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VALIDATION OF THE PMSS MODELLING SYSTEM IN URBAN ENVIRONMENTS AND APPLICABILITY IN CASE OF AN EMERGENCY

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Abstract: Releases of harmful airborne materials may pose a serious threat to the population in case of an accident or a malevolent action. In such a situation, a reliable and rapid assessment of the impacted areas is of highest interest for the security services and their authorities to make decisions and take appropriate protection measures. As these events are more likely to occur in built-up (industrial or urban) places, only 3D flow and dispersion models are adequate to address these complex environments in possibly evolving meteorological conditions. This paper aims to evaluate the PMSS modelling system that comprises a diagnostic and momentum solving flow model and a Lagrangian Particle Dispersion model. PMSS is validated on a panel of experimental test cases from the COST Action ES1006 for both idealized and real urban mock-ups, wind tunnel and in field trials, continuous and puffs releases. The concentrations predicted in various configurations of PMSS are compared to measurements on the basis of statistical metrics. PMSS proves to be compliant with the validation criteria established in literature in the large majority of the test cases and robust enough to be used in the context of emergency response, when fast but still reliable results are needed.

Key words: PMSS modelling system, wind tunnel and field data validation, COST Action ES1006.

INTRODUCTION

Atmospheric releases of potentially hazardous materials may originate from accidents affecting industrial plants or malicious activities (sabotage or terrorist attack). As a threat for the population, they are a major concern for the rescue team and their local or national authorities seeking for reliable health impact assessment of such events to take appropriate protection measures of the people.

Last years, improvements in modelling capabilities and computational resources have made 3D numerical simulations more and more capable to deal with rugged terrain and complicated buildings geometry in evolving meteorological conditions. However, flow and dispersion modelling in an industrial or urban built-up area remains very challenging given the complex characteristics of this environment.

Most of the fast response systems devoted to dispersion in built-up areas rely on standard or modified Gaussian models able to account for the effects of the individual buildings and the global street network. However, they hardly apply to complex layouts or transient phenomena, like flow channeling and vortices inside streets. By contrast, Computational Fluid Dynamics (CFD) models provide reference solutions by solving the Navier-Stokes equations, thus properly account for complex flows in built-up areas, but suffer from extreme computational times even on very large computers. Thus, a trade-off is needed between the accuracy of the flow resolution and the response time, especially on limited calculation resources.

In this context, the Micro-SWIFT-SPRAY (MSS) (Tinarelli *et al*. 2013) modelling system was developed in order to provide a simplified, but rigorous solution of the flow and dispersion in built-up environments in a limited amount of time. SWIFT is a 3D diagnostic, mass-consistent, terrain-following model taking account of the buildings and providing the 3D fields of wind, turbulence, and temperature. SPRAY is a 3D Lagrangian Particle Dispersion Model able to account for the presence of buildings. In recent years, parallel versions of SWIFT and SPRAY have been developed leading to the PMSS system (Oldrini *et al*., 2017). Moreover, a momentum solver has been implemented in SWIFT (Oldrini *et al*., 2014) to simulate more accurately velocity and pressure fields in built-up environments than obtained with the diagnostic flow model; this solver has been validated on academic test cases (Oldrini *et al*., 2016).

After a brief description of the experimental test cases, this paper is dedicated to the validation of (P)MSS on experimental test cases from the COST Action ES1006 (Trini Castelli et al., 2016; Armand et al., 2016). The tests include idealized and realistic urban mock-ups, wind tunnel and field trials, continuous and puff releases. In view of determining the sensitivity and robustness of (P)MSS, the computations were performed by independent teams of modelers making various choices regarding the meteorological input data or the numerical options in (P)MSS. All predicted results were compared to measurements and the performances of (P)MSS evaluated through a statistical analysis based on the fractional bias (FB), the normalized mean square error (NMSE), and the fraction of predictions over measurements in a factor of 0.5 to 2 (FAC2). Following Hanna and Chang (2012), the reference acceptance criteria for the results of atmospheric dispersion in built environments are: $|FB| < 0.67$, $NMSE < 6$, and $FAC2 > 0.30$.

BRIEF DESCRIPTION OF THE EXPERIMENTAL TEST CASES

Within the scope of COST Action ES1006, the boundary layer wind tunnel facility at the Environmental Wind Tunnel Laboratory of Hamburg University was used for the measurements in controlled conditions.

The Michelstadt experiment was designed as the first test for the validation of dispersion models in an urban layout with the building structure representing an idealized Central-European city. The urban wind field was measured from a densely spaced grid. Six different point sources were used and two opposite wind directions were simulated. The concentration measurements were positioned to be representative of affected areas in various building configurations. Continuous and puff releases were carried out and both non-blind and blind test cases established. In the blind tests, minimum information for the inflow was available, as it would be the case during a real incidental or accidental situation.

The Complex Urban Terrain Experiment (CUTE) was designed to test dispersion models in real urban areas and it included results from field and wind tunnel measurements. The experimental campaign was carried out in the densely built-up downtown of a Central-European city. In the real-field test, the source was located on a boat. SF_6 was released continuously during the test and the samples at 20 measurement points were analyzed after the trial by means of gas chromatography. In the wind tunnel tests, the scaled model of the city center was used and both continuous and puff releases were considered.

ANALYSIS OF MICHELSTADT WIND TUNNEL SIMULATION RESULTS

Continuous and puff releases from three source locations S2, S4 and S5 for the non-blind test and from four source locations S5, S6, S7 and S8 for the blind test were considered for the Michelstadt case study. Three configurations of (P)MSS were run by independent teams of modelers. As a matter of fact, even if all relevant, the choices operated by users applying the same model may bring to rather different results. Thus, the goal was to investigate the sensitivity of (P)MSS results to the the version of the modelling suite, the setting of the physical variables in input and the numerical simulation parameters. The model performances were evaluated by statistically comparing the numerical results with the observations successively for the continuous releases and the puff releases, for both the non-blind and blind tests.

Michelstadt wind tunnel continuous releases

The scatter plots in **Figure 1** compare the predicted and observed mean concentrations at the sensor locations for all continuous releases. The spread between predictions and observations is not negligible, yet a large part of the data lies inside the factor of two area. The results of the blind test cases are slightly less satisfying than the results of the non-blind test cases. The agreement is better for a release taking place in an open square (like for the S2 source) than for a release occurring in a complex environment, in street-canyon (S4 and S5 sources), at a crossroad (S6 and S7 sources) or inside a courtyard (S8 source).

These considerations are confirmed when analyzing the predicted mean concentration in terms of the statistical metrics FB, NMSE and FAC2 as can be seen in **Table 1**. Regarding FB, the results are mostly acceptable according to the acceptance criterion |FB| < 0.67. The results for FB are larger than zero, indicating that the model applied for continuous sources tends to underestimate the observed mean concentrations. Regarding NMSE, the model results are within the acceptance threshold value of 6 in the non-blind test cases, while blind case results are above the acceptance criteria except for MSS_A. In fact, NMSE is sensitive to far outliers, corresponding to predicted values that largely differ from observations, even though they might occur rarely. Regarding FAC2, there is a satisfactory agreement of the model results within the criterion applying to this statistical metric for both non-blind and blind tests.

Michelstadt wind tunnel puff releases

The scatter plots in **Figure 2** compare the predicted and observed mean dosages and puff mean durations at the sensor locations for all puff releases. The ranges of observed and predicted dosages are rather different. In numerical simulations, minimum concentrations are of order 0.1 ppmv with dosages taking very low values. For the dosages calculated from the measurements, only the puffs which exceeded 5 ppmv s were included in the evaluation. Given the challenging complexity of the tests, both blind and non-blind cases show fair enough results, since they timely capture the passage of the puff even if with some underestimation of the dosage. While the simulated mean dosages are under-predicted, a reasonable accuracy is obtained for the values greater than 10^3 ppmv s. Less satisfying results are observed in the blind cases due to the scarce input information. Finally, for the puff duration results, only few points are outside the factor of two area for all non-blind and blind tests, well within the acceptance range.

The predicted mean dosage, mean peak concentration averaged over 15 s, and mean duration are analyzed in terms of the statistical metrics FB, NMSE and FAC2 as reported in **Table 2**. (P)MSS tends to under-estimate the mean dosage, given that FB exceeds the acceptance limit 0.67 in most of the cases, but the scatter estimated through the NMSE keeps inside the limit of NMSE < 6. The FAC2 value is acceptable only for PMSS_B in the non-blind case. The poor performance indicates that the model realization does not capture the statistics of the puff PDF for this parameter. The quality of the results is not systematically better for the non-blind case than for the blind one. This suggests that the performance of the model is well established and the difficulty in catching the mean dosage is linked to the complexity of the test scenario and uncertainties of puff releases and dispersion. The mean puff duration is very well caught by the model with all acceptance criteria, especially FAC2, respected. The quality of the results is also fair for the 15 s mean peak concentration and FAC2 is within the acceptance threshold alternatively for one of the two models in non-blind and blind test cases.

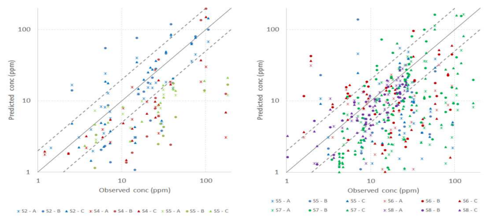

Figure 1. Michelstadt continuous releases. Scatter plots of the predicted and measured mean concentrations, for the non-blind test cases (left: blue for S2, red for S4 and green for S5) and the blind test cases (right: blue for S5, red for S6, green for S7, purple for S8), for MSS_A (asterisks), PMSS_B (dots) and PMSS_C (triangles) configurations.

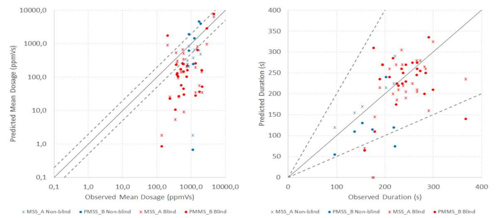

Figure 2. Michelstadt puff releases. Scatter plots of the predicted and measured mean dosages (left) and puff mean durations (right), for the non-blind test cases (S2, S4 and S5 sources, blue colour) and the blind test cases (S5, S6, S7 and S8 sources, red colour). for MSS_A (asterisks) and PMSS_B (circles) configurations.

Table 1. Michelstadt continuous releases. COST ES1006 statistical metrics for the three (P)MSS runs. Non-blind releases from sources S2, S4 and S5 and blind releases from sources S5, S6, S7 and S8.

	Model	FB	NMSE	FAC2
Non-blind tests	MSS_A	0.68	4.35	0.46
	PMSS_B	0.11	2.15	0.64
	PMSS_C	0.73	4.02	0.51
Blind tests	MSS_A	0.64	2.07	0.41
	PMSS_B	0.36	9.01	0.45
	PMSS_C	0.67	11.55	0.38

Table 2. Michelstadt puff releases. COST ES1006 statistical metrics for two (P)MSS runs. Non-blind releases from sources S2, S4 and S5 and blind releases from sources S5, S6, S7 and S8.

		Model	FB	NMSE	FAC2
Mean dosage	Non-blind tests	MSS_A	1.53	1.04	0.01
		PMSS_B	0.68	6.30	0.38
	Blind tests	MSS_A	1.25	4.94	0.15
		PMSS_B	1.17	3.84	0.08
15-s peak conc.	Non-blind tests	MSS_A	1.25	3.05	0.13
		PMSS_B	-0.40	1.55	0.38
	Blind tests	MSS_A	0.65	2.81	0.31
		PMSS_B	0.35	3.93	0.08
Mean duration	Non-blind tests	MSS_A	0.09	0.07	0.92
		PMSS_B	0.03	0.06	0.96
	Blind tests	MSS_A	0.11	0.18	0.86
		PMSS_B	0.35	0.27	0.86

ANALYSIS OF CUTE FIELD AND WIND TUNNEL EXPERIMENTS SIMULATION RESULTS

For CUTE, both field and wind tunnel continuous and puff releases experiments were carried out. Here, the goal was to investigate the sensitivity of the simulations to alternative (diagnostic or momentum solving) flow models and meteorological input driving the dispersion of the tracer in (P)MSS.

Sensitivity to the turbulence intensity – Two sets of lower and higher turbulence input data were evaluated for computing the wind field driving PSPRAY model. The turbulence intensity is partially depending on the land-use, which here is very complex due to the heterogeneities related to the presence of a river, an industrial harbour area and the urban pattern. As expected, a stronger turbulence spreads and dilutes more the plume so that the high concentration zones extend less far downwind the source. Having information about e.g. the variances of the velocities, allows better reproducing the turbulence level in the domain.

Sensitivity to the wind direction profile – For the field experiment continuous release, two simulations were performed using MSS scalar version. In MSS_W1, a vertical wind profile was calculated starting from the only available measurement at 175 m given to the modelers, keeping the direction homogenous in vertical. In MSS_W2, data coming from a nearby weather mast were used to build a wind profile with directions that vary in the vertical following the available measurements. The different inputs have the effect to make the plume deviating in slightly different directions, so that the affected areas are different.

Sensitivity to the flow model – Flow computations were performed with both the diagnostic and the momentum versions of PSWIFT. The momentum version of PSWIFT was found to be superior in solving the flow inside the street canyons. Hence, it is expected to provide a more physically sound and reliable distribution of the tracer gas in a complex geometry. Still, in this test case, it turned out that the PSPRAY concentration patterns were not drastically different when one wind model or the other was used.

CUTE in field and wind tunnel experiment continuous releases

The scatter plots in **Figure 3** compare the predicted and observed mean concentrations at the sensor locations for CUTE both field and wind tunnel continuous release tests. They show a tendency towards underestimation and a quite high degree of scatter for the weak concentrations while the simulation of the highest concentrations is more satisfying. For the field experiment, the best agreement is obtained in the configuration MSS_W2 because a more relevant wind direction profile was used in this case. For the wind tunnel experiment, a fair agreement of the predictions with the measurements is obtained in all configurations, especially for the highest concentrations. (P)MSS performances are similar to that found in the Michelstadt wind tunnel test cases with the influence of some input conditions illustrated.

These considerations are confirmed when analyzing the predicted mean concentration in terms of the statistical metrics FB, NMSE and FAC2 as can be seen in **Table 3**. For the field experiment, the statistical measures show a certain variability among the configurations of (P)MSS. Half of the results indicate biased FB and NMSE larger than the acceptance limits while a FAC2 greater than 0.3 complying with the acceptance criterion is documented. Given the low absolute concentrations, also the differences between observed and predicted data are small, but they have a large relative weight. Here, results obtained with the momentum (M) and diagnostic (D) flow models in PSWIFT perform equivalently well in terms of FAC2 while there is more scatter in PMSS_M compared to PMSS_D. Noticeably, concentrations are no more systematically under-predicted when using the momentum flow model as it was the case with the diagnostic one. For the wind tunnel, the statistical metrics are better than for the field experiment and all configurations meet the acceptance limits, giving FAC2 values much better than the required limit. FB and FAC2 results obtained with PMSS_M improve with respect to results using PMSS_D.

CUTE wind tunnel puff releases

The scatter plots in **Figure 4** compare the predicted and observed mean integrated concentration or dosage and the mean duration at the sensor locations for CUTE wind tunnel puff releases. The paired data are few, thus the comparison and the related statistics do not represent a comprehensive validation test, yet they provide interesting insights. In both (P)MSS runs, there is a tendency to underestimate the integrated concentrations ranging between 10^2 and 10^3 ppmv s, whereas the highest observed values are well reproduced by the predictions. These results are in line with the findings in Michelstadt cases for puff releases. PMSS_D run tends to generate a longer mean duration than experimentally observed while the mean durations predicted by MSS fits well the observed values.

The predicted mean dosage, mean peak concentration averaged over 15 s and the mean duration are analyzed in terms of the statistical metrics FB, NMSE and FAC2 as reported in **Table 3**. As for the wind tunnel continuous release, the puff releases results demonstrate predominantly fair performance of the model in both configurations. While MSS generates some better results compared to PMSS_D, the latter one still gives acceptable results.

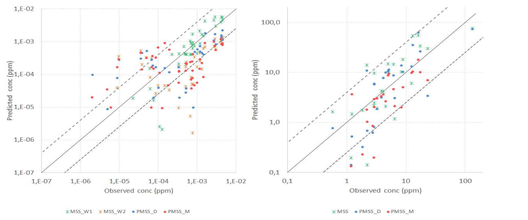

Figure 3. CUTE field experiment continuous release (left) and wind tunnel continuous release (right). Scatter plot of the predicted and measured concentrations, for (left) MSS_W1 (green asterisks), MSS_W2 (orange asterisks), PMSS_D (blue circles), PMSS_M (red circles), and for (right) MSS (green asterisks), PMSS_D (blue circles), PMSS_M (red circles).

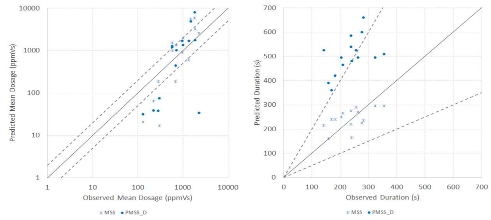

Figure 4. CUTE wind tunnel puff releases. Scatter plot of the predicted and measured mean dosage (left) and mean duration (right), for MSS (asterisks) and PMSS_D (circles).

Table 3. CUTE continuous and puff releases. COST ES1006 statistical metrics for various (P)MSS runs.

			Model	FB	NMSE	FAC2
Field Experiment	Cont. release	Mean conc.	PMSS_D	0.03	5.59	0.35
			PMSS_M	-1.07	23.01	0.32
			MSS_W1	0.96	11.37	0.30
			MSS_W2	-0.30	3.01	0.57
Wind tunnel	Cont. release	Mean conc.	PMSS_D	-0.34	1.75	0.38
			PMSS_M	-0.07	2.09	0.47
			MSS	-0.21	2.27	0.35
	Puff releases	Mean dosage	PMSS_D	-0.47	2.63	0.38
			MSS	-0.53	1.67	0.44
		15-s peak conc.	PMSS_D	0.77	2.71	0.38
			MSS	-0.17	0.44	0.50
		Mean duration	PMSS_D	-0.72	0.64	0.27
			MSS	-0.03	0.04	1.00

CONCLUSIONS

The validation of (P)MSS has been performed against the experimental results performed in the frame of the COST Action ES1006 with an increase in the complexity level, from the wind tunnel mock-up scale to full scale real situations, from stationary plumes to highly variable puff releases, also from a diagnostic flow model to a model solving the momentum equation. Only a part of the (P)MSS validation exercise is presented is this paper; the reader can find a more exhaustive presentation in Trini Castelli *et al.* (2018).

The statistical analysis for (P)MSS in various configurations has shown that in most of the test cases, the (P)MSS performances are within the acceptance criteria defined for modelling in urban environments. Moreover, (P)MSS proved to be robust even when dealing with poor information input (as is the case during the response phase of an accidental or malicious situation) and various physical and numerical parametrizations of the modelling system.

Even for the puff releases, (P)MSS was able to replicate the deflection of the plume axis with respect to its initial direction due to the effect of building structures on ground-level wind flow in Michelstadt and CUTE test cases. Notwithstanding the variability of the results from the different model configurations, the dispersion patterns and the the areas affected by the plumes are always consistent among them.

Sensitivity tests on the input flow data showed that slightly different wind directions or turbulence levels lead to substantially distinct affected areas. Thus, proper meteorological data are of outmost importance in achieving reliable simulations. For accidental or malicious releases, it may be not easy to have accurate and timely observed data. However, the planning of a sensor network, to assure a continuous monitoring of the meteorological situation, is certainly feasible for sensitive industrial sites.

Besides its own interest, the validation of (P)MSS addresses the capability and reliability of Lagrangian particle models in the conditions of an emergency in built-up environment. In practical applications, first responders and stakeholders are provided with the results of simplified models, which are not appropriate tools in a built-up environment. Consequently, response procedures based on simplified models may be not effective or incisive, or even misleanding. On the contrary, (P)MSS succeeds in a trade-off between accuracy and timeliness of the computations, demonstrating that such a modelling system is a valuable support to the emergency preparedness and response, what is a real benefit for this field of research.

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