



# Implementation of Lagrangian particle dispersion model for mesoscale and regional air quality studies

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## ABSTRACT

The possible simplifications of the Lagrangian particle dispersion model are examined in order to develop an efficient tool for mesoscale applications. Computer time requirements for different model versions are also presented.

## INTRODUCTION

The goal of the presented research is the development of an efficient modeling tool to perform intensive calculations of air pollution dispersion on mesoscale and regional scales. Lagrangian particle models linked to numerical meteorological models have recently become a very important tool for studying dispersion [7, 8]. However, despite advances of computer technology, these models are still computationally expensive for mesoscale or regional applications when it is necessary to track a large number of particles for long distances and for a long time. The paper systematically examines possible simplifications of the particle models related to the representation of particle turbulent diffusion.

The Lagrangian particle dispersion (LPD) model used in the study was originally developed on an IBM PC at Warsaw University of Technology as a part of a Mesoscale Dispersion Modeling System (MDMS) where it was linked to a 3-D meteorological mesoscale model (MESO) [9, 10, 11]. Recently, the LPD model has been utilized with other meteorological models including the CSU RAMS (Regional Atmospheric Modeling System). This paper is limited to a consideration of passive tracer dispersion, however, the more advanced model version includes linear chemistry, dry deposition, buoyancy effects and gravitational settlement of heavy particles.

## LAGRANGIAN PARTICLE DISPERSION MODEL

Pollution dispersion in the LPD model is simulated by tracking a large set of particles. Subsequent positions of each particle representing a discrete element

of pollutant mass are computed from the relations

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

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

$$Z(t + \Delta t) = Z(t) + (w + w')\Delta t \quad (3)$$

The resolvable scale components of wind velocity  $u$ ,  $v$  and  $w$  are obtained directly from the meteorological model. Three Markov chain schemes (LPD2a, LPD2b, LPD2c) and two fully random walking schemes (LPD1b, LPD1c) are considered to create the turbulent wind components  $u'$ ,  $v'$ , and  $w'$ . The most advanced model, LPD2a, is used as a reference and all other model versions are obtained by its subsequent simplifications. In addition an option without turbulent diffusion (LPD0) where particles are moved explicitly by the resolved wind can be used to calculate resolvable trajectories and streaklines.

### Model LPD2a

The Markov process including wind velocity covariances is defined by the scheme proposed by Zannetti [12]:

$$u'(t) = \phi_1 u'(t - \Delta t) + \sigma_{ru} \eta_u \quad (4)$$

$$v'(t) = \phi_2 v'(t - \Delta t) + \phi_3 u'(t) + \sigma_{rv} \eta_v \quad (5)$$

$$w'(t) = \phi_4 w'(t - \Delta t) + \phi_5 v'(t) + \phi_6 u'(t) + (\sigma_{rw} \eta_w + w_d) \quad (6)$$

The coefficients  $\phi_1, \dots, \phi_6$  are expressed by the wind velocity variances,  $\sigma_u^2$ ,  $\sigma_v^2$ ,  $\sigma_w^2$ , covariances,  $\overline{u'w'}$ ,  $\overline{v'w'}$ ,  $\overline{u'v'}$ , and Lagrangian autocorrelations  $R_u$ ,  $R_v$ ,  $R_w$ . The last terms are random normally-distributed components;  $\eta_u$ ,  $\eta_v$ , and  $\eta_w$  are random numbers from a standard Gaussian distribution. The random component of vertical velocity has a nonzero mean value  $w_d$ , called a drift velocity, to prevent the spurious accumulation of particles in regions of low turbulence. [4].

The time step  $\Delta t$  used to move particles in the Markov chain model versions is variable in inhomogeneous turbulence and depends on the Lagrangian time scale,  $T_{Lw}$ :  $\Delta t = \max(0.1T_{Lw}, \Delta t_{min})$ . The minimum time step  $\Delta t_{min}$  is arbitrarily prescribed to avoid a zero time step near the ground surface.

### Model LPD2b

If the covariances of wind velocity components are neglected, the model LPD2a is simplified to the form:

$$u'(t) = R_u u'(t - \Delta t) + (1 - R_u^2) \sigma_u \eta_u \quad (7)$$

$$v'(t) = R_v v'(t - \Delta t) + (1 - R_v^2) \sigma_v \eta_v \quad (8)$$

$$w'(t) = R_w w'(t - \Delta t) + (1 - R_w^2) \sigma_w \eta_w + w_d \quad (9)$$

### Model LPD2c

The model is further simplified by neglecting the horizontal turbulent wind components:

$$u'(t) = 0 \quad (10)$$

$$v'(t) = 0 \quad (11)$$

$$w'(t) = R_w w'(t - \Delta t) + (1 - R_w^2) \sigma_w \eta_w + w_d \quad (12)$$

### Model LPD1b

This model version is obtained from the model LPD2b by increasing the time step

$\Delta t$  used to move particles. Assuming that  $\Delta t$  is much larger than the Lagrangian time scales, the scheme is derived where particles have no memory and move fully randomly at each time step:

$$u'(t) = \sigma_u \eta_u \quad (13)$$

$$v'(t) = \sigma_v \eta_v \quad (14)$$

$$w'(t) = \sigma_w \eta_w + w_d \quad (15)$$

The time step  $\Delta t$  is kept constant (typically  $\Delta t = 180$  s).

### Model LPD1c

After neglecting the horizontal turbulent velocity components in the model LPD1b the simplest variant is obtained:

$$u'(t) = 0 \quad (16)$$

$$v'(t) = 0 \quad (17)$$

$$w'(t) = \sigma_w \eta_w + w_d \quad (18)$$

### Turbulence parameterization

The wind velocity variances and covariances required by the LPD model are calculated diagnostically from available meteorological information using a simplified second-order closure technique developed by Mellor and Yamada [5, 3, 1]. A so-called level 2.5 scheme modified for a case of growing turbulence [3] is applied if the fields of wind, potential temperature, and turbulent kinetic energy, are provided by the meteorological model which uses the same turbulence parameterization. This scheme is based on the prognostic equation for the turbulent kinetic energy solved in the meteorological model. A simpler level 2.0 scheme is used if only wind and potential temperature fields are available from the meteorological model or observations. This scheme assumes an exact balance between production of turbulent energy and dissipation. The Lagrangian time scales are calculated from wind velocity variances

$$T_{Lu} = cl/\sigma_u, \quad T_{Lv} = cl/\sigma_v, \quad T_{Lw} = cl/\sigma_w \quad (19)$$

where  $l$  is the turbulent length scale, and the constant  $c$  is assumed to be 2 in order to obtain a good agreement between the Lagrangian time scales simulated in the model and given by empirical formulae [2] for an idealized case of a horizontally homogeneous atmospheric boundary layer.

Concentration calculation In order to reduce the uncertainty related to concentration calculations from the particle distributions, the simplest version of the kernel density estimation technique is used. The concentration is obtained with the aid of the uniform kernel with constant bandwidths which are equal to the increments of the grid assumed for the concentration calculations.

## BENCHMARK TESTS

Computation time for the LPD model strongly depends on the number of particles to be tracked as well as on meteorological conditions and the variant of turbulent diffusion parameterization used. Only particles traveling within a specified area are considered. Figure 1 compares computer time required by an IBM RISC 6000/550 workstation to trace 10000 particles during 1 hour using different meteorological input:

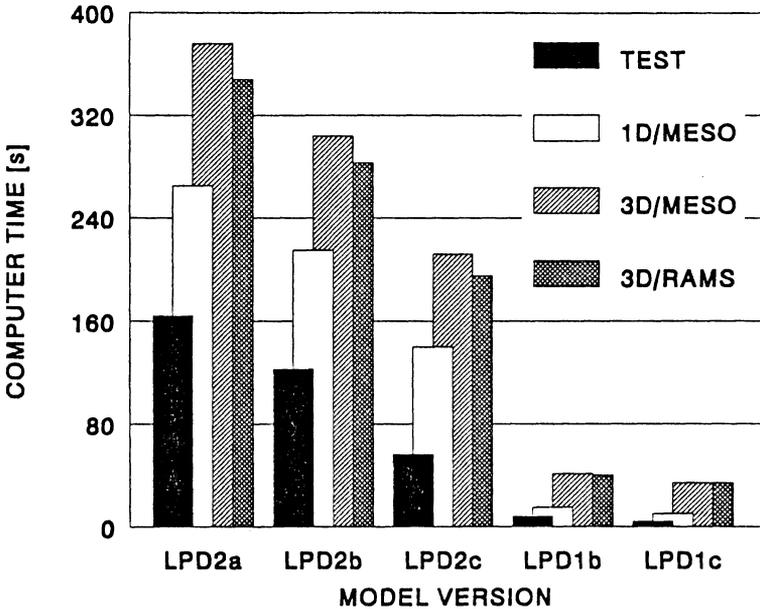


Figure 1. Computer time required by different versions of the LPD model to trace 10000 particles for 1 hour on IBM RISC-6000/550 workstation

- a test homogeneous meteorology;
- 1-D simulation of a horizontally homogeneous boundary layer using the MESO model (60 levels up to 3 km);
- 3-D simulation of a mesoscale circulation using the MESO model ( $67 \times 67$  horizontal grid points,  $\Delta x = 6$  km, 30 levels up to 5 km);
- 3-D simulation of a mesoscale circulation using the CSU RAMS (2 nested grids, particles were traced on the internal grid:  $73 \times 53$  horizontal grid points,  $\Delta x = 12.5$  km, 13 levels up to 3 km).

The particles were released randomly within a  $200 \times 200 \times 1$  km volume at the start of the test simulations. It should be pointed out that additional computer time is needed to read meteorological fields created by the meteorological model, to perform diagnostic calculations of turbulent variables, and to interpolate all variables in space for the position of each particle at each time step of the model. The interpolation may require more computer time than the advection of particles, especially, in the case of 3-D high resolution meteorological fields.

#### SENSITIVITY TESTS

The different versions of the LPD model were examined with the aid of the meteorological simulation performed for a region of complex terrain in the eastern United States [11]. The modeling domain ( $550 \times 550 \times 5$  km;  $67 \times 67 \times 30$  gridpoints)

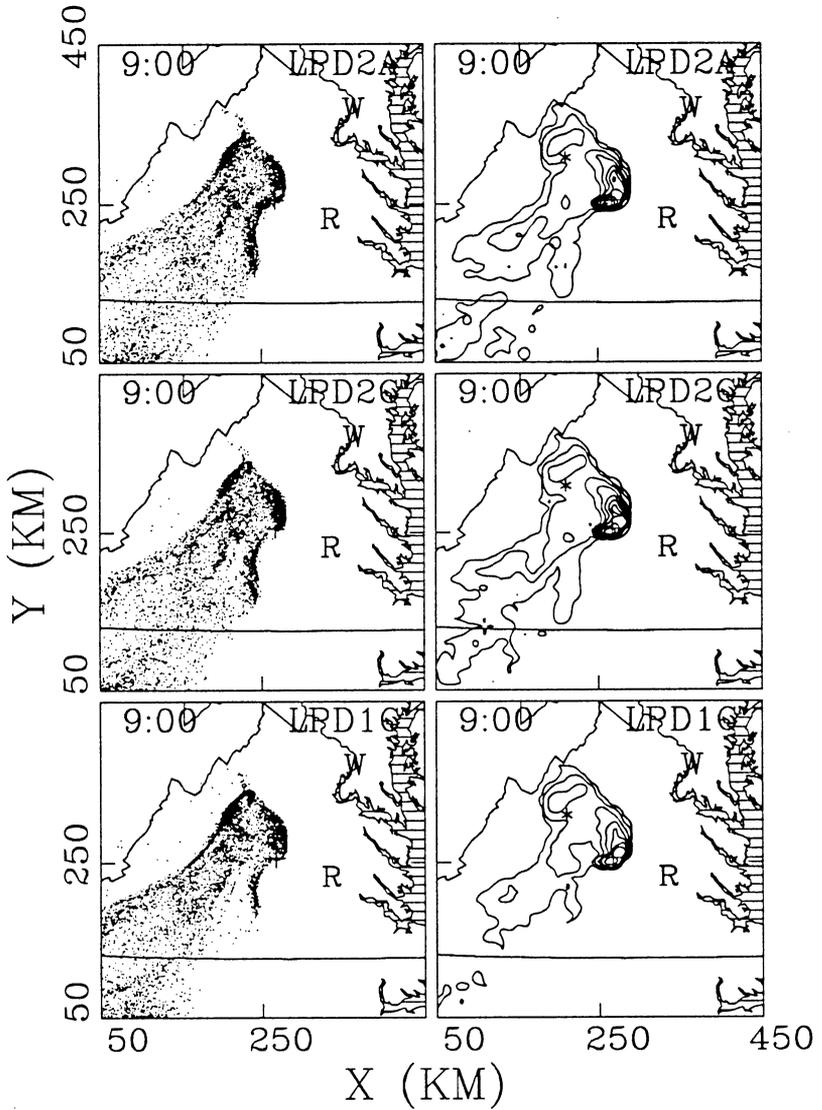


Figure 2. Particle distributions at 00:00 LST (2nd day of meteorological simulation) and  $\text{SO}_2$  surface concentration fields simulated by models LPD2a, LPD2c, and LPD1c (contours of concentration: 0.1, 0.5, 2, 4, ..., 8, 10, 20, ...  $\mu\text{g m}^{-3}$ )



covers the state of Virginia and includes the Chesapeake Bay in the eastern part and the Appalachian and Blue Ridge mountains in the northwestern part. A 60-hour 3-D meteorological simulation (from 0400 LST on day 1 till 1600 LST on day 3) with the model MESO was performed for cloudless June conditions with a steady synoptic wind of 5 m/s from the northeast. Dispersion conditions in the atmosphere are characterized by a complicated mesoscale circulation resulting from the interaction of synoptic flow, sea-land breeze circulations and mountain-valley winds.

SO<sub>2</sub> concentration fields from the VA Power-Cumberland power station with an SO<sub>2</sub> emission rate of 489.8  $g s^{-1}$  were simulated by each version of the LPD model. Particles were released continuously at a rate 1440 particles per hour starting at 2400 LST at an effective stack height calculated with the aid of a plume rise algorithm adopted from Nettetville [6]. A time series of 3-hour average surface concentration fields were calculated from each particle simulations using  $10 \times 10 \times 0.1$  km boxes. Figure 2 demonstrates examples of particle distributions and surface concentrations. The differences between simulations were analyzed in terms of the root mean square difference (RMS). The RMS was calculated using concentration fields from each couplet of simulations and normalized by the maximum concentration taken as a mean from these two simulations (Figure 3). The differences between all three Markov chain simulations are very small and also differences between the two random walk simulations are negligible. Differences between the most advanced model (LPD2a) and each of the random walk version are evident, however, as expressed by the RMS they do not exceed 15% of the maximum concentrations. The RMS was also calculated for concentration fields sorted from maximum to minimum values. This operation does not significantly change the RMS which means that the random walk version predicts similar concentration patterns as the Markov chain version but they may under- or overestimate maximum concentrations. This conclusion is confirmed by the time series of SO<sub>2</sub> concentration calculated for a receptor located in Shenandoah National Park (Figure 4).

## CONCLUSIONS

The performed simulations indicate that in mesoscale and regional applications horizontal turbulent diffusion of pollutants is not important and may be neglected. There is also no need for more refined particle models (e.g., models including wind covariances). The random walk particle models predict the same concentration pattern as the more advanced particle models, although some differences in maximum concentrations are evident. These simplified particle models are a very attractive tool for mesoscale studies since they can be an order of magnitude faster than the Markov chain models. The presented analysis of the particle models are being extended for a larger set of mesoscale dispersion simulations.

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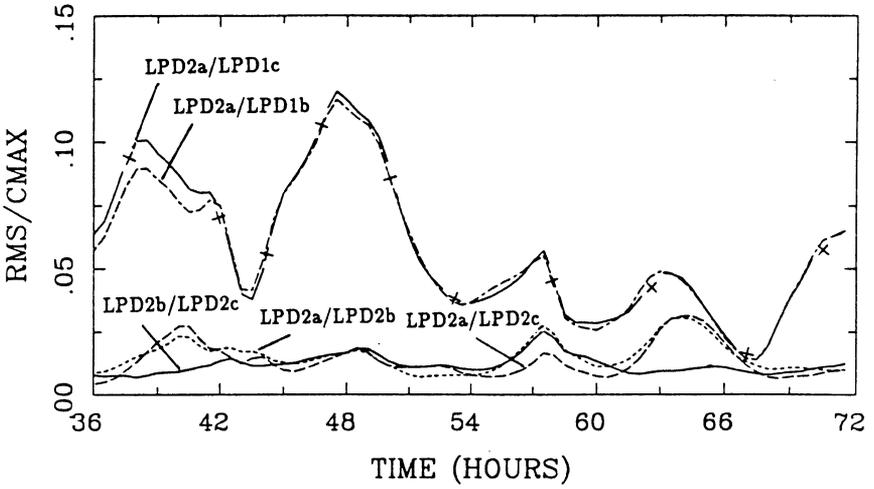


Figure 3. Time variations of differences between surface SO<sub>2</sub> concentration fields predicted by different versions of the LPD model

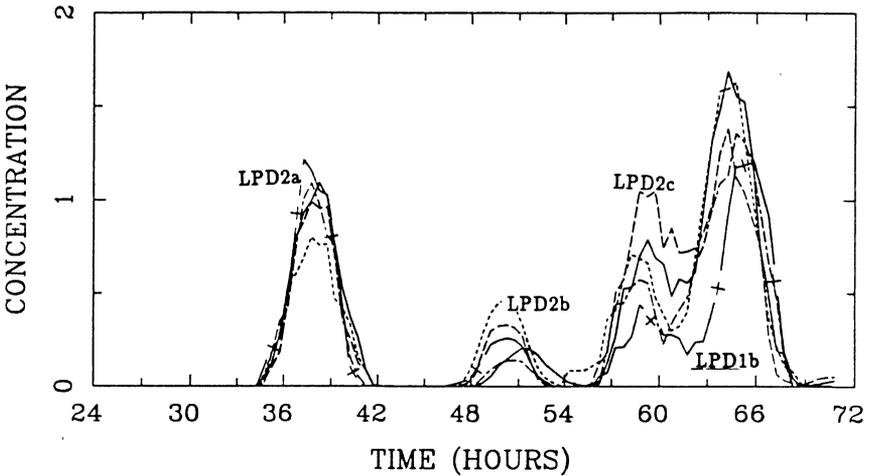


Figure 4. Time series of surface SO<sub>2</sub> concentration ( $\mu\text{g m}^{-3}$ ) at Shenandoah National Park predicted by different versions of the LPD model



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