

Particle Modeling Simulation of Atmospheric Dispersion using the MC-LAGPAR Package

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ABSTRACT

A Monte Carlo model and computer code (MC-LAGPAR) for simulating atmospheric transport and diffusion of plumes are described. The turbulent diffusion is simulated by the semi-random motion of Lagrangian particles. The particles are emitted by a point source and dispersed in a computational domain by pseudo-velocities derived from vertical profiles of meteorological variables.

The MC-LAGPAR code includes the implementation of special algorithms for the simulation of a dynamic plume rise, chemical decay, deposition and resuspension effects. Furthermore, computer-graphics displays have been developed. The model, here used in its two dimensional version, is validated in the well-known case of homogeneous and stationary turbulence. In this case, we compared the concentration fields obtained by our model with those calculated by the known analytical solution. In both computations, the standard deviations of wind velocities are calculated according to the Taylor formulas.

In the nonhomogeneous case, the vertical structure of turbulence is parameterized according to the scheme suggested by Hanna. As an example of the non-homogeneous case, we present numerical simulations in convective (unstable) conditions in which the influence of updraughts and downdraughts is empirically taken into account.

KEYWORDS: Air pollution, Lagrangian modelling, Monte Carlo, Particle Models, Homogeneous and Nonhomogeneous turbulence.

1. INTRODUCTION

Atmospheric diffusion processes in the Planetary Boundary Layer (PBL) are strongly affected by phenomena characterized by turbulent eddies of different scales, i.e., semi-random atmospheric motion that is strongly auto- and cross-correlated. The emission of pollutants in the PBL, due to natural and anthropogenic sources, generates concentration fields whose evolution is strongly dependent upon the turbulent properties of the atmosphere.

Deterministic air quality models are an important tool for providing unambiguous source-receptor relationships, i.e., the assessment of the fraction of concentration caused by each source in each receptor area. In particular, only the use of a reliable deterministic simulation model allows the definition and implementation of appropriate and cost-effective emission control strategies in a certain region.

Dispersion models simulate: 1) atmospheric transport; 2) atmospheric turbulent diffusion; 3) chemical and photochemical processes; and 4) ground deposition (dry and/or wet).

Models can be divided into two main categories: Eulerian and Lagrangian models. Eulerian models (e.g., K-theory grid models, Mc Rae et al. [1]) use a fixed reference system, while Lagrangian models (e.g., puff models, Zannetti [2]) either use a reference system that travels with the average atmospheric motion (e.g., a photochemical Lagrangian box model, Drivas et al. [3]) or split the plumes into "elements" and calculate the separate dynamics of each element. This second category (Lagrangian models) seems to be the most appropriate for simulating atmospheric dispersion processes.

The most recent and powerful computational tool for the numerical discretization, in a Lagrangian frame, of a physical system is provided by particle modeling techniques (Hockney and Eastwood [4]). Using particle methods in air pollution applications, emitted polluting material is characterized by "fictitious" computer particles. Each particle is "moved" at each time step by pseudo-velocities, that take into account both the average wind transport and the (seemingly) random turbulent fluctuations of the wind components.

Several air quality studies have applied particles methods (Lamb [5], Lange [6], Hanna [7], De Baas et al. [8], Baerentsen and Berkowicz [9], McNider [10], Pielke et al. [11], Segal et al. [12]). Potentially, the method is superior in both numerical accuracy and physical representativeness. However, much research is still needed to extract, from meteorological measurements (most of them Eulerian ones) the Lagrangian input required to run these models, i.e., the generation scheme of the pseudo-velocities that move each particle at each time step. Most particle models use Monte-Carlo techniques (random number generation methods) to generate the pseudo-velocities.

The approach and formulation of one of the aforesaid models, i.e., MC-LAGPAR (Zannetti [13]) is described in the following section. Then, simulation outputs relative to cases of both homogeneous and nonhomogeneous turbulence are presented and discussed. Finally, conclusive remarks are provided in the last section.

* Computational Mechanics Publications

Paper received on 15 May 1987 and in final form on 10 September 1987.

Referees: Prof. Roger Pielke and Dr. Steve Hanna

2. MC-LAGPAR MODEL

The MC-LAGPAR model was originally formulated (Zannetti [14]) to allow the simulation of air parcel motion with both autocorrelation and cross-correlation terms. In particular the method includes the (negative) cross-correlation $\overline{u'w'}$ between the horizontal (along wind) and vertical fluctuations of the wind vector. This term sometimes plays an important role and its inclusion provides better simulation capabilities in comparison with other particle models.

The basic scheme assumes that each particle is moved at each time step Δt by a pseudo-velocity $\underline{V}(x,y,z,t,p)$ that is a function of space and time and that is particle dependent. If we assume that the x-axis is chosen along the average wind direction, it is $\underline{V}(\overline{U}+u', v', \overline{W}+w')$ where u' , v' and w' are the fluctuations above the average values \overline{U} , 0, and \overline{W} , which are either known or available as an output of an Eulerian meteorological model. The fluctuations of each particle p are updated at each Δt by the following Monte-Carlo scheme:

$$u'(t+\Delta t) = f_1 u'(t) + u''(t+\Delta t) \quad (1)$$

$$v'(t+\Delta t) = f_2 v'(t) + v''(t+\Delta t) \quad (2)$$

$$w'(t+\Delta t) = f_3 w'(t) + f_4 u'(t+\Delta t) + w''(t+\Delta t) \quad (3)$$

where u'' , v'' , w'' are random values generated by Monte-Carlo methods. If the statistics of the fluctuations u' , v' , w' are known (i.e., variance, autocorrelation and cross-correlation $\overline{u'w'}$), the parameters f_1 , f_2 , f_3 , f_4 and the variances of u'' , v'' , w'' can be computed, for each particle at each time step, using algebraic manipulations (Zannetti [13]):

$$f_1 = \frac{r}{u'} \quad (4)$$

$$f_2 = \frac{r}{v'} \quad (5)$$

$$f_3 = \frac{\frac{r}{w'} - f_1 \frac{r^2}{u'w'}}{1 - f_1^2 \frac{r^2}{u'w'}} \quad (6)$$

$$f_4 = \frac{\frac{r}{u'w'} \frac{\sigma}{w'} (1 - f_1 \frac{r}{w'})}{\sigma_{u'} (1 - f_1^2 \frac{r^2}{u'w'})} \quad (7)$$

$$\sigma_{u''}^2 = \sigma_{u'}^2 (1 - f_1^2) \quad (8)$$

$$\sigma_{v''}^2 = \sigma_{v'}^2 (1 - f_2^2) \quad (9)$$

$$\sigma_{w''}^2 = \sigma_{w'}^2 (1 - f_3^2) - f_4^2 \sigma_{u'}^2 - 2 f_1 f_2 f_4 \frac{r}{u'w'} \frac{\sigma}{u'} \frac{\sigma}{w'} \quad (10)$$

The MC-LAGPAR model has been recently expanded (Zannetti [15]) to incorporate all three cross-correlations $\overline{u'v'}$, $\overline{v'w'}$, $\overline{u'w'}$ in a generic (x,y,z) reference system. The simulations presented in this paper have been obtained, however, using the simpler scheme of Eqs. 1-3.

MC-LAGPAR incorporates several optional routines for the treatment of a dynamic plume rise ([16], [17], [18]); chemical decay, ground deposition/absorption/resuspension are taken into account with simple exponential formulas:

$$p_x = 1 - e^{-\frac{-\Delta t}{T_x}}$$

where p_x and T_x are the probability and the time scale of removal or deposition or absorption or resuspension effects.

The model can simulate the nonstationary evolution of a single puff release or the behaviour of a continuously emitted plume in stationary conditions. The former case (single puff) is simulated by an instantaneous generation of particles with the same initial velocity fluctuations. It is commonly claimed that this generation allows the representation of relative diffusion, even though this assumption has been recently challenged (Hanna, personal communication). The latter case (continuous plume) is simulated by a continuous generation of particles with initial velocity fluctuations randomly extracted from the velocity distributions at the source heights. This assumption allows a correct simulation of the "ensemble" properties of the plume. In the rest of the paper we focus only on the simulation of a continuous plume, using assumptions that pertain to one-hour averaging times.

Particles hitting the ground are allowed to be reflected. In this case, however, the "memory" w' of the reflected particle is forced to change sign in order to correctly treat the reflection phenomena. A similar condition can be prescribed for the upper boundary.

The current version of the MC-LAGPAR computer code is written in APL. The code performs dispersion simulations in a three dimensional domain with flat terrain and requires emission and meteorological input. The meteorological input is dependent only upon the altitude and must be specified at user-selected elevations. This input is: the average wind components (\overline{U} , \overline{V} , \overline{W}), the variances and autocorrelations of the fluctuations u' , v' and w' , the cross-correlation $\overline{u'w'}$, and the potential temperature gradient (only to calculate the plume rise). These user-specified values are linearly interpolated at each step to provide the values at each particle's elevation. Meteorological measurements can be used to directly or indirectly evaluate the above meteorological parameters. In particular, a set of suitable algorithms has been proposed (Hanna [19]) that provides the above variances and autocorrelations using the mixing height h_i , the Monin-Obukhov length L , the convective velocity scale w_{*c} , the friction velocity u_{*} , the roughness length z_0 , and the Coriolis parameter f ; all parameters can be either directly measured or evaluated from meteorological measurements. In addition, the T_x time scales need to be inputted. Finally, the number of particles n and the time step Δt of the simulation must be done.

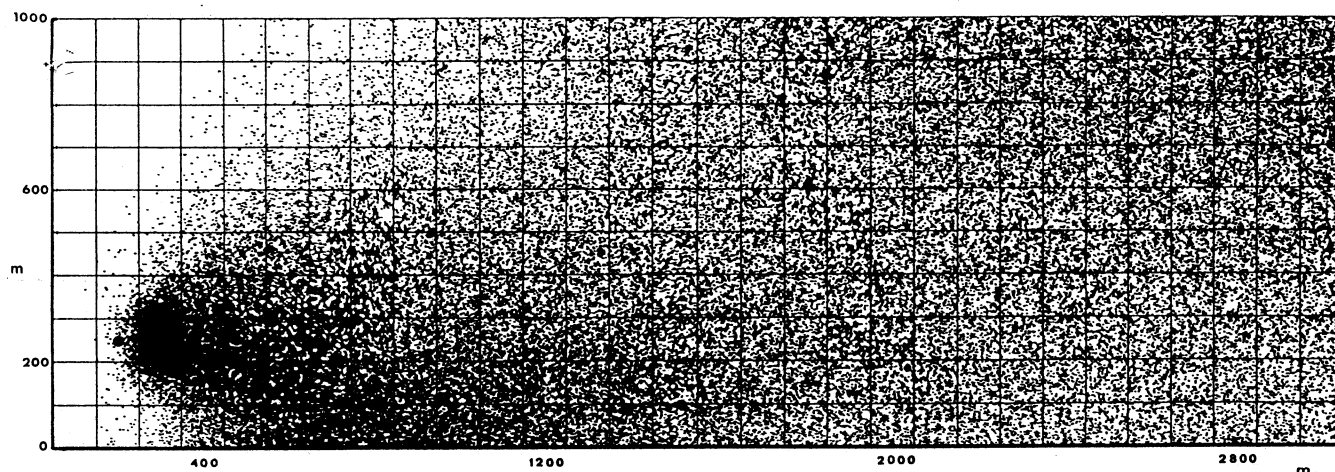


Fig. 1. Example of plume simulation in unstable condition with particle release at 250m.

The main output is a file containing the coordinates (x,y,z) of each particle at each time step. Using an interactive package (written in FORTRAN-77), it is possible to display the "puff" of particles (Fig. 1), to calculate and plot the concentration of pollutant on a suitably selected grid, to draw the isoconcentration lines on the x-y or x-z planes, to determine the standard deviations and centerline of the plume, and so on. Some examples of these possibilities are showed in the following figures.

3. SIMULATION OF HOMOGENEOUS TURBULENCE

When turbulence is homogeneous, its average properties are uniform in space. Therefore the turbulent statistics used in performing the simulations, i.e., σ_u and σ_w (the standard deviation of wind velocity fluctuations) and T_L (the Lagrangian integral time scale), were kept constant with respect to the space coordinates.

It can be shown that MC-LAGPAR generates trajectories whose standard deviations reproduce quite well the particle displacements theoretically deduced by Taylor [20]:

$$\sigma_{\text{Taylor}}(n \cdot \Delta t) = 2 \sigma_{u'} T_L^2 \left[\frac{n \cdot \Delta t}{T_L} - \left(1 - e^{-\frac{n \cdot \Delta t}{T_L}} \right) \right] \quad (11)$$

Fig. 2 shows the result of this comparison. The agreement is noticeable.

Then, we performed the computation of the concentration field in the (x,z) plane of material continuously emitted by a point source. The parameters of the simulation were the following:

$$H_s = 400\text{m}, \bar{u} = 3\text{m/s}, T_L = 144\text{s}, \sigma_{u'} = \sigma_{w'} = 0.34\text{m/s}, \Delta t = 60\text{s}$$

where H_s is the source height and \bar{u} is the wind speed. The dimensions of the grid cell used to compute the concentrations were defined by $\Delta x = u \cdot \Delta t = 180\text{m}$ and $\Delta z = 50\text{m}$.

The latter value ($\Delta z = 50\text{m}$) seems to be the best choice in our case, and was evaluated by analyzing several simulations with Δz in the range between 5m and 100m: the more the cell increases, the more the concentration tends to reduce its variability. However, Δz cannot be too large in order to well represent ground-level concentrations with sufficient spatial resolution.

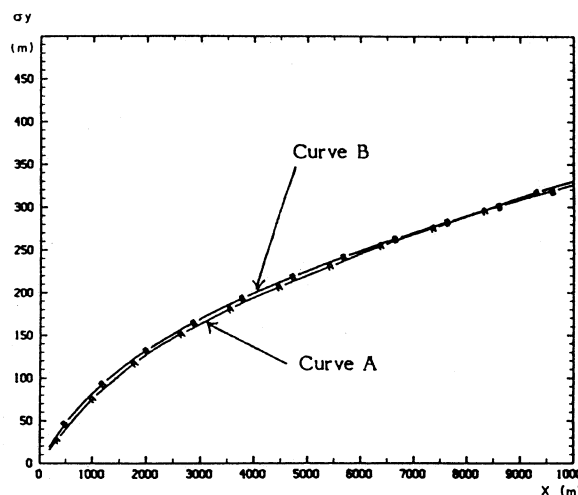


Fig. 2. Standard deviation along cross-wind direction as a function of downwind distance. Curve A: numerical simulation with 3000 particles. Curve B: Eq. 11.

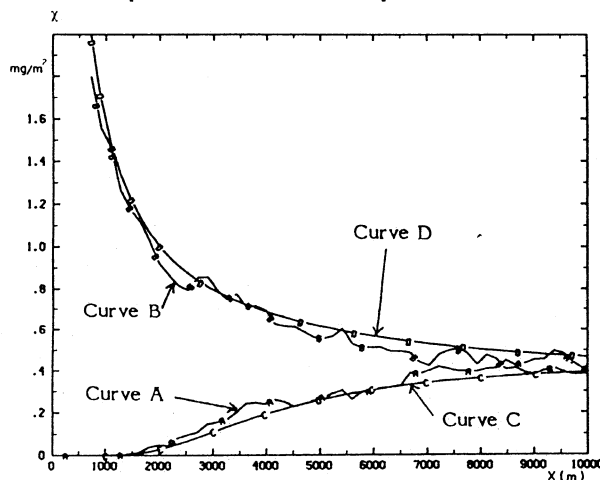


Fig. 3. Concentration as a function of a downwind distance.

- Curve A: ground-level with MC-LAGPAR numerical simulation.
- Curve B: centerline plume level with MC-LAGPAR numerical simulation.
- Curve C: ground-level with analytical solution.
- Curve D: centerline plume level with analytical solution.

The results of our simulations have been compared (at ground level and at the centerline plume level) with the results obtained by the two-dimensional analytical solution in homogeneous turbulence (i.e., the Gaussian model), in which σ_z was evaluated by Eq. 11. Fig. 3 shows the results of such a comparison, which clearly appears to be satisfactory.

4. SIMULATION OF NONHOMOGENEOUS (CONVECTIVE) CONDITIONS

To prescribe the values of the meteorological parameters (stability and height dependent) needed to simulate turbulent diffusion in the planetary boundary layer, we choose the scheme suggested by Hanna [19]. This scheme provides different parametrization of the vertical profiles of

$$\sigma_{u'}, \sigma_{v'}, \sigma_{w'}, T_{L_{u'}}, T_{L_{v'}}, T_{L_{w'}}$$

for different stability conditions (unstable, neutral, stable), where $T_{L_{u'}}, T_{L_{v'}}, T_{L_{w'}}$ are the Lagrangian time scales.

In unstable conditions, Hanna suggests :

$$\sigma_{u'} = \sigma_{v'} = \sigma_{w'} = u_*' (12 + 0.5 h_i / |L|)^{1/3}$$

$$\sigma_{w'} = \begin{cases} = 0.96 \cdot w_*' \left(\frac{3z}{h_i} - \frac{L}{h_i} \right)^{1/3} & \text{for } z < 0.03 h_i \\ = w_*' \cdot \min \left[0.96 \cdot w_*' \left(\frac{3z}{h_i} - \frac{L}{h_i} \right)^{1/3}; 0.763 \left(\frac{z}{h_i} \right)^{0.175} \right] & \text{for } 0.03 h_i < z < 0.4 h_i \\ = 0.722 \cdot w_*' \left(1 - \frac{z}{h_i} \right)^{0.207} & \text{for } 0.4 h_i < z < 0.96 h_i \\ = 0.37 \cdot w_*' & \text{for } 0.96 h_i < z < h_i \end{cases}$$

$$T_{L_{u'}} = T_{L_{v'}} = 0.15 \frac{h_i}{\sigma_{u'}} \\ T_{L_{w'}} = \begin{cases} = 0.1 \left(\frac{z}{\sigma_{w'}} \right) \frac{1}{0.55 + 0.38 (z - z_0) / |L|} & \text{for } z < 0.1 h_i \text{ and } (z - z_0) < |L| \\ = 0.59 \frac{z}{\sigma_{w'}} & \text{for } z < 0.1 h_i \text{ and } (z - z_0) > |L| \\ = 0.15 \frac{h_i}{\sigma_{w'}} \left(1 - e^{-\left(\frac{5z}{h_i} \right)} \right) & \text{for } z > 0.1 h_i \end{cases}$$

In our simulations we set :

$$h_i = 1000 \text{ m}, w_*' = 1.6 \text{ m/s}, \bar{u} = 2.5 \text{ m/s},$$

$$u_*' = 0.2 \text{ m/s}, z_0 = 0.2 \text{ m} \text{ and } L = -5 \text{ m}$$

Since in nonhomogeneous turbulence the wind profile is not constant with height, the cross-correlation term $u'w'$ must be taken into account (Zannetti [13]). In our simulations, $u'w'$ was set equal to $-u_*'^2$ near the surface and allowed to approach zero linearly with the height at the top of the PBL. This trend of $u'w'$ with height was derived from fig. 6.7 of Plate (1982) [21].

Fig. 4 shows the differences on the ground-level concentrations due to two vertical wind profiles: 1) constant and 2) power law with height. In the case of the power law profile, its exponent was chosen in order to give an average wind velocity in the PBL equal to the value of the constant wind profile. It appears that using a power law profile, the maximum ground-level concentration comes near the source and its value slightly increases.

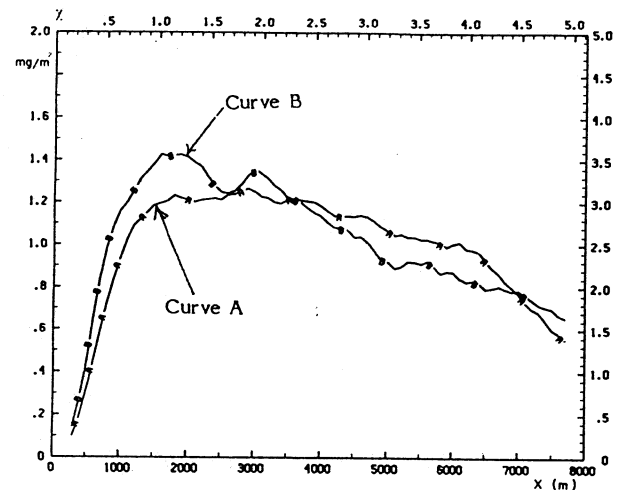


Fig. 4. Ground-level concentration as a function of a downwind distance with:

curve A: constant wind profile ($\bar{u} = 2.5 \text{ m/s}$)

curve B: power law wind profile ($u = 1.378 \cdot z^{0.1}$)

the top and right scales report nondimensional distance $(w_*'/\bar{u}) \cdot (x/h_i)$ and concentration $(Q/h_i \cdot \bar{u})$.

The effects of the convective plumes on the pollutant dispersion were empirically considered. The measurements of Yamamoto et al. [22] show that the average ascent velocity w of plumes is constant with height in the PBL and it can be calculated that its value is about 0.5-0.6 times w_*' . A suitable value for the velocity of descent is $0.4 \cdot w_*'$ (Briggs 1975 [16]). Therefore, we added to the turbulent vertical velocities a constant vertical velocity due to the convective cells. In other words, to each trajectory a constant vertical velocity (up or down) was attributed in such a way that \bar{w} is zero over all the trajectories and all the heights. This means that the number of particles N_u in updraft, having an higher velocity w_u , are less than those (N_d particles) in downdraft. They are calculated by:

$$N_d = N_u \frac{w_u}{-w_d}$$

As also done by Baerentsen and Berkowicz [9], each particle is allowed to jump from an updraft to a downdraft and vice versa with probabilities that depend on the time scales T_{Lu} and T_{Ld} of the two phenomena. That is, setting

$$T_{Lu} = \frac{h_i}{w_u}$$

the probability of a particle to jump from updraft to downdraft is

$$P_{u \rightarrow d} = 1 - e^{-\frac{\Delta t}{T_{Lu}}}$$

To be sure that the same number of particles jumps from up- to downdraft and viceversa we retrieve (for $\Delta t \ll T_{Lu}$ and $t \ll T_{Ld}$)

$$T_{Ld} = \frac{h_i}{-w_d}$$

and the probability of a particle to jump from downdraft to updraft is

$$P_{d \rightarrow u} = 1 - e^{-\frac{\Delta t}{T_{Ld}}}$$

Figs. 5, 6 and 7, show the comparison between the ground-level concentrations obtained from MC-LAGPAR simulations (curve A) and the water-tank experiments of Willis and Deardorff [23],[24],[25] (circles). These last refer to three different source heights (the emissions are nonbuoyant):

$$H_s / h_i = 0.067, 0.24, \text{ and } 0.49$$

and Figs. 5, 6 and 7 refer respectively to the same cases.

Fig. 8 shows MC-LAGPAR simulation referred to a source height

$$H_s / h_i = 0.75$$

Concentrations are averaged values over the interval $z / h_i < 0.05$ except for the source height $H_s / h_i = 0.067$, where the average is over $z / h_i < 0.01$. In Figs. 5, 6, 7 and 8, maximum ground-level concentrations according to the Briggs formula (ref. Eq. 14 in De Baas et al. [8]) are also reported (squares). $-w_d$ and w_u in our simulations have been set equal to 0.4 and 0.6 times w_{x*} , respectively.

Looking at Figs. 5, 6, 7 and 8, it appears that the agreement between MC-LAGPAR simulations and experimental data is satisfactory. In particular, the simulations are able to well reproduce the typical behaviour of airborne pollutant dispersion in convectively unstable conditions. In fact, if particles are released near the ground, they first remain at the surface and then rise to the middle level of the PBL, whereas if they are emitted from elevated stacks, they first descend and then rise to middle level [8]. This fact is clearly shown in Figs. 9, 10, 11 and 12, where the contours of the nondimensional concentrations

$$\chi = \left(\frac{Q}{h_i \cdot u} \right)$$

of the four numerical simulations are plotted in the x - z plane. The goodness of the agreement is particularly interesting, as the simulations were performed by inserting in the Hanna scheme for unstable conditions a very simple mechanism taking into account the ascent of hot natural plumes.

It must be pointed out that, in our simulations, we did not encounter any unreasonable accumulation of particles in regions of low σ_w , and, therefore, we found no need to include semi-empirical drift velocity corrections, as performed, for example, by Legg and Raupach [26]. We believe that our realistic treatment of the downdrafts and updrafts, together with the inclusion of the cross-correlation $u'w'$ whose effects are mostly noticeable near the ground, is the main reason why particle accumulation is correctly avoided.

5. CONCLUSIONS

A Monte-Carlo model to simulate a turbulent diffusion of pollutants in the atmosphere is presented. The numerical scheme and the input-output assumptions are shown. The results of simulations in homogeneous conditions are in good agreement with those obtained by the analytical solution. Numerical experiments performed in atmospheric convective conditions (nonhomogeneous turbulence) produce concentration fields that satisfactorily agree with Willis and Deardorff's water-tank experiments. Therefore, the MC-LAGPAR computer code has proved to be a flexible and reliable tool to simulate air pollution dispersion in different meteorological situations.

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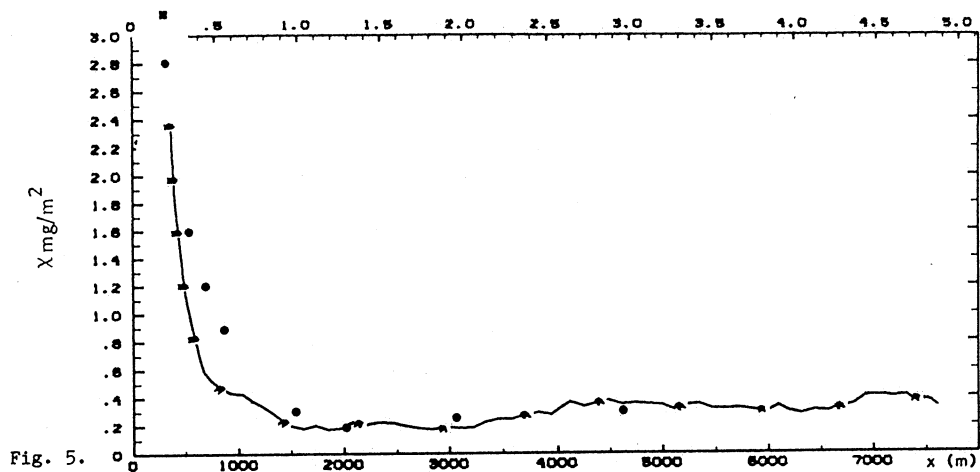


Fig. 5.

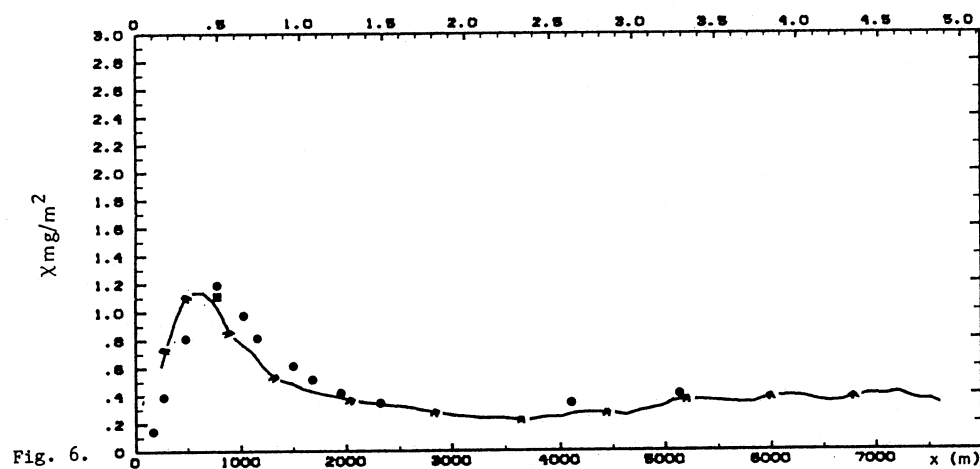


Fig. 6.

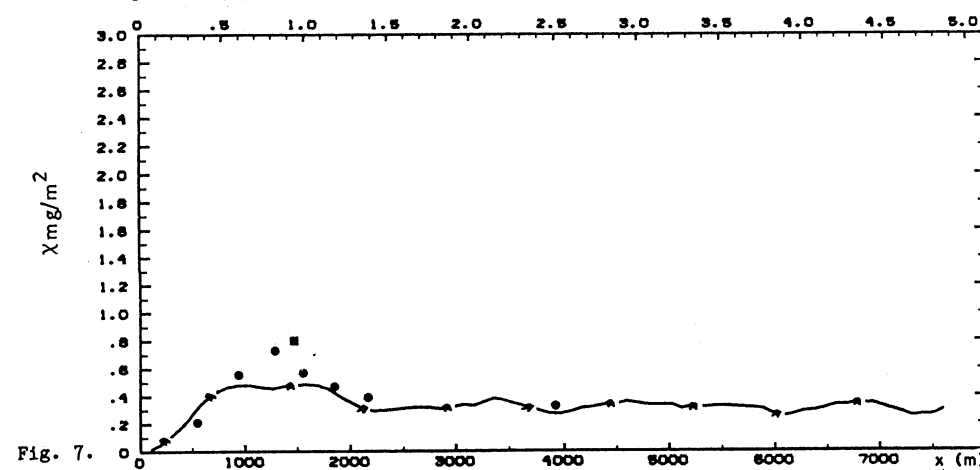


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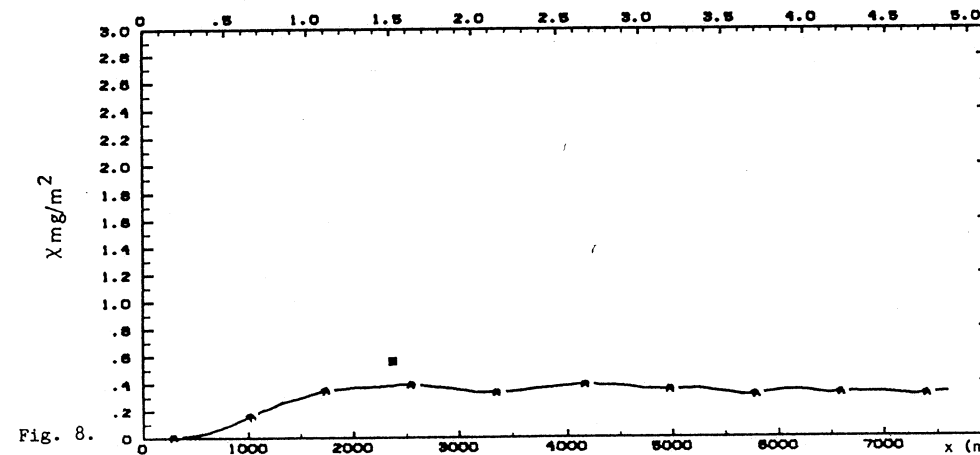


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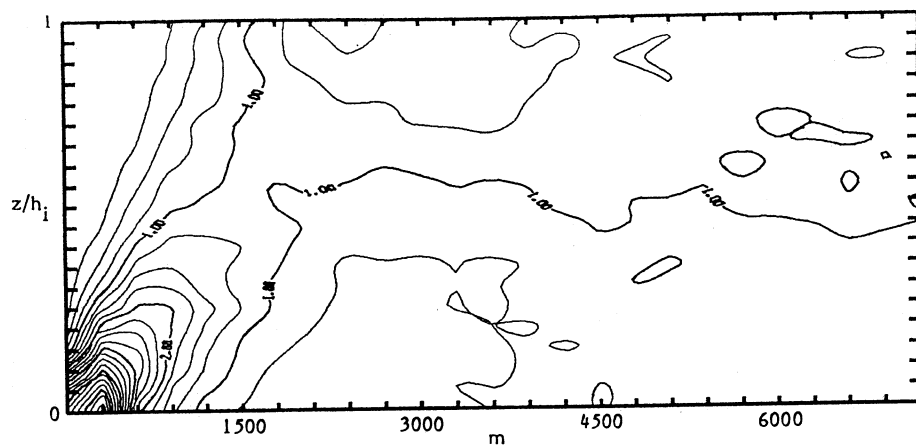


Fig. 9.

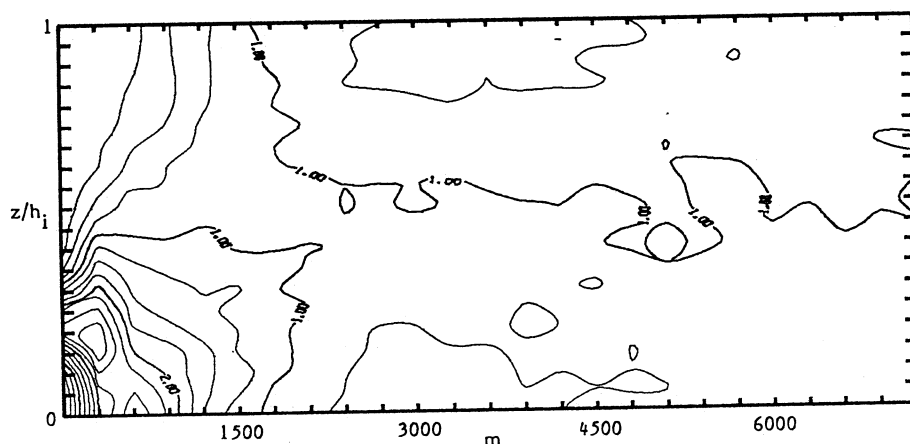


Fig. 10.

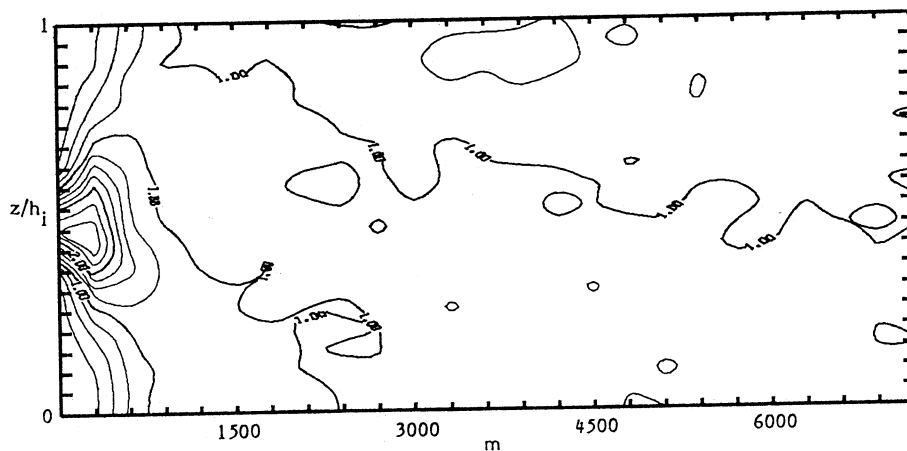


Fig. 11.

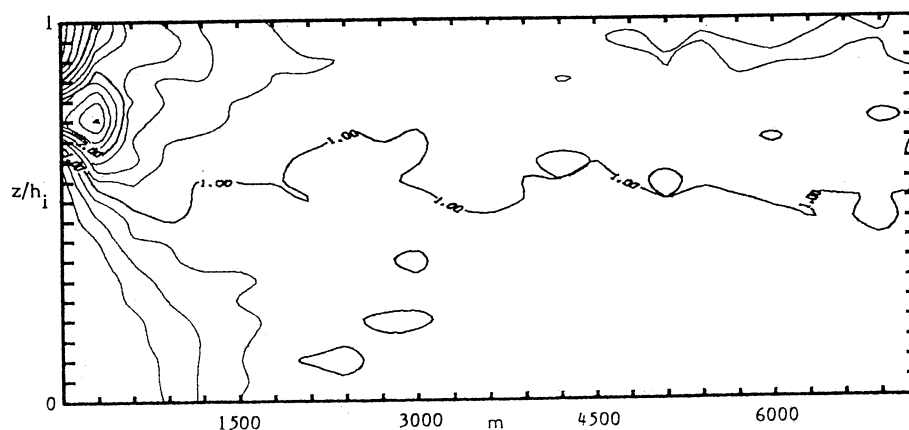


Fig. 12.

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