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# Monte Carlo Simulation of Plume Dispersion in Homogeneous and Nonhomogeneous Turbulence

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## INTRODUCTION AND OVERVIEW

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 which 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 dependend upon the turbulent properties of the atmosphere.

Deterministic air quality models are an important tool for providing unambiguous source-receptor relationship, 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 which 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 the simulation of the 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, which take into ccount both the average wind transport and the (seemingly) random turbulent fluctuations of the wind components.

Several air quality studies have applied particle methods (Lamb[5] , Lange[6] , Hanna[7] , De Baas et al.[8] , Baerentsen and Berkowicz[9]). 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 which 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[10]) is described in the following section. Then, simulation outputs relative to both cases of homogeneous and non-homogeneous turbulence, are presented and discussed. Finally, conclusive remarks are provided in the last section.

## MC-LAGPAR MODEL

The MC-LAGPAR model was originally formulated (Zannetti[11]) 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.

The basic scheme assumes that each particle is moved at each time step Dt by a pseudo-velocity $\underline{V}(x,y,z,t,p)$ which is a function of space, time and 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 considered known. The fluctuations of each particle p are updated at each Dt by the following Monte-Carlo scheme:

$$u'(t+Dt) = f_1 u'(t) + u''(t+Dt) \qquad (1)$$

$$v'(t+Dt) = f_2 v'(t) + v''(t+Dt) \qquad (2)$$

$$w'(t+Dt) = f_3 w'(t) + f_4 u'(t+Dt) + w''(t+Dt) \qquad (3)$$

where $f_1$, $f_2$, $f_3$ and $f_4$ are constants and 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 using algebrical manipulations (Zannetti[10]). The MC-LAGPAR model has been recently expanded (Zannetti[12]) to incorporate all three cross-correlations $\overline{u'v'}$, $\overline{v'w'}$, $\overline{u'w'}$. 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 the plume rise and the probabilistic computation of ground deposition/absorption/resuspension effects. The model can simulate the non-stationary evolution of a single puff release or the behaviour of a continuously emitted plume in stationary conditions. This latter case requires the release of particles with a suitable initial velocity distribution in order to correctly simulate the "ensemble" properties of the plume.
Particles hitting the ground are allowed to be reflected. In this case, however, the "memory" w' of the reflected particle is forced to a positive value (i.e., if negative the sign is changed) 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 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: variances and autocorrelations of the fluctuations u', v' and w', and cross-correlation $\overline{u'w'}$. 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[13]) which provides the above variances and autocorrelations using the mixing height Zi, the Monin-Obukhov length L, the convective velocity scale $w_*$, the friction velocity $u_*$, the roughness height $z_0$ and the Coriolis parameter f, all parameters that can be either measured or evaluated from meteorological measurements.

HOMOGENEOUS TURBULENCE SIMULATIONS

When the turbulence is homogeneous the average properties are uniform in space. Therefore the turbulent statistics used in performing the simulations (i.e., $\sigma_{u'}$ and $\sigma_{w'}$ 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[14] :

$$\sigma_{Taylor}\left(n\,\Delta T\right) = 2\,\sigma_{u'}^{2}\,T_L^2\left[\frac{n\Delta T}{T_L} - \left(1 - e^{-\frac{n\Delta T}{T_L}}\right)\right] \quad (4)$$

Fig. 1 shows the result of this comparison. As it can be seen the agreement is noticeable.

Then, we performed the computation of the concentration field in the X-Z plane of material continuosly emitted by a point source. The parameters of the simulation were the following:

Hs = 400m, $\bar{u}$ = 3m/s, $T_L$ = 144s, $\sigma_{u'} = \sigma_{w'}$ = 0.34m/s, Dt = 60s

where Hs is the source height and u is the wind speed. The dimensions of the grid cell used to compute the concentrations were defined by DX = u·Dt = 180m and DZ = 50m. Fig. 2 shows the ground level concentrations as a function of the downwind distance. The various curves refer to different choices of DZ, i.e. : 5,10,30,50,100m. As can be seen the more the cell height increases, the more the concentration trend tends to reduce its variability. However we see that the curve corresponding to DZ = 100m is much too high in the downwind distance interval 1000m-4000m; here the ground level concentration is overestimated as it includes particles which still belong to the plume and which have not yet reached the ground. Thus, in this case, DZ = 50m seems to be the best choice. Obviously if the emission height were lower, DZ should be lower and therefore a greater number of particles would be needed to reduce the scatter of ground level concentration trends.

The results of our simulations have finally been compared (at ground level and at the centerline plume level) to the results obtained by the two-dimensional analytical solution in homogeneous turbulence (i.e. the gaussian model) in which $\sigma_z$ was evaluated through eq. (4).
Fig. 3 show the results of such a comparison which clearly appears to be quite satisfactory.

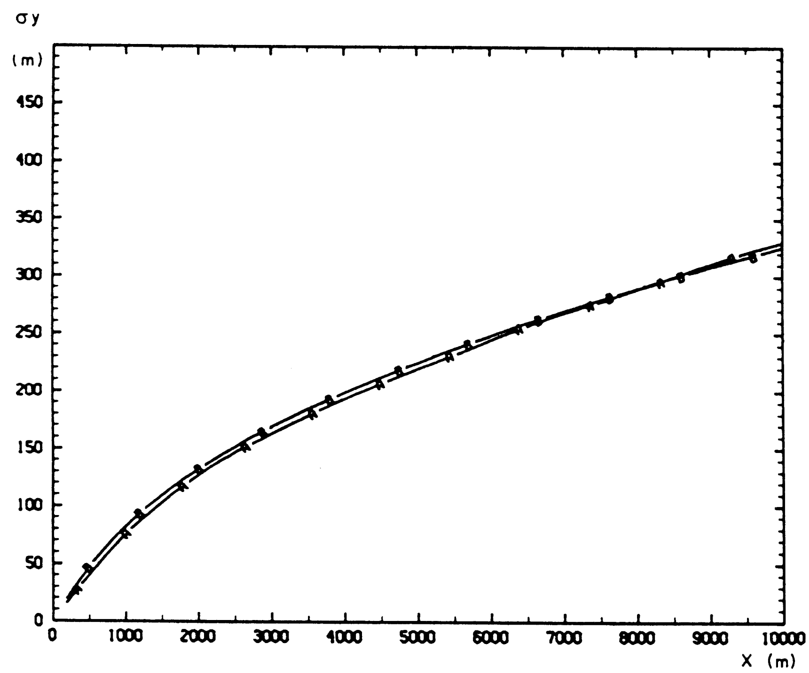



Figure 1. Standard deviation along cross-wind direction as a function of downwind distance. Curve A: numerical simulation with 3000 particles. Curve B: Results from Eq. (4).

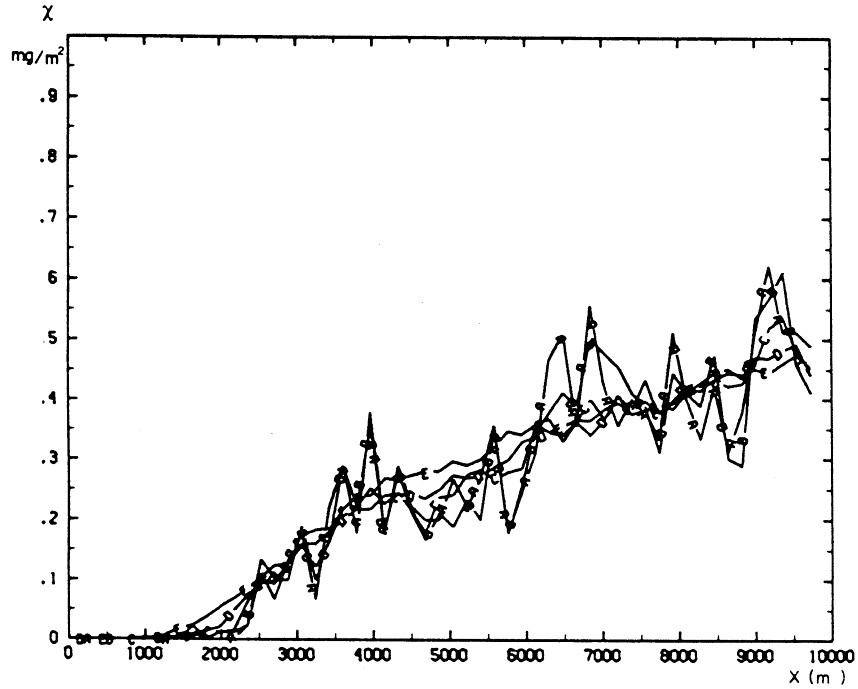



Figure 2. Ground level concentration as a function of the downwind distance with 1000 particles and emission rate Q = 1 Kg/s:

curve A: Dz = 5 m
curve B: Dz = 10 m
curve C: Dz = 30 m
curve D: Dz = 50 m
curve E: Dz = 100 m

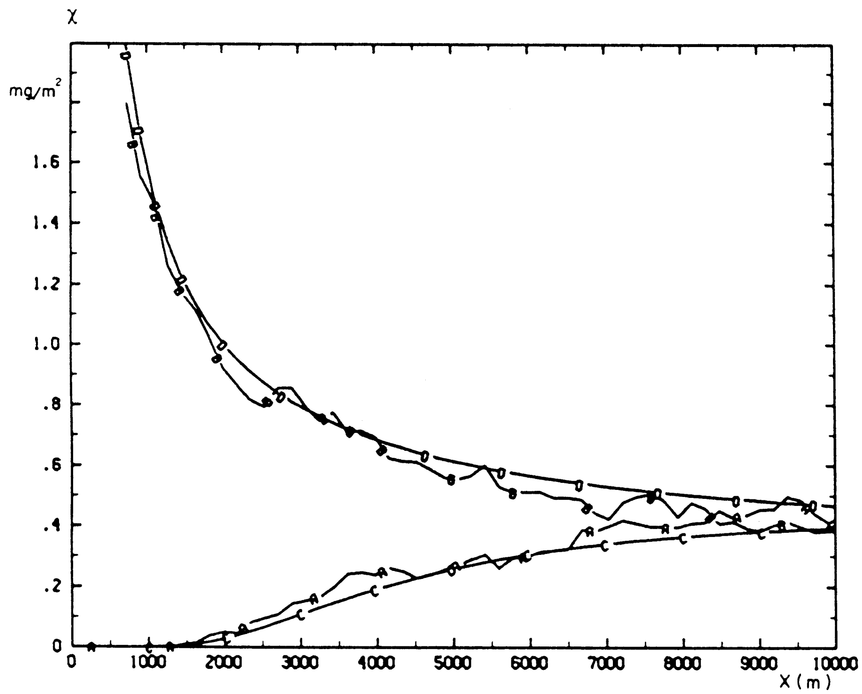



Figure 3. Concentrations as a function of downwind distance.

curve A: ground level with MC-LAGPAR numerical simulation

curve B: center-line plume level with MC-LAGPAR numerical simulation

curve C: ground level with analytical solution

curve D: centerline plume level with analytical solution

NONHOMOGENEOUS TURBULENCE SIMULATIONS

To prescribe the values of the quantities (stability and height dependent) needed to simulate the turbulent diffusion of the planetary boundary level we choose the scheme suggested by Hanna[13].
Different parametrization of $\sigma_{u'}$, $\sigma_{w'}$, $\sigma_{v'}$, $T_{Lu'}$, $T_{Lw'}$, $T_{Lv'}$ vertical profiles are suggested by that scheme with reference to the different stability contitions (unstable, neutral, stable).

To illustrate the results that can be obtained by MC-LAGPAR code with Hanna's scheme, we show in Fig. 4 the standard deviation curves along cross-wind direction in the three stability conditions. They are compared to the ones suggested by Singer-Smith[15].

It can be pointed out that if the constant vertical wind profile is substituted by a power law, all the other conditions remaining unchanged, the maximum ground level concentration comes near the source and its value slightly increases.
When the wind profile is not constant with height the cross-correlation term $\overline{u'w'}$ must be taken into account (Zannetti[10]). In our simulations $\overline{u'w'}$ was set equal to $u_*^2$ near the surface and let to decrease linearly with the height till the top of the PBL, where it is assumed to be equal to zero.
Fig. 5 show the differences on the ground level concentrations due to the two wind profiles. 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.

In unstable conditions we considered the effects on the dispersion of the thermal plumes. With reference to the measurements of Yamamoto et al.[16], we added to the turbulent vertical velocities a constant vertical velocity due to the convective cells. To each trajectory a vertical velocity (up or down) was attributed in such a way that w over all the trajectories and all the heights is zero. This means that the number of particles in updraft, having an higher velocity, are less than those in downdraft. As also done by Baerentsen and Berkowicz[9], each particle is allowed to jump from an updraft to a downdraft and viceversa with probabilities which depend on the time scales of the two phenomena. In our case, using the Hanna's schema for instable conditions, we set :

$Zi = 1000m$, $w_* = 1.6 m/s$, $\bar{u} = 2.5 m/s$, $u_* = 0.2 m/s$, $L = -10m$,

$w_{up} = 0.6 \cdot w_*$, $w_{down} = -0.4 \cdot w_*$,

$T_{L_{up}} = Zi/w_{up}$, $T_{L_{down}} = Zi/w_{down}$.

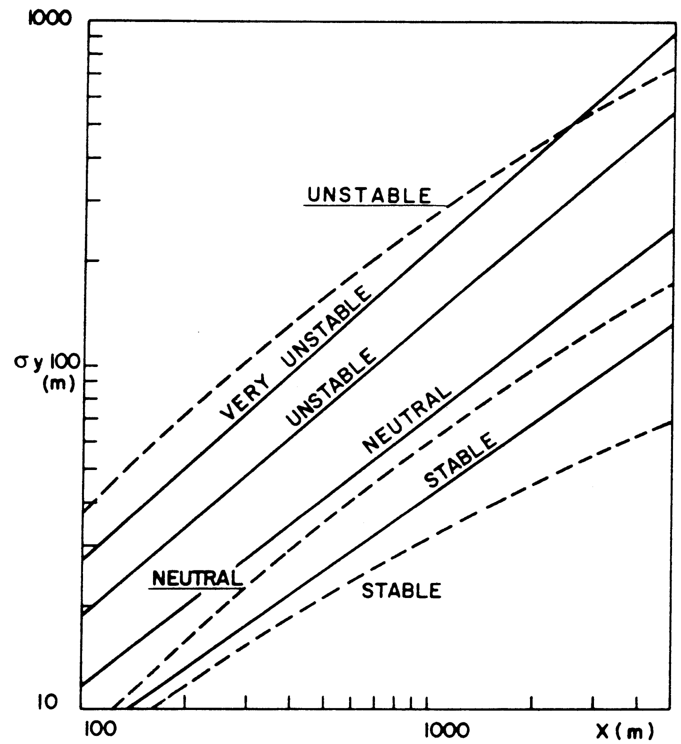



Figure 4. Standard deviations along cross wind direction as a function of downwind distance. Solid lines are Singer-Smith curves. Dashed lines are MC-LAGPAR results with: $\bar{u}$ = 2.5 m/s, $z_0$ = 0.2 m, $u_*$ = 0.2 m/s, $w_*$ = 1.6 m/s and L = -5 m (for unstable case), L = 100m (for stable case).

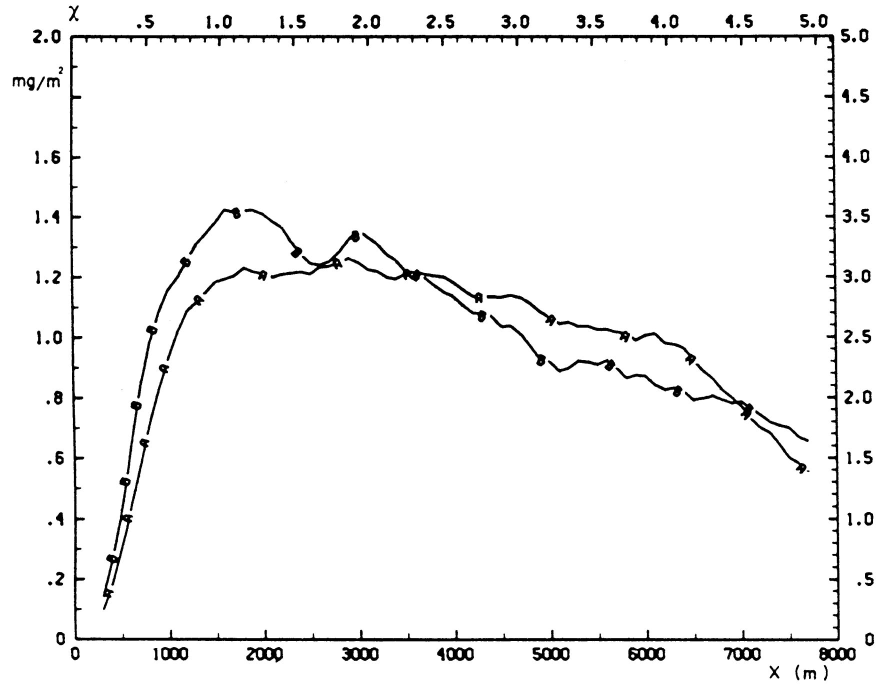



Figure 5. Ground level concentration as a function of a downwind distance with:
curve A: constant wind profile ($\bar{u}$ = 2.5 m/s)
curve B: power law wind profile ($u = 1.378\ z^{0.1}$)

On the top and right scales are reported non-dimensional distance $(w_*/\bar{u}) \cdot (x/zi)$ and concentration $(Q/zi \cdot \bar{u})$.

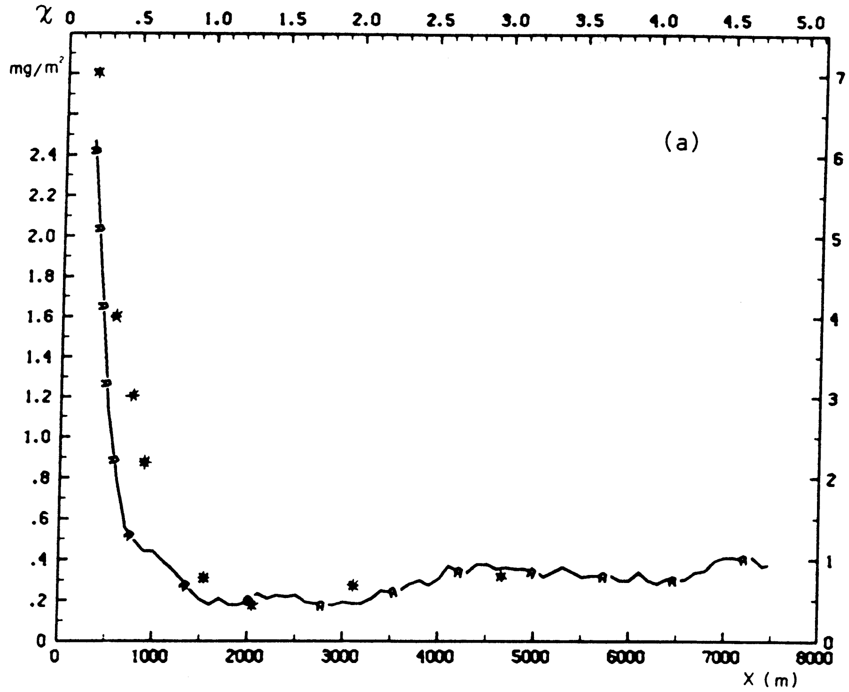



Figure 6. Ground level concentrations as a function of downwind distance for the source heights:

(a) $Hs/_{zi} = 0.067$

(b) $Hs/_{zi} = 0.24$

(c) $Hs/_{zi} = 0.49$

The results of MC-LAGPAR model with 3000 particles are indicated by a curve A and the measurements of Willis and Deardorff by stars.

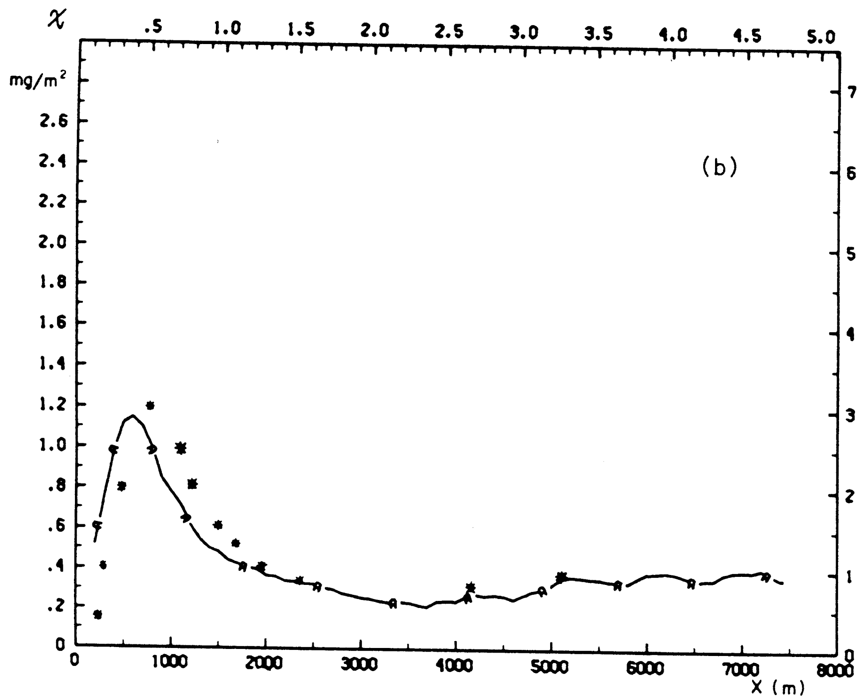
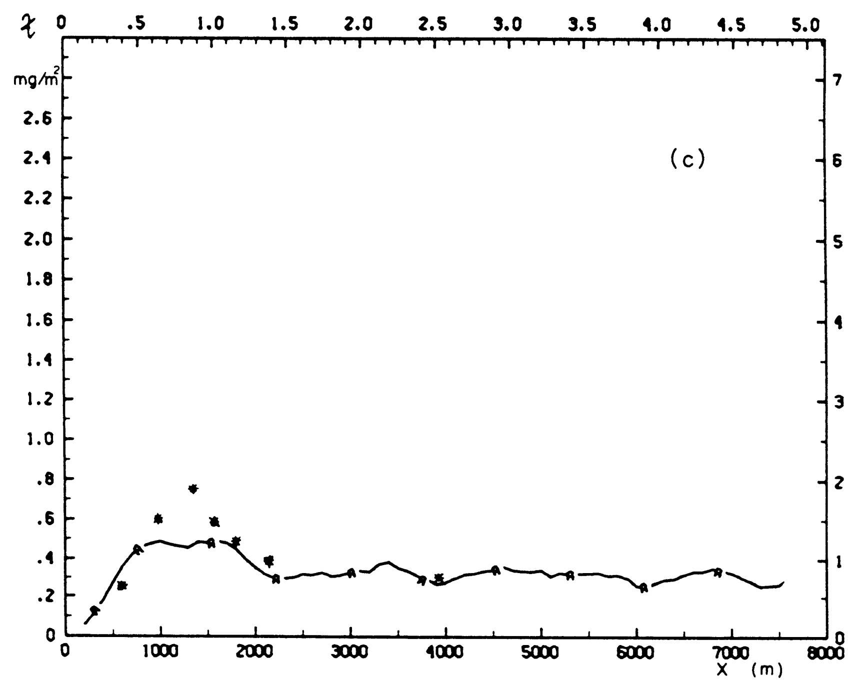



Figure 6.



Figs. 6 shows the comparison between the ground level concentrations obtained from MC-LAGPAR simulations and the water-tank experiments of Willis and Deardorff [17, 18, 19]. Concentrations are average values over the interval Z/Zi < 0.05 except for the source height Hs/Zi = 0. 067 where the average is over Z/Zi < 0.01.

## CONCLUSIONS

MC-LAGPAR computer code has proved to be a flexible tool to simulate air pollution dispersion in different meteorological situations. It is possible to select wind and turbulent parameters vertical profiles. Furthermore the physical mechanisms which play a significant role in the pollutant dispersion in the atmosphere could be simulated.

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