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**A SENSITIVITY ANALYSIS FOR A LAGRANGIAN PARTICLE DISPERSION MODEL IN
EMERGENCY-RESPONSE TEST CASES**

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Abstract: Different setups of the modelling system MSS (MicroSwiftSpray) have been tested and analysed in application to flow and dispersion in built environments. Case studies from the COST Action ES1006 have been considered, with the aim of assessing the modelling tools in the emergency response context. Examples from the sensitivity analysis are here proposed, to evaluate the effects of different configurations of the models and different initial conditions.

Key words: *flow and dispersion modelling, built environment, emergency response.*

INTRODUCTION

In the frame of the modelling exercises carried out in COST Action ES1006 (Baumann-Stanzer et al., 2015), considering accidental releases in urban environments, a sensitivity analysis was performed for MicroSpray Lagrangian particle model (Tinarelli et al., 2007 and 2012). Different groups have been using the same model but applied in different configurations. MicroSpray model is integrated with the mass consistent diagnostic flow model MicroSwift in a modelling system, and it was run (1) in a standalone configuration, named as MSS, (2) in the parallel version for a standalone configuration, named PMSS, and (3) in its version inserted in a modelling suite providing advanced GIS-embedded software for modelling air quality in cities, named ARIA City.

The simulations were run in a standard setup and here we show results related to releases for the Michelstadt and CUTE test cases, where flow and dispersion data were collected. In Michelstadt wind-tunnel test case, a typical European urban site is reproduced, designed to characterise the neighbourhood-scale urban areas across Europe. Several continuous and puff releases in different locations were reproduced and both non-blind and blind tests were performed. CUTE test case refers to a real-field campaign, then reproduced also in the wind tunnel, with continuous and puff releases in a European city with a harbour. CUTE exercise was run in a blind way.

THE MSS MODELLING SYSTEM

MSS, and its parallel version PMSS, is a modelling system integrating the diagnostic mass-consistent model MicroSwift with MicroSpray Lagrangian particle dispersion model. MicroSwift interpolates the input wind profile on the simulation 3D domain through an objective analysis based on the mass conservation equation. In MSS the total turbulence is obtained summing the local one, produced by the flow distortion around the obstacles, plus a background level obtained by standard boundary-layer parameterizations. The local turbulence is estimated on the basis of a mixing-length closure, with the mixing length being a function of the distance to the obstacle or the ground. MicroSpray is able to take into account the presence of obstacles. The dispersion of an airborne pollutant is simulated following the motion of a large number of fictitious particles. The mean (“transport”) component of the particle velocity is provided by the meteorological driver. The stochastic (“turbulent”) component of the particle motion is obtained by solving a 3-D form of the Langevin equation for the random velocity.

MICHELSTADT TEST CASE

The **Michelstadt** modelling exercise is based on data gathered in a flow and dispersion experiment performed in the atmospheric boundary layer wind tunnel at the Environmental Wind Tunnel Laboratory in Hamburg. The measurements were carried out in an idealized Central-European urban environment model. Five point sources were used non-simultaneously in continuous and short-term release mode, and two wind directions were investigated. For the modelling exercise, both non-blind and blind tests were performed.

Here we discuss the results obtained, when MSS model is applied by different users in different configurations: the Lagrangian particle model is integrated with the mass consistent diagnostic flow model in a modelling system, hereafter named as MC&L (CONF_2). This system can be run in its parallel version (PMC&L hereafter), in a standalone configuration (CONF_1) or in a modelling suite providing advanced GIS-embedded software for modelling air quality in cities (CONF_3). In Table 1 we report the details of the model configurations as applied in three different setups. The simulations were run in a standard setup and here we show results related to the non-blind continuous release for different emission locations.

Table 1. Details on the configurations of the three different runs

	CONF_1	CONF_2	CONF_3
Model	PMC&L stand alone	MC&L standalone	PMC&L in modelling suite
Scale	Full		
Buildings	Shape file derived from dxf file available in COST ES1006 Action		
Wind velocity	Power law fitting experimental profile	Logarithmic law extrapolation below 9.9 m (with experimental friction velocity u^* and roughness length $z_0=1.53$ m) Experimental profile above 9.9 m	MC automatic logarithmic extrapolation below 99.9 m using roughness length $z_0=1$ m 6 m/s at 99.9 m and power law above 99.9 m
Background turbulence	Fitted to experimental : Urms=1.2m/s, Vrms=1.2m/s, Wrms=0.86m/s	z_0 and u^* imposed to fit experimental Urms and Vrms profile between 1m/s and 1.5m/s , Wrms profile between 0.8m/s and 1.2m/s	« Urban » landuse type in the modelling suite $z_0 = 1$ m. Leading to Urms and Vrms ~ 1m/s and Wrms~0.8m/s
Horizontal resolution	1.5 m	2 m	3 m
Vertical grid	1 m below 27m, top = 200m; 40 points	1m below 12m, top=200m 21 points	2 m from the first level to the top=200m; 21 points
Emission time step	1 s	3 s	1 s
N particles/dt	1275	1000	100
Averaging period	2700s(+900s for steady state)	3600s (+1200s)	3600s(+1200s)
CPU time	15 minutes	1 hour	2 minutes
Hardware	8 cores (3.2GHz)	1 core Intel i7 2.67 Ghz	7 cores Intel Xeon 2.8 GHz

In Figure 1 the differences among the inlet wind speed profiles as used in the three setups can be appreciated and are compared to the experimental data. In Figure 2 the contours of concentration data are plotted for the three setups. In general, the agreement with the observed values (squares) is fair for all cases. We notice that downwind the source, the area with highest concentrations inside the longitudinal and diagonal canyons extends further for CONF_1 simulations than for the others. The tracer distribution is generally well captured in the longitudinal canyon, while in the diagonal one the predicted concentrations are higher than the observed. The area with medium concentration values has a larger downwind extension for CONF_2 and CONF_3, thus far from the source, in the cross section at street-

level, the concentrations are lower for CONF_1 than for CONF_2 and CONF_3. We note that in CONF_1 a very fine vertical meshing is used, allowing to better detail the flow inside and at the top of the canopy level, at the same time detecting larger vertical wind velocity gradients. The vertical transfer at the top level may become strong and, consequently, part of the tracer is trapped in the street canyons near the source while another part is pushed above the buildings by a quick airflow. The vertical mesh of CONF_2 has the same resolution but for shallower layer, while CONF_3 vertical mesh is coarser. Thus the vertical velocity gradients are smoother and lead to a weaker transfer from the canopy towards the inertial atmospheric sublayer above it. The area of smallest concentration values is more extended for CONF_1 at the boundary of the plume - this might be linked to the higher number of particles used in CONF_1 run, increasing the statistics of the particle dispersion. In Figure 3 we compare the concentrations predicted with the three different setups for three continuous releases, named as S2, S4 and S5, through scatter plots. A larger spread occurs between CONF_1 and CONF_2, especially in case of S4 source, while the agreement looks slightly better in the other cases.

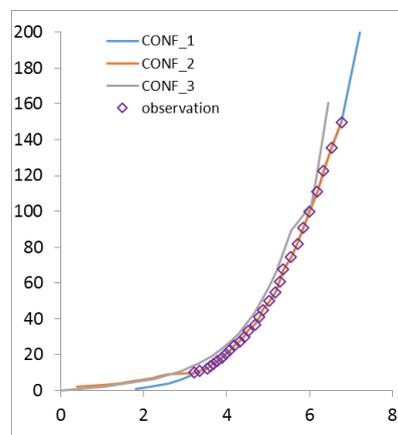


Figure 1. Michelstadt case. Inlet wind speed profile as used in the three different configurations (solid lines, blue for 'CONF_1', dark red for 'CONF_2' and green for 'CONF_3') and experimental data (diamonds).

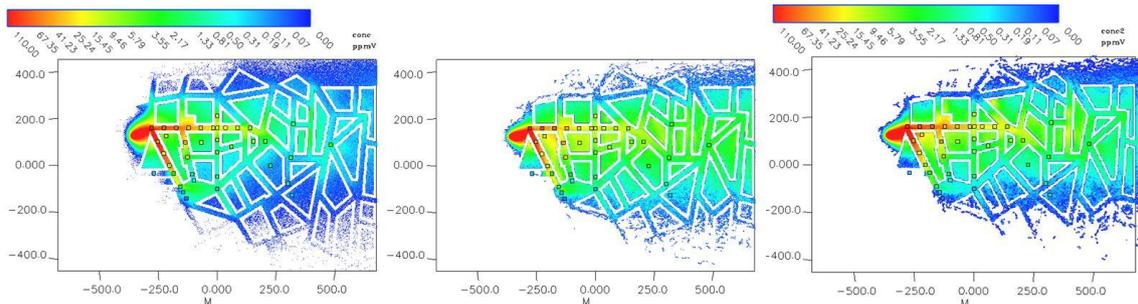


Figure 2. Concentration contours in the simulation domain for CONF_1, CONF_2 and CONF_3 (from left to right). The coloured squares represent the observations in the same colour scale as for the simulations.

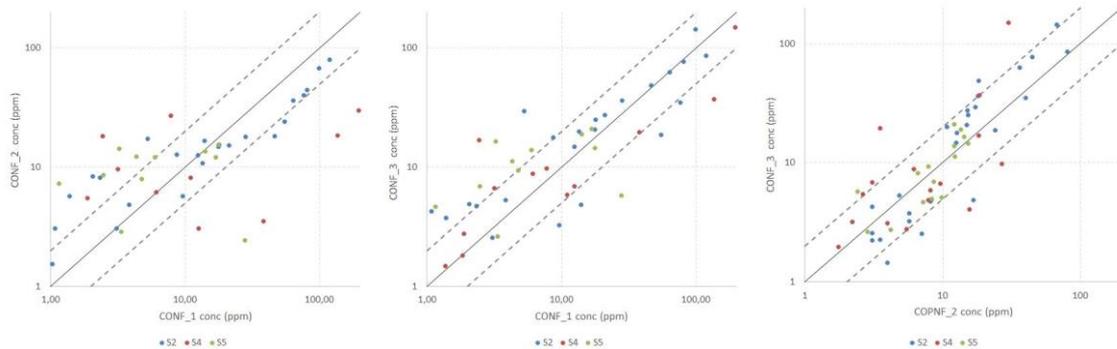


Figure 3. Scatter plots (logarithmic scale) of the different setups predicted concentration values at the measuring locations for the release at sources S2 (blue points), S4 (red points) and S5 (green points)

CUTE TEST CASE

In CUTE test case data from both a field experiment in a real city and its reproduction in the EWTL wind tunnel were gathered. Continuous and puff releases from a boat towards a harbour area were carried out. Concentrations were detected by 20 measurement stations located at different positions in the field experiment, while more than 30 recording stations were used in the wind tunnel.

For CUTE case a sensitivity analysis on the initial conditions is proposed to address the problem of their uncertainty, which is particularly high in case of accidental release and which may strongly influences the model results. Test simulations were run for both the field and wind tunnel experiments, continuous release, in neutral conditions. Alternative wind velocity and turbulence input settings were considered to verify the variability of model outputs to different driving meteorological data. For the wind, two different simulations were run, in the first one (W#1) a vertical wind profile was calculated starting from the only measurement at 175m provided to all modellers in COSTES1006 Action exercise, keeping the direction homogenous in vertical. In the second one (W#2) all data available at the weather mast were used to build a wind profile having directions that vary in the vertical following the available measurements. In Figure 4 the effect of the different wind direction in input is clear, the plume deviates in slightly different directions and the affected areas are thus different, having an impact on the possible response. The performance of the run W#2 were found to be better than for W#1 initialization.

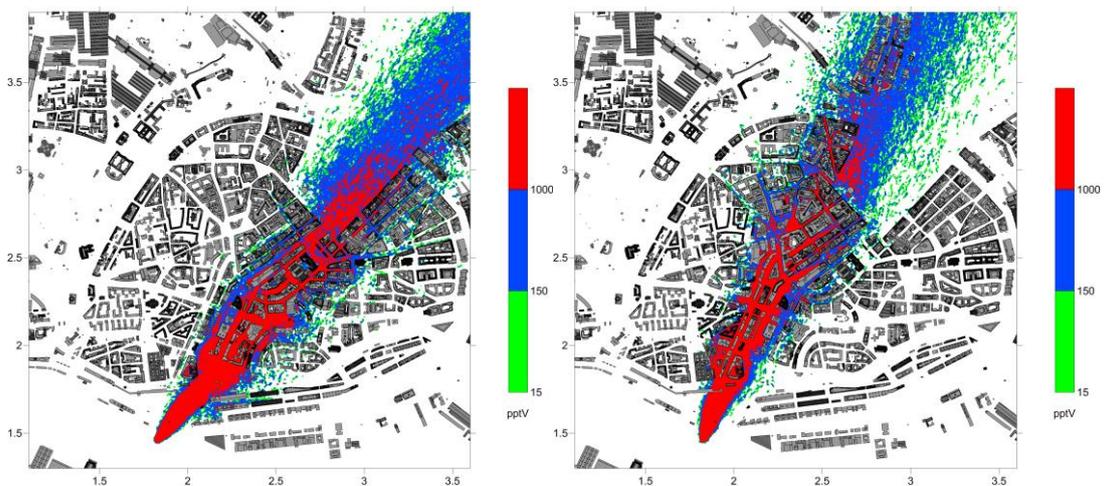


Figure 4. CUTE case, field experiment. Comparison of concentration field with two wind inlet profiles, W#1 on the left and W#2 on the right.

The turbulence input was estimated with an analytical formulation, for neutral atmosphere using two roughness values, so that T#1 corresponds to a stronger turbulence than the one determined in T#2:

T#1: $z_0=1\text{m}$; in the field case $u_*=1.31\text{m/s}$; $\text{TKE}(z=10\text{m})=6.4\text{m}^2/\text{s}^2$; in the wind tunnel case $u_*=1.26\text{m/s}$ and $\text{TKE}(z=10\text{m})=5.9\text{m}^2/\text{s}^2$

T#2: $z_0=0.1\text{m}$; in the field case $u_*=0.33\text{m/s}$; $\text{TKE}(z=10\text{m})=0.4\text{m}^2/\text{s}^2$; in the wind tunnel case $u_*=0.31\text{m/s}$; $\text{TKE}(z=10\text{m})=0.39\text{m}^2/\text{s}^2$

The resulting concentrations fields, plotted in Figure 5 for the field experiment, highlight the impact of the different turbulence, where a stronger turbulence spreads and dilutes more the plume so that the zones with high concentration extend less far downwind the source.

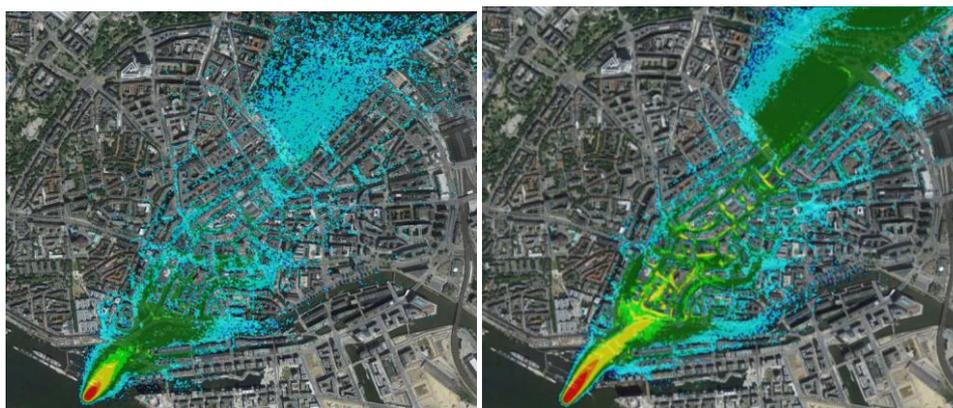


Figure 5. CUTE case, field experiment. Comparison of concentration field with two turbulence inlet profiles, T#1 on the left, T#2 on the right.

CONCLUSIONS

The sensitivity tests allowed confirming the robustness of the dispersion model, since even in different configurations, with different input conditions and turbulence parameterizations, and using it in different modelling systems or suites, the quality of the results is comparable and the simulations provide reliable outputs. The analysis also highlighted that, besides the physical quantities, there are key quantities handled by the users that can help improving the performances, such as the number of particles and the horizontal and vertical grid resolution. We notice that the possibility to run the model in a parallel configuration allows largely reducing the computational time, which however keeps being small also when using the model on a single CPU.

The sensitivity test on the initial conditions proved the importance of having appropriate local measurements, possibly characterizing also the vertical variability, to achieve more reliable simulations of an accidental release. While in general it is not easy to have such kind of observed data available, in case of known sensitive sites, where for instance industrial plants are located, a proper planning of the net of sensors becomes fundamental to support emergency response tools.

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