VALIDATION OF THE LAGRANGIAN PARTICLE MODEL DIPCOT FOR MESOSCALE AND LONG-RANGE ATMOSPHERIC DISPERSION OVER COMPLEX TERRAIN

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INTRODUCTION

The stochastic (Lagrangian) particle atmospheric dispersion model DIPCOT (*Davakis et. al,* 2001, *Davakis et. al,* 2000) is evaluated by simulating a mesoscale (TRANALP campaign) and a long-range (European Tracer Experiment-ETEX) dispersion experiments. The effect of the method of calculation of the pollutant concentration is also examined, by comparing the results of three methods: a box counting method with variable box dimensions and two Gaussian-shaped density kernels. The evaluation procedure is based on the statistical and graphical comparison of the predicted concentrations against the observed ones, using some well-known performance indices and various types of plots.

THE DISPERSION MODEL AND THE CONCENTRATION CALCULATION

The Lagrangian particle dispersion model DIPCOT is a 3D model aiming at the study of atmospheric dispersion over complex topography. The mass of a pollutant is distributed to a certain number of fictitious particles, which are displaced within the computational domain, following the wind flow, and assuming that turbulent diffusion can be modelled as a Markov process. Calculating the trajectories of these particles simulates atmospheric dispersion. Further details about DIPCOT can be found in *Davakis, S. et. al.* (2000).

In the Lagrangian atmospheric dispersion models two methods are used for the estimation of concentration at a given location: the box counting method and the density kernel estimation method. In the box counting method the concentration is computed by counting the number of the particles that fall into an imaginary volume around the location of interest. There are no strict rules determining the size of the sampling box. However, a too small volume would lead to large fluctuations of concentration, while a too large volume, would result in over-smoothed concentrations. This problem can be overcome (*de Haan, P.*, 1999, *Uliasz, M.*, 1994) by increasing the number of released particles, in expense, however, of computing time and resources. In the density kernel method the mass of a particle has a specified spatial distribution, called density kernel (*de Haan, P.*, 1999). The concentration at the location of interest is calculated by summing the contributions of all the particles. The number of particles that can be used in this method is smaller than in the box counting methods (e.g., *Yamada, T. and S. Bunker*, 1988). The main parameters that must be predefined are the shape of kernel and its bandwidth (i.e. the width as a function of the particle mass distribution).

In this paper the following concentration calculation methods are intercompared in the framework of the model DIPCOT: i) a box counting method (from now on called as CM1) as described by (*Uliasz, M.*, 1994), with a modification concerning the box dimensions that are set equal to the maximum variance of the displacement of the all particles at each dimension, ii) a Gaussian-shaped density kernel method (from now on referred to as CM2), where the bandwidths are equal to the variance of the particle dispersion σ_x, σ_y, σ_z, as proposed by *Yamada,*

T. and S. Bunker (1988) and iii) a Gaussian-shaped density kernel method (from now on referred to as CM3), where the bandwidths are set equal to the variances of the particle distribution around each observation point, taking into account only the particles within a pre-defined distance from that point.

THE EXPERIMENTAL DATA SETS

The TRANSALP 90 campaign (*Ambrosetti, P. et. al*, 1994) was conducted in South Switzerland on 29 September 1990 and involved the release of a passive tracer inside a mountain valley and the subsequent dispersion in a highly complex terrain in the Alps. The wind flow simulations were performed by the mesoscale prognostic meteorological model ADREA-I (*Varvayanni, M. et. al.*, 1998).

The European Tracer Experiment ETEX (http://rtmod.ei.jrc.it/etex/) was performed in October 1994 and involved the release of a passive non-depositing gas in western France and the subsequent dispersion over Europe. The analysed meteorological data supplied by the ECMWF have been processed in this paper, to drive the dispersion model.

THE EVALUATION PROCEDURE

The model was applied for each one of the two experiments, using the three predefined concentrations calculations methods (CM1, CM2, CM3). The simulations where performed using 20000 particles for the released gas in all cases.

For the analysis of the TRANSALP case, the calculated concentrations were artificially shifted in time because there was a systematic under-prediction of the wind speed from the meteorological pre-processor, especially in the area near the source, causing a time difference, typically of two hours, between the observed and the predicted concentrations. In the ETEX experiment, the "Global analysis" data set described by *Mosca, S. et al* (1998) was adopted, which included all the significant zeros at each sampling site. This means that at each receptor the experimental data set consists of all the zero values 6 hrs before the cloud arrival and 6 hrs after the cloud departure, as well as all the zeros between non zero values.

The evaluation of the model was performed by comparing the predicted ground level concentrations with the observed ones using scatter and Quantile-Quantile (Q-Q) plots and by calculating statistical indices with the **ME**teorological and **DI**spersion **STAT**istics code (*Deligiannis, P. et al.*, 1997), which is based on the Bootstrap resampling method (*Hanna*, *S.R.*, 1989). Well known "performance indices" have been calculated such as the mean Fractional Bias (FB), the Geometric Mean bias (GM), the Normalised Mean Square Error (NMSE) and the Factor-of-Two (*FACT2*).

RESULTS

The results of the model evaluation process are presented in Tables 1 and 2 for the statistical indices, and in Figures 1 and 2 for the scatter and Q-Q plots.

The FB values for both examined cases and for all concentration calculation methods (Tables 1 and 2) are larger than 0. This indicates an underestimation of the observed concentrations by the model. However the 0 value is included in the 95% confidence intervals of the FB for the ETEX case (Table 2), which means that the FB is not significantly different than 0. This is not the case of the TRANSALP experiment, where the underestimation is systematic by all methods.

Table 1. Statistical Indices FB, MG, NMSE and FACT2 for the TRANSALP experiment

Concentration Calculation Method	CM1	CM2	CM3
FB	0.4707	0.3744	.26437
95% Conf. Int.	(0.280|0.661)	(0.1499|0.5989)	(7.583E-02|0.4529)
MG	0.2515	0.5385	0.4908
95% Conf. Int.	(0.1365|0.4633)	(0.3255|0.7516)	(0.2344|0.7472)
NMSE	1.4338	1.3403	1.0756
FACT2	21.3483	20.2247	41.5730

Table 2. Statistical Indices FB, MG, NMSE and FACT2 for the ETEX experiment

Concentration Calculation Method	CM1	CM2	CM3
FB	0.75624	0.3744	0.7569
95% Conf. Int.	(-0.2402|1.752)	(-0.8816|1.3062)	(-0.2324|1.7463)
MG	.3155	0.3280	0.3124
95% Conf. Int.	(.2078|0.4790)	(0.1914|0.5619)	(0.1919|0.5084)
NMSE	27.2325	13.8227	26.0639
FACT2	35.6890	34.9823	34.9116

Underestimation is also indicated by the MG values, that are smaller than 1 for both examined cases and for all concentration calculation methods (Tables 1 and 2). According to MG the underestimation is systematic since 1 is not included in the 95% confidence intervals in any case and for any method. It is reminded that the MG gives equal weight to all concentration values, while the FB gives more weight to the large concentration values.

The NMSE values for the ETEX case are one order of magnitude larger than the TRANSALP case, indicating a larger scatter of values for the former case. The FACT2 values in the ETEX case are larger than in the TRANSALP case, indicating a better overall model performance in the former case by all methods.

For the comparison between the three concentration calculation methods, it appears that for the TRANSALP case the best performing method, according the FACT2 is CM3. For the ETEX case, based on the FB and the NMSE, the best performing method is CM2.

The plots, presented in Figures 1 and 2, support the conclusions drawn by the statistical indices. The scatter plots indicate a larger scatter of values in the ETEX case, but also a more even distribution around the 1:1 line. From the Q-Q plots it is apparent that the underestimation is more pronounced for the small concentration values.

CONCLUSIONS

This paper presents a validation study of the model DIPCOT for a mesoscale and a long - range atmospheric dispersion cases, applying three different methods of concentration calculation, and using statistical analysis and graphical representation of the results.

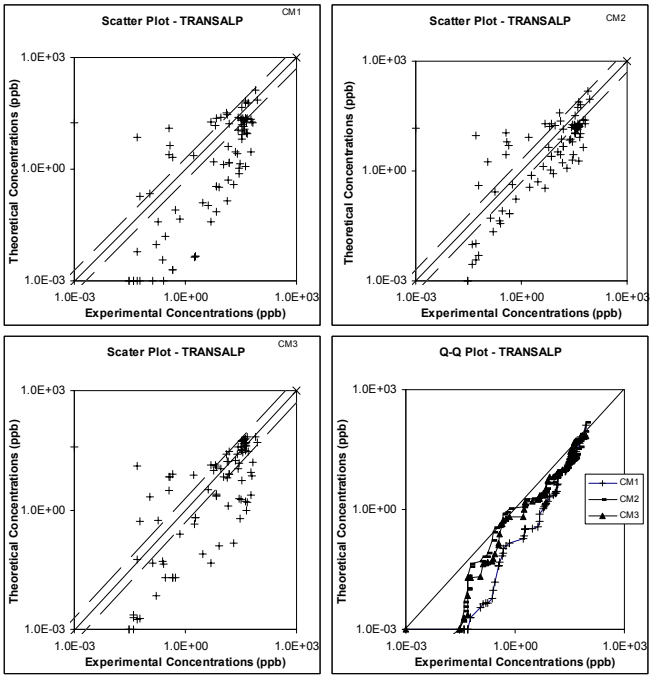

Figure 1: Scatter and Q-Q plots for the TRANSALP case

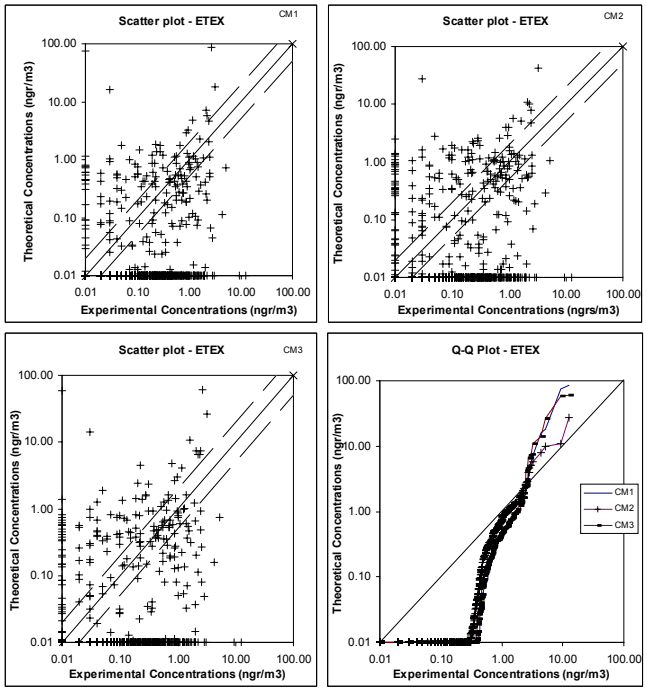

Figure 2: Scatter and Q-Q plots for the ETEX case

The two density-kernel methods performed slightly better in both simulated experiments than the box counting method. This is attributed to the large number of particles required by the latter method, especially in cases of highly complex terrain or long-range dispersion examined here. Further testing of the box counting method is needed with increasing number of particles. All the examined concentration calculation methods performed rather satisfactorily for the large concentrations, while they exhibited a systematic underprediction of the small ones. Given that the small concentration values mostly occur far from the source, the underpredictions can be attributed to the ever-growing bandwidth of the kernel or box size, as the plume moves away of the source. Therefore, it is the authors' opinion that the growth of this characteristic size must be controlled, especially far from the source. So, limitations of the characteristic size in each method must be further examined. Moreover, the use of the "optimal" bandwidth proposed by *de Haan P*. (1999) for the kernel density methods, can be considered.

The differences of the model performance in the two examined cases are attributed to two factors: i) the complex terrain effects, that are more pronounced in the meso-scale application (TRANSALP) and introduce a larger degree of uncertainty, and ii) the meteorological data, that in the meso-scale case are purely prognostic, while in the long-range case (ETEX) are "analysed" weather-prediction data, and therefore introduce contain less uncertainties.

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