1.22 PR-PLPM (PLUME RISE PHOTOCHEMICAL LAGRANGIAN PARTICLE MODEL): FORMULATION AND VALIDATION OF THE NEW PLUME RISE SCHEME

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INTRODUCTION

PLPM (Photochemical Lagrangian Particle Model) is a Lagrangian three-dimensional dispersion model, interfaced to the diagnostic meteorological model CALMET.
Physical model formulation together with a preliminary evaluation, performed on the Kincaid data set (*Bowne, N.E. and Londergan, R.J.*,1983) were presented at the 8th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes (*Zanini, G. et al.,* 2002). Interesting results have been achieved by this first validation as far as the inter-comparison of different density reconstruction methods are concerned. Nevertheless, *residual analysis* suggested the development of a new plume rise scheme (able to simulate the physical, gradual rise of buoyant plumes) as the first aim to enhance model performances.
Indeed, only a very simple plume rise scheme based on the empirical Briggs formulae virtual effective height computation was introduced in the previous version of PLPM.
Then an Eulerian plume rise scheme has been adapted and introduced within PLPM, on the basis of the experience of *Webster, H. and Thompson, D.* (2002). The choice of such an integrated approach is based on a suitable way of dealing with atmospheric parameters and particle physical dynamics. This approach uncouples meteorological quantities: particle properties and the randomness of particle motion can be treated separately.
A comparison between the enhanced model PR-PLPM and the old PLPM together with the complete validation of the new model have been carried out according to the standard Kincaid experimental data set and the statistic methodology proposed by the Model Validation Kit (*Olesen*, 1998).

NEW PLUME RISE SCHEME DESCRIPTION

The Ooms Eulerian Model of the Plume Rise

The plume rise algorithm nested within PLPM is based on the scheme proposed by *Ooms, G.* (1972). The corresponding set of scalar ODEs describing the plume rise phenomenon is based on the conservation of mass, momentum and heat (enthalpy) of a plume slice. The ODEs system has been discretized in order to obtain the final implemented equation, resolved with a simple forward-in-time numerical technique.

Nesting the Eulerian Plume Rise scheme within PLPM

Following the examples of *Anfossi, D. et al.* (1993) and *Webster, H. and Thompson, D.* (2002), an Eulerian plume rise scheme has been nested within a Lagrangian framework. Both theoretical and implementation issues are involved when two different modelling approaches (i.e., the Eulerian and the Lagrangian ones) have to be integrated.
The basic idea of Lagrangian particle models is the independence of particle motions. The problem of including plume rise within a Lagrangian model is that the rise of each particle is influenced by the buoyancy of the plume *as a whole*. This problem has been overcome by the introduction of the concept of the *plume-particle*. The adopted plume rise scheme considers each particle as a plume and solves an integral system based on the governing conservation

equations following each particle separately, using local mean flow properties. The rise of each particle responds to local conditions and it is modelled as a small plume driven by local ambient conditions.
In Lagrangian particle models, each particle moves along its trajectory in the spatial domain by the effect of the sum of a deterministic velocity $\boldsymbol{u}$ and a stochastic term $\boldsymbol{u}'$, due to the effect of air turbulence:

$$\boldsymbol{x}\,(t+\Delta t) = \boldsymbol{x}\,(t) + \Delta t\,(\boldsymbol{u} + \boldsymbol{u}') \qquad (1)$$

At each time-step the new particle velocity is computed and the updated particle position in the spatial domain is obtained.
In the new release of the PLPM model (called PR-PLPM), the deterministic particle velocity includes also the plume rise in the first phase of plume dispersion. In other words, the mean velocity term is replaced by the plume-particle velocity, achieved by solving the conservation equation system: then the equation (1) becomes

$$\boldsymbol{x}\,(t+\Delta t) = \boldsymbol{x}\,(t) + \Delta t\,(\boldsymbol{u}_p + \boldsymbol{u}') \qquad (2)$$

where the deterministic term $\boldsymbol{u}_p$ represents the velocity of each particle, including also plume rise effect. Equation (2) is valid as long as a buoyancy force acts on the particle. When the plume-particle reaches the equilibrium with the surrounding atmosphere, the particle starts to be transported passively by the wind, and its motion can be described by equation (1).
The achievement of dispersion simulations for a wider range of meteorological conditions and the introduction of detailed wind and temperature fields are the main advantages of this miscellaneous approach. Finally, the entrainment of ambient air is considered throughout the plume rise process.
The structure of equation (2) allows an easy integration in terms of implementation issues. As far as implementation details are concerned, the plume rise module has been nested within the original routine calculating, at each time-step, the new particle position. According to the conditional instruction regulating the duration of plume rise effect, the update particle position is calculated by using the plume-particle velocity or, simply, the local mean wind speed. For each iteration the plume rise routine is triggered only if the vertical component of $\boldsymbol{u}_p$ is significantly larger than the vertical component of $\boldsymbol{u}_a$ or if the particle is more aged than 30 minutes. Those conditions allow the evaluation of the phase of plume dispersion, controlling the end of the rising phase and the beginning of the passive advection of the particle.
Even if the plume rise module is triggered for each particle at each time-step, the global computational time has not significantly increased and the differences between PR-PLPM and PLPM, in terms of computational time performances, can be considered as negligible.

PR-PLPM AND PLPM INTERCOMPARISON

The new model PR-PLPM has been validated and intercompared with the old PLPM on the well known Kincaid experimental data set .

Input Data

For each experimental day, the meteorological input file has been achieved by running the meteorological pre-processor CALMET.
In order to compare properly the old PLPM results with the new ones, the same set of simulations has been produced using the original PLPM model running on the same computer (i.e., using the same processor and the same random number generating algorithm).
Both PR-PLPM and PLPM have been initialized according to the same spatial domain of the Kincaid experiment and the geometrical features of the source.
Hourly emissions have been divided in 60 puffs released every 60 seconds, each containing 30 particles, for a total emission rate of 1800 particles/hour.

RESULTS

A preliminary qualitative evaluation of the plume rise effect has been carried out by the analysis of centre of mass height of the plume as a function of the distance from the source. As expected, the height of the PR-PLPM plume centreline grows gradually in proximity of the source, from the edge of the stack (h = 187 m), and tends to converge to the effective height predicted by Briggs formulae, according to old PLPM plume rise scheme (see Figure1).

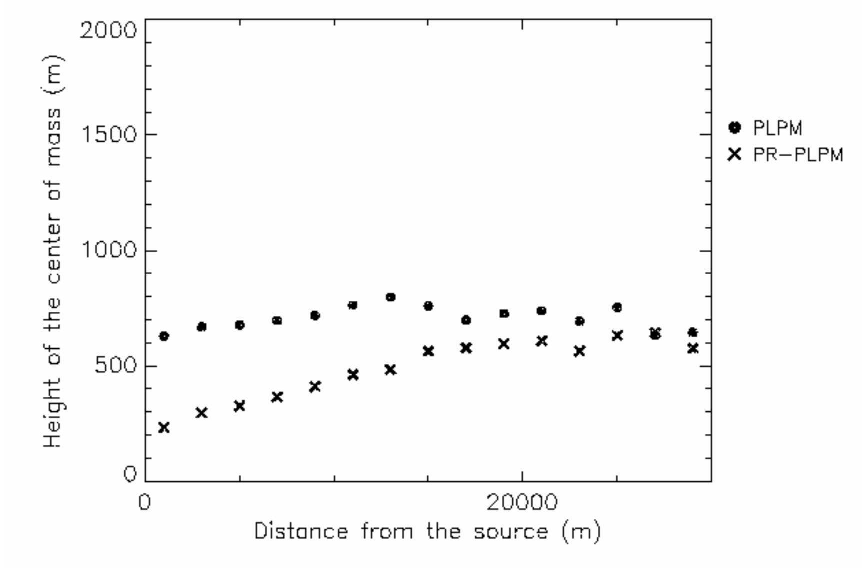

Figure 1. Plume centre of mass height as a function of the distance from the source. Kincaid, 31 5 1981, h 13.

As far as near source behaviour is concerned, also residual analysis shows as PR-PLPM performances are better than PLPM ones. In Figure2 five percentiles (5th, 25th, 50th, 75th and 95th) of both PLPM and PR-PLPM residual distributions for different distances from the source are shown; for short distances, 50th percentiles of PR-PLPM distributions are closer to unity than the corresponding PLPM ones.

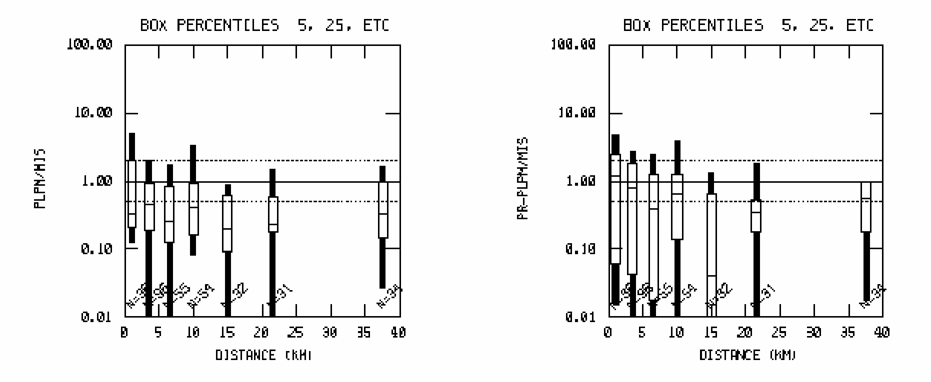

Figure 2. Residual analysis (Q=3) for PLPM and PR-PLPM, varying the distance from the source

Actually percentiles analysis of values distributions shows that both PLPM and PR-PLPM generally under predict ground concentrations but only PR-PLPM seems to reproduce the trend of the measures with maximum concentrations some kilometers away from the source (see Figure 3).

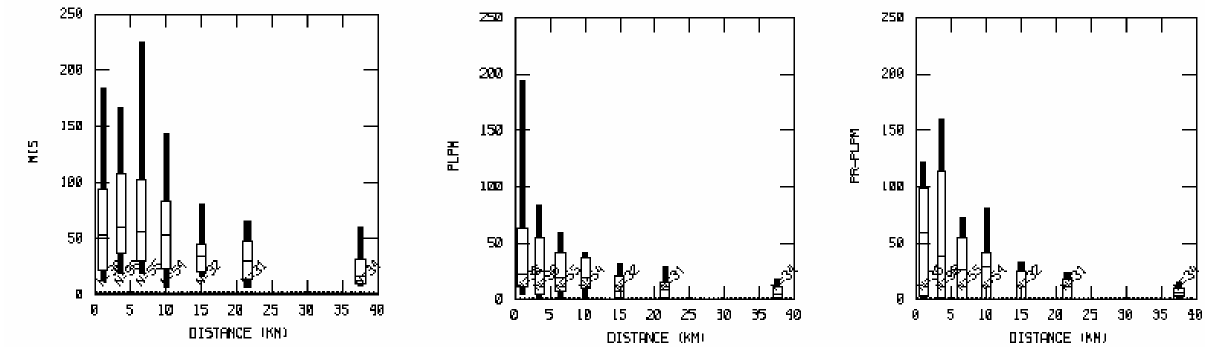

Figure 3. Percentiles analysis (Q=3) for measures and PLPM and PR-PLPM predicted values, varying the distance from the source.

Also ground concentration maps (Figure 4) confirm that PR-PLPM performs better at short distances.

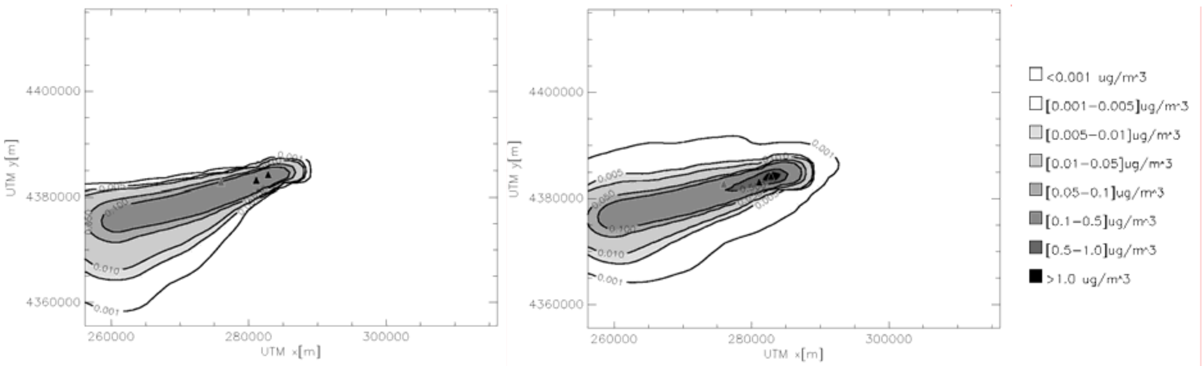

Figure 4. PLPM (left) and PR-PLPM (right) estimated concentration at ground level. Triangle colour indicate measured concentrations at receptors positions. Kincaid, 31 5 1981, h 12.

In addition residual analysis varying emission parameters was conducted. Figure 5 shows that at high emission temperature (when the effect of buoyant plume rise is more important) 50th percentiles of PR-PLPM residual distributions are closer to unity than the corresponding PLPM ones.

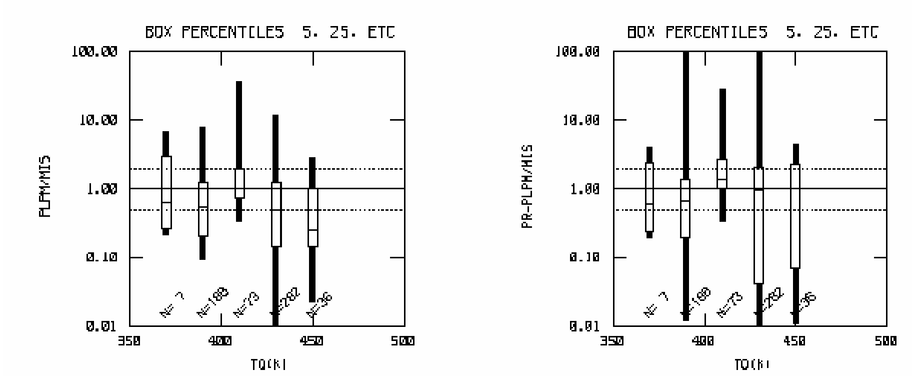

Figure 5. Residual analysis (Q=2,3) for PLPM and PR-PLPM, varying emission temperature

Finally, in Table 1 statistics for PR-PLPM and PLPM are shown; usual performance indexes were calculated on Kincaid subset with quality index Q=3.
In Table 2 performance indexes are shown for the statistics of the ratios $C_{predicted}/C_{observed}$.

Table 1. Performance indexes on normalized concentration values subset with Q=3 (N=338)

	Mean	Sigma	Bias	NMSE	R	FAC2	FB	FS
Measures	54.34	40.25	0.0	0.0	1.0	1.0	0.0	0.0
PLPM	22.85	25.18	31.49	2.57	0.029	0.302	0.816	0.461
PR-PLPM	32.02	39.26	22.31	2.00	0.056	0.361	0.517	0.025

Table 2. Performance indexes on C_p/C_o subset (Q=3)

	Mean	Sigma	Bias	NMSE	FAC2	FB
Measures	1.0	0.0	0.0	0.0	1	0.0
PLPM	0.64	0.92	0.36	1.51	0.302	0.435
PR-PLPM	0.83	1.06	0.17	1.38	0.361	0.182

Results shows that PR-PLPM performs better than older PLPM under all points of view.

CONCLUSIONS

A new Lagrangian dispersion model PR-PLPM has been developed by nesting an Eulerian plume rise scheme within the existing PLPM model.
Performances of the new model have been evaluated in terms of particle dispersion simulation and density reconstruction (i.e. concentration field).
A comparison between the old and the new models simulation performances leads to encouraging conclusions. PR-PLPM performs better than older PLPM: an enhanced estimation of concentration fields is achieved, especially at short distances from the source.

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