's and three $\sigma_{u''}$'s) from statistical variables possessing meteorological significance (i.e., wind fluctuation variances, autocorrelations and cross-correlations).

Let us multiply the three Eqs. (9) by $u'_x(t_1)$, $u'_y(t_1)$, $u'_z(t_1)$, respectively. Then, if the processes (9) are stationary with $t_2 = t_1 + \Delta t$, and remembering that, by definition, u''_x, u''_y, u''_z are totally uncorrelated, we obtain, after averaging,

$$\overline{u'_x(t_2)\, u'_x(t_1)} = f_1\, \sigma^2_{u'_x} \tag{10a}$$

$$\overline{u'_y(t_2)\, u'_y(t_1)} = f_2\, \sigma^2_{u'_y} + f_3\, \overline{u'_x(t_2)\, u'_y(t_1)} \tag{10b}$$

$$\overline{u'_z(t_2)\, u'_z(t_1)} = f_4\, \sigma^2_{u'_z} + f_5\, \overline{u'_y(t_2)\, u'_z(t_1)} + f_6\, \overline{u'_x(t_2)\, u'_z(t_1)}\,. \tag{10c}$$

But, using Eqs. (9) the three unknown terms in the right side of Eqs. (10b) and (10c) can be expressed as

$$\overline{u'_x(t_2)\, u'_y(t_1)} = f_1\, r_{xy}\, \sigma_{u'_x}\, \sigma_{u'_y} \tag{11a}$$

$$\overline{u'_y(t_2)\, u'_z(t_1)} = f_2\, r_{yz}\, \sigma_{u'_y}\, \sigma_{u'_z} + f_3\, f_1\, r_{xz}\, \sigma_{u'_x}\, \sigma_{u'_z} \qquad (11b)$$

$$\overline{u'_x(t_2)\, u'_z(t_1)} = f_1\, r_{xz}\, \sigma_{u'_x}\, \sigma_{u'_z} \qquad (11c)$$

where r_{xy}, r_{yz}, r_{xz} are the cross correlations between u'_x and u'_y, u'_y and u'_z, u'_x and u'_z, respectively. By substituting Eqs. (11) into Eqs. (10), we obtain

$$r_x\, \sigma^2_{u'_x} = f_1\, \sigma^2_{u'_x} \qquad (12a)$$

$$r_y\, \sigma^2_{u'_y} = f_2\, \sigma^2_{u'_y} + f_3\, f_1\, r_{xy}\, \sigma_{u'_x}\, \sigma_{u'_y} \qquad (12b)$$

$$r_z\, \sigma^2_{u'_z} = f_4\, \sigma^2_{u'_z} + f_5\, (f_2\, r_{yz}\, \sigma_{u'_y}\, \sigma_{u'_z} + f_3\, f_1\, r_{xz}\, \sigma_{u'_x}\, \sigma_{u'_z}) + f_6\, f_1\, r_{xz}\, \sigma_{u'_x}\, \sigma_{u'_z} \qquad (12c)$$

where r_x, r_y and r_z are the auto-correlations of the fluctuations u'_x, u'_y and u'_z, respectively, with time lag Δt.

Additional equations are required to solve the entire system. By multiplying Eq. (9a) by Eq. (9b) and averaging, we obtain

$$r_{xy}\, \sigma_{u'_x}\, \sigma_{u'_y} = f_1\, f_2\, r_{xy}\, \sigma_{u'_x}\, \sigma_{u'_y} + f_1\, f_3\, r_x\, \sigma^2_{u'_x} + f_3\, \sigma^2_{u''_x} \qquad (13a)$$

while by multiplying Eq. (9b) by Eq. (9c) and averaging we obtain

$$r_{xz}\, \sigma_{u'_x}\, \sigma_{u'_z} = f_1\, f_4\, r_{xz} + f_1\, f_5\, (f_2\, r_{xy}\, \sigma_{u'_x}\, \sigma_{u'_y} + f_3\, r_x\, \sigma^2_{u'_x}) + f_1\, f_6\, r_x\, \sigma^2_{u'_x} + (f_5\, f_3 + f_6)\, \sigma^2_{u''_x} \qquad (13b)$$

and by multiplying Eq. (9b) by Eq. (9c) and averaging we obtain

$$r_{yz}\, \sigma_{u'_y}\, \sigma_{u'_z} = f_2\, f_4\, r_{yz}\, \sigma_{u'_y}\, \sigma_{u'_z} + f_2\, f_5\, r_y\, \sigma^2_{u'_y} + f_2\, f_6\, f_1\, r_{xy}\, \sigma_{u'_x}\, \sigma_{u'_y} + f_3\, f_4\, f_1\, r_{xz}\, \sigma_{u'_x}\, \sigma_{u'_z} + f_3\, f_5\, r_{xy}\, \sigma_{u'_x}\, \sigma_{u'_y} + f_3\, f_6\, \sigma^2_{u'_x} + f_5\, \sigma^2_{u''_y} \ . \qquad (13c)$$

Moreover, by taking the variances of Eqs. (9) and using Eqs. (11), we obtain

$$\sigma^2_{u''_x} = \sigma^2_{u'_x}\, (1 - f_1^2) \qquad (14a)$$

$$\sigma^2_{u''_y} = \sigma^2_{u'_y}\, (1 - f_2^2) - f_3^2\, \sigma^2_{u'_x} - 2\, f_2\, f_3\, f_1\, r_{xy}\, \sigma_{u'_x}\, \sigma_{u'_y} \qquad (14b)$$

$$\sigma^2_{u''_z} = \sigma^2_{u'_z}\, (1 - f_4^2) - f_5^2\, \sigma^2_{u'_y} - f_6^2\, \sigma^2_{u'_x} - 2\, f_4\, f_5 (f_2\, r_{yz}\, \sigma_{u'_y}\, \sigma_{u'_z} + f_3\, f_1\, r_{xz}\, \sigma_{u'_x}\, \sigma_{u'_z}) - 2\, f_4\, f_6\, f_1\, r_{xz}\, \sigma_{u'_x}\, \sigma_{u'_z} - 2\, f_5\, f_6\, r_{xy}\, \sigma_{u'_x}\, \sigma_{u'_y} \ . \qquad (14c)$$

The above equations allow a solution of the Monte-Carlo scheme of Eqs. (9) following the computational sequence below:

- from Eq. (12a) we obtain

$$f_1 = r_x \qquad (15)$$

- from Eq. (14a) $\sigma_{u''_x}$ can be computed
- Eqs. (12b) and (13a) give a system of two equations in the two unknowns f_2 and f_3, providing the solution

$$f_2 = \frac{r_y - r_x\, r^2_{xy}}{1 - r_x^2\, r^2_{xy}} \qquad (16)$$

$$f_3 = \frac{r_{xy}\, \sigma_{u'_y}\, (1 - r_x\, r_y)}{\sigma_{u'_x}\, (1 - r_x^2\, r^2_{xy})} \qquad (17)$$

- from Eq. (14b) $\sigma_{u''_y}$ can be computed
- Eqs. (12c), (13b) and (13c) give a system of three equations in the three unknowns f_3, f_4, and f_5 which allow a numerical computation of f_4, f_5 and f_6 (an analytical solution for f_4, f_5, and f_6 could be derived but is too cumbersome).
- from Eq. (14c) $\sigma_{u''_z}$ can be computed

The above scheme has been successfully tested and is able to provide a multiple time series of fluctuations u'_x, u'_y and u'_z with <u>any</u> physically acceptable degree of auto- and cross-correlation using the meteorological input $\sigma_{u'_x}$, $\sigma_{u'_y}$, $\sigma_{u'_z}$, r_x, r_y, r_z, r_{xy}, r_{xz}, r_{yz} which can be either measured or inferred from meteorological analyses and assumptions. This meteorological input can be easily assumed to vary with space and time. Space variations are accounted by using meteorological values interpolated at the particle location $\mathbf{x}_p(t_1)$; time variations can be included by performing particle simulations as a sequence of different steady-state conditions (e.g., 15-minute periods).

The meteorological input for Eqs. (9) is estimated at $\mathbf{x}_p(t_1)$, but is assumed to represent the meteorological parameters along the trajectory from $\mathbf{x}_p(t_1)$ to $\mathbf{x}_p(t_2)$. Therefore, Δt must be chosen sufficiently small to avoid a large variation of the meteorological parameters along such trajectory (i.e., the particle displacement must be smaller than the meteorological length scales). Vertical displacements are particularly critical, due to the sometimes large vertical variation of $\sigma_{u'_z}$ near the ground. This factor probably plays a major role in the inaccurate mass accumulation effects often found in layers with lower $\sigma_{u'_z}$.

An accurate, cost-effective simulation can still be performed using a relatively large Δt if particle trajectories are allowed to be "split," when necessary, for properly taking into account the varying meteorological input (mainly $\sigma_{u'_z}$) encountered from $\mathbf{x}_p(t_1)$ to $\mathbf{x}_p(t_2)$.

Finally, particles should be reflected by the ground surface, but reflection should be followed by setting the particle "memory" u'_x, u'_y, u'_z to zero.

3. THE MC-LAGPAR II MODEL

The algorithms and considerations presented in the previous section have been incorporated into a computer program, MC-LAGPAR II, which allows Monte-Carlo Lagrangian particle simulations of a single source in flat terrain. This prototype model has been written using the APL interactive language. The key APL routine for the recursive computation of u'_x, u'_y, and u'_z is illustrated in Figure 1, in which the APL function MC3D extracts the meteorological input from the input vector IN: autocorrelations (RX, RY, RZ; previously r_x, r_y, r_z), standard deviations (SX, SY, SZ; previously σ_{u_x}, σ_{u_y}, σ_{u_z}) and cross correlations RXY, RXZ, RYZ; previously, r_{xy}, r_{xz}, r_{yz}). Results are saved in the output vector OUT: the six parameters F1, F2, F3, F4, F5, F6 (previously f_1, f_2, f_3, f_4, f_5, f_6) and the variances of the Gaussian noises S2X, S2Y, S2Z (previously $\sigma^2_{u''_x}$, $\sigma^2_{u''_y}$, $\sigma^2_{u''_z}$). The solution of the linear system for F3, F4, F5 is performed in the statement [23] using the primitive APL operator ⌹.

```
     ∇OUT←MC3D IN

[1]   ⍝
[2]   ⍝ COMPUTATION OF THE PARAMETERS F's
[3]   ⍝ AND THE GAUSSIAN NOISE VARIANCES
[4]   ⍝
[5]   RX←IN[1],0⍴RY←IN[2],0⍴RZ←IN[3]
[6]   SX←IN[4],0⍴SY←IN[5],0⍴SZ←IN[6]
[7]   RXY←IN[7],0⍴RXZ←IN[8],0⍴RYZ←IN[9]
[8]   F1←RX
[9]   S2X←(SX*2)×1-F1*2
[10]  F2←(RY-RX×RXY*2)÷DEN←1-(RX*2)×RXY*2
[11]  F3←(RXY×SY×1-RX×RY)÷DEN×SX
[12]  S2Y←(-((F2*2)×SY*2))+(-((F3*2)×SX*2))
[13]  S2Y←(SY*2)+S2Y-2×F2×F3×F1×RXY×SX×SY
[14]  A←3 3⍴0
[15]  A[1;]←SZ,((F2×RYZ×SY)+F3×F1×RXZ×SX),F1×RXZ×SX
[16]  A[2;1]←F1×RXZ×SZ
[17]  A[2;2]←(F1×F2×RXY×SY)+(F1×F3×RX×SX)+F3×SX×1-F1*2
[18]  A[2;3]←(F1×RX×SX)+SX×1-F1*2
[19]  A[3;1]←(F2×RYZ×SY×SZ)+F3×F1×RXZ×SX×SZ
[20]  A[3;2]←(F2×RY×SY*2)+(F3×RXY×SX×SY)+S2Y
[21]  A[3;3]←(F2×F1×RXY×SX×SY)+F3×SX*2
[22]  B←(RZ×SZ),(RXZ×SZ),RYZ×SY×SZ
[23]  FI←B⌹A
[24]  F4←FI[1],0⍴F5←FI[2],0⍴F6←FI[3]
[25]  S2Z←(SZ*2)+(-(F4*2)×SZ*2)+(-(F5*2)×SY*2)+(-(F6*2)×SX*2)
[26]  S2Z←S2Z+(-2×F4×F5×((F2×RYZ×SY×SZ)+F3×F1×RXZ×SX×SZ))
[27]  S2Z←S2Z+(-2×F4×F6×F1×RXZ×SX×SZ)+(-2×F5×F6×RXY×SX×SY)
[28]  OUT←F1,F2,F3,F4,F5,F6,S2X,S2Y,S2Z
```

Figure 1. Main APL routine for computing the parameters of Eqs. (9).

The above parameter evaluation allows the recursive computation of the fluctuations UX, UY, UZ (previously u'_x, u'_y, u'_z) for each particle I, as illustrated in Figure 2, in which UXO, UYO, UZO are the "old" fluctuations UX, UY, UZ computed at the previous time step Δt. The APL function GN gives a Gaussian random number with variance S2X, S2Y, or S2Z, respectively.

```
[···]UX[I]←(F1×UXO[I])+GN S2X
[···]UY[I]←(F2×UYO[I])+(F3×UX[I])+GN S2Y
[···]UZ[I]←(F3×UZO[I])+(F5×UY[I])+(F6×UX[I])+GN S2Z
```

Figure 2. APL routine for the recursive updating of the particle velocity fluctuations.

4. CONCLUSIONS

The new Monte-Carlo scheme presented in this paper allows a numerical simulation of air quality dynamics which is more realistic than other simpler Monte-Carlo methods, since it is able to incorporate fully three-dimensional auto- and cross-correlated wind fluctuations. However, it requires advanced statistical information on wind fluctuation characteristics, which is generally not available.

With the continuous improvement of meteorological measurement techniques and the on-going research on the relationship between Eulerian measurements and Lagrangian properties, methods such as the MC-LAGPAR II approach proposed in this article, could become, in the near future, valuable numerical tools for advanced simulations of atmospheric turbulence dispersion phenomena that would make full use of the extensive on-going monitoring efforts in this field.

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