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ASSESSMENT OF A LAGRANGIAN STOCHASTIC PARTICLE MODEL FOR CONCENTRATION VARIANCE WITH FIELD DATA

Enrico Ferrero[1], Stefano Alessandrini[2], Scott Meech [2] and Dietmar Oettl [3]

[1]Università del Piemonte Orientale, Alessandria, Italy
[2]NCAR, Boulder (CO), US
[3]Air Quality Control, Government of Styria, Austria

Abstract: A stochastic Lagrangian model for concept fluctuations is tested by comparing simulation results with data measured in a small-scale dispersion experiment. To account for the scale of the experiment, the parameterisations of standard deviations and Lagrangian timescales are varied with appropriate constants. The results show a fairly good agreement between the simulated and observed values for the stable cases while discrepancies are observed for the neutral and stable cases.

Key words: *Dispersion model, Concentration fluctuations, Lagrangian model***.**

INTRODUCTION

Generally, atmospheric dispersion models prescribe the mean concentration field, noting that mean concentration is the key parameter to evaluate air quality for regulatory purposes. However, in a wide range of cases, such as the dispersion of toxic, flammable, or chemical reacting gases, evaluating the mean concentration field may not be sufficient, and the knowledge of the concentration variance is needed. In the case of odour annoyance estimation, models use a postprocessing module to calculate the 90th percentile throughout the peak-to-mean method. Our model is able to give an evaluation of the 90th percentile thanks to the estimation of the fluctuation intensity. Furthermore, this is obtained on-line which allows a fast response in the case of an emergency due to toxic or flammable releases

A new scheme for the concentration variance calculation, based on the works of Manor et al. (2014), Ferrero et al. (2017), Ferrero and Oettl (2019), is assessed using field experiment data. The scheme is introduced in a Lagrangian Stochastic Particle Model (LSPM), Open-Source code SPRAY-WEB (Università del Piemonte Orientale et al.; Tinarelli et al., 1994; Alessandrini et al., 2013; Bisignano et al., 2017). The model provides on-line mean concentrations and concentrations' variance 3D fields; thus, it does not need any off-line postprocessing. The model is tested against the FFT07 field experiment. A number of trials called "FUsing Sensor Information from Observing Networks (FUSION) Field Trial -2007" (or FFT-07) were performed at Dugway Proving Ground, Utah, USA (Storwald, 2007; Platt et al., 2008) that involved releases of tracers. This short-range (500 m) highly instrumented experiment was mainly exercised for intercomparing Source Term Estimation (STE) prototypes and algorithms. In this work, we use the data set in order to assess the ability of the new model in predicting the concentration variance at the ground level with a high spatial resolution of a tracer emitted from a point source. It is worth noticing that the spatial-temporal scale is very small. The domain size is few hundred meters and the plume dispersion is observed for about ten minutes. Preliminary results, are shown, and the model's performance is evaluated through statistical analysis. The model performances are also compared with those obtained with a simpler LSPM in which the mean concentration and the concentration variance calculation are carried out off-line.

THE NUMERICAL SIMULATIONS

Meteorological simulations, which provide the input for SPRAYWEB, are carried out using WRF (Skamarock et al., 2008) and the Global Climatological Analysis Tool (GCAT, Alessandrini et al., 2017). This simulation is quadruply nested with 67x67 grid points for each nest and the inner nest having 1.1-km grid spacing. There are 38 vertical levels in the atmosphere with a model top at 50 hPa. The WRF runs last from 13:09:2007 at 00:00:00 to 17:09:2007 at 00:00:00. As far as the configuration of the physical parameterizations is concerned we use, for the microphysics the WSM 6-class graupel scheme a new scheme with ice, snow and graupel processes suitable for high-resolution simulations; for the long-wave radiation RRTM scheme the Rapid Radiative Transfer Model, an accurate scheme using look-up tables for efficiency and accounting for multiple bands, trace gases, and microphysics species; for the short-wave radiation, Dudhia scheme, simple downward integration allowing for efficient cloud and clear-sky absorption and scattering; for the surface-layer, the Monin-Obukhov Similarity scheme, based on Monin-Obukhov with Carslon-Boland viscous sub-layer and standard similarity functions from look-up tables; for the land-surface, the Noah Land-Surface Model, unified NCEP/NCAR/AFWA scheme with soil temperature and moisture in four layers, fractional snow cover and frozen soil physics; for the boundary layer the Mellor-Yamada-Janjic (Eta) TKE scheme; for the cumulus parameterization, the Kain-Fritsch (new Eta) scheme, deep and shallow sub-grid scheme using a mass flux approach with downdrafts and CAPE removal time scale. While the meteorological fields are directly obtained from the WRF output, the turbulent parameterization for wind components standard deviations and Lagrangian time scales, needed for the dispersion simulations, are calculated using the interface code WSI (Bisignano et al. 2017). For the simulation presented here, we decided to use the Hanna (1982) parameterization. The computational domain used for the SPRAYWEB simulations is 72×72 km^2 corresponding to the inner grid of the WRF simulation. The cells in which the domain is divided are of size $\Delta x=\Delta y$ = 100m in the horizontal direction, Δz = 15m is the first layer depth. The time step for the particle trajectories simulation is Δt = 1 s.

Table 1. Monin-Obukhov lengths L of the different Trials

Trial	**7**	**14**	**15**	**22**	**30**	**45**	**46**
L	40	-126	12	8	22	-3	149

Table 1 shows the Monin-Obukhov length L values for the different trials. As can be seen, there is one unstable case (Trial 45), two neutral cases with opposite L values and four cases with increasing stability (Trials 7, 30, 15 and 8). The experiment therefore allows the model to be tested under a variety of stability conditions.

Preliminary analyses were conducted using a simpler version of the code using an offline approach. First the model simulates the mean concentration field and then the fluctuation concentration fields is calculated with the same stochastic equation and the same turbulence parameterisations. Two examples of the simulation results are shown in Figure 1 and 2 for a unstable case (Trial 45) and a stable case (Trial 7). In the plots are also indicated the measurements location and those that get measured non-zero values and those in which both simulated and measured values are non-zero. It can be observed that the patterns in the two cases are very different

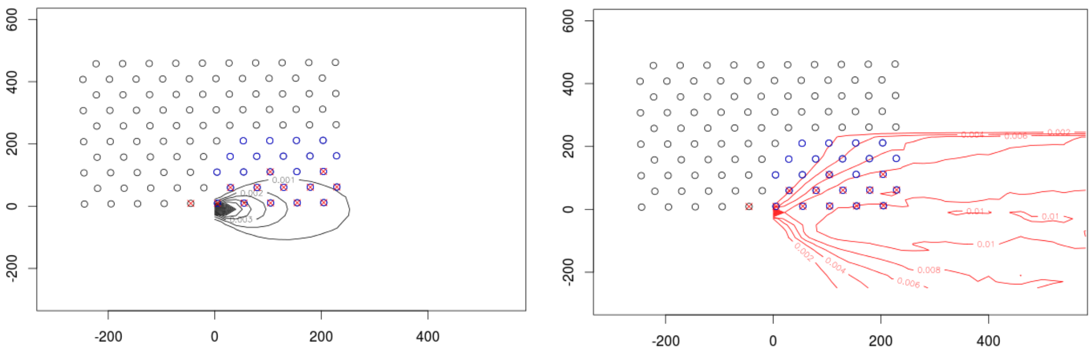

Figure 1. Pattern of the simulated mean concentration and concentration fluctuation for the unstable case (Trial 45). Left panel shows the mean concentration, right panel the concentration fluctuation. Black circles indicate the measurement points; blue circles refer to the probes giving non-zero value while crossed dots indicate where both measured and simulated non zero values are found.

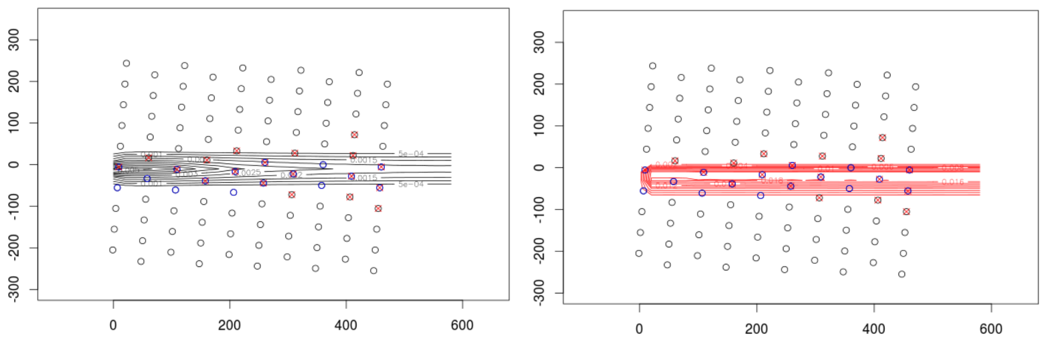

Figure 2. As in Figure 1 but for the stable Trial 7

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