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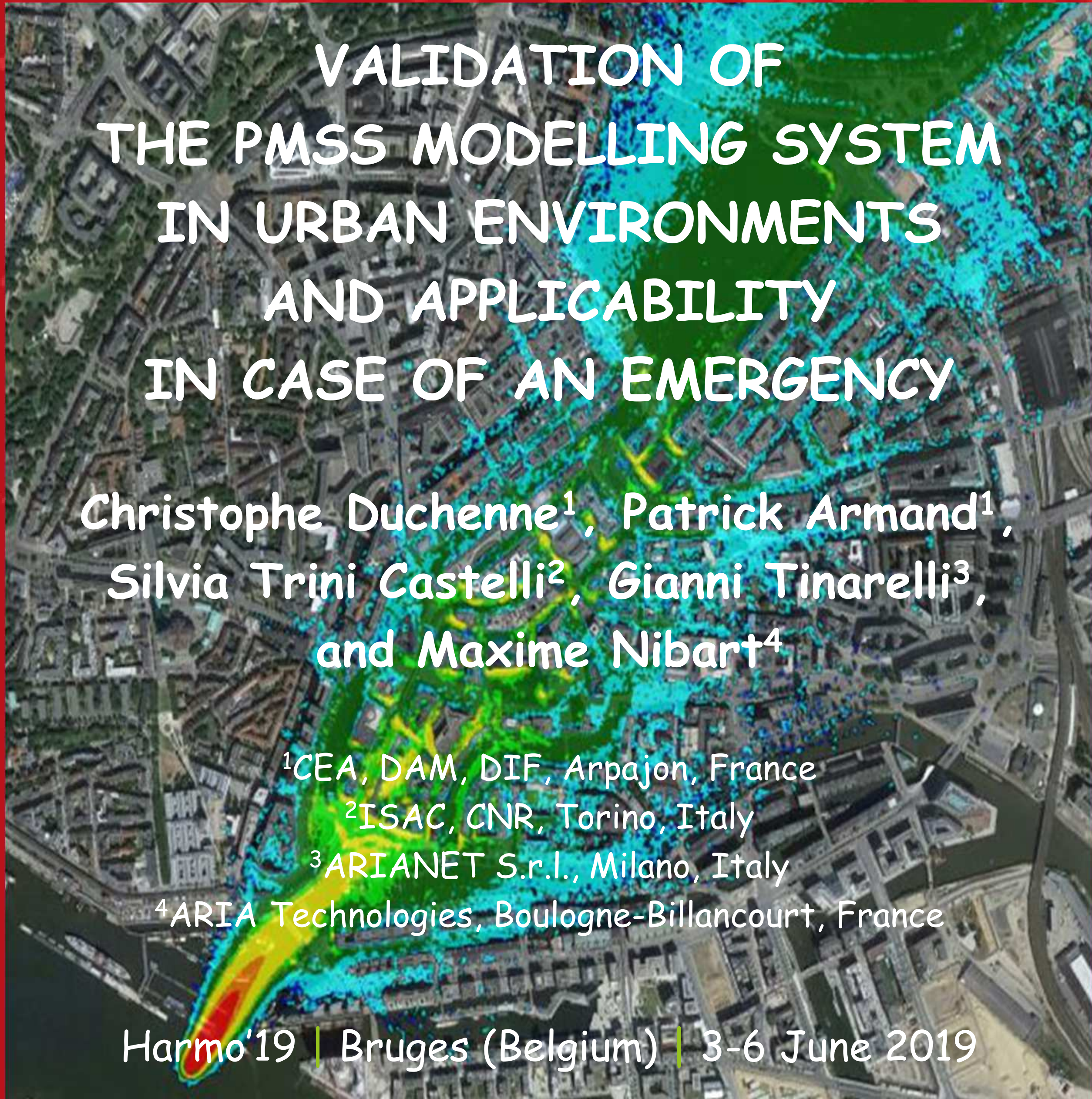

VALIDATION OF THE PMSS MODELLING SYSTEM IN URBAN ENVIRONMENTS AND APPLICABILITY IN CASE OF AN EMERGENCY

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INTRODUCTION AND RATIONALE (1)

- Atmospheric releases of hazmat are a huge concern for the rescue teams and their authorities seeking for reliable health impact assessment to take appropriate protection measures of the population

- Most of the fast-response systems devoted to dispersion in built-up areas rely on modified Gaussian models able to account for the street network, but hardly apply to complex layouts or transient effects

- By contrast, Computational Fluid Dynamics (CFD) models provide reference solutions by solving the Navier-Stokes equations, but suffer from extreme computational times even on very large computers

- Thus, Micro-SWIFT-SPRAY (MSS) (Tinarelli et al. 2012) modelling system was developed as a trade-off between the accuracy of the flow resolution and the response time (even with limited resources)
  - ✓ SWIFT is a 3D diagnostic mass-consistent flow model accounting for the buildings
  - ✓ SPRAY is a 3D Lagrangian Particle Dispersion Model with dry and wet depositions
  - ✓ Parallel versions of SWIFT and SPRAY have been developed leading to PMSS (Oldrini et al., 2017)
  - ✓ A momentum solver has been implemented in SWIFT (Oldrini et al., 2014) for a better simulation of the velocity and pressure fields, and validated on academic test cases (Oldrini et al., 2016)

INTRODUCTION AND RATIONALE (2)

- After a description of the test cases, the paper & presentation are devoted to the validation of (P)MSS on experimental test cases from COST Action ES1006 (Armand et al., 2016; Trini Castelli et al., 2016)

- Tests include idealized & realistic urban mock-ups, wind tunnel & field trials, continuous & puff releases

- In view of determining the sensitivity and robustness of (P)MSS, the computations were performed by three independent teams of modelers making different choices regarding the meteorological input data or the numerical options in (P)MSS (see more details in Trini Castelli et al., 2018)

- 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), the fraction of predictions in a factor of two of the measurements (FAC2), the geometric mean (MG) and the geometric variance (VG)

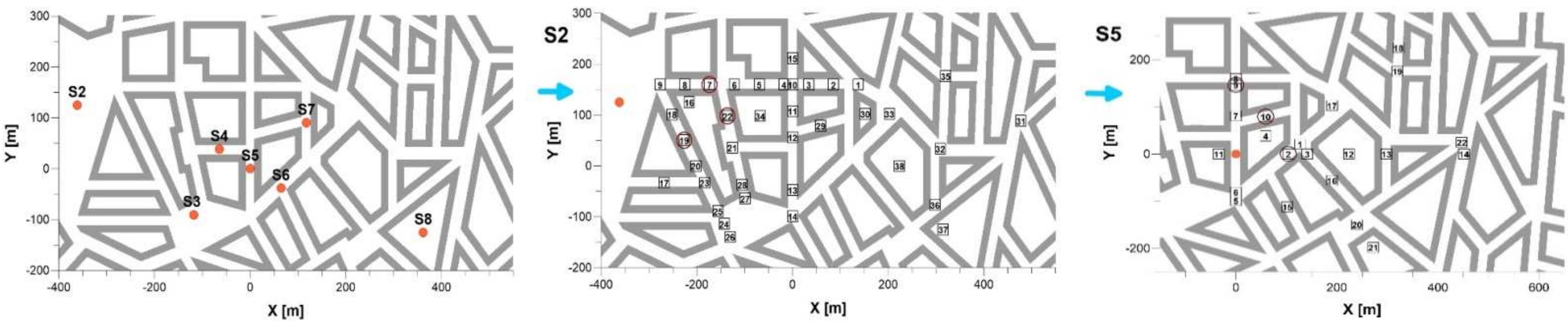
- The reference acceptance criteria for the results of atmospheric dispersion in built environments are:
  $|FB| < 0.67$, $NMSE < 6$, and $FAC2 > 0.30$ (Hanna and Chang, 2012)

DESCRIPTION OF THE EXPERIMENTAL TEST-CASES (1)

- In COST Action ES1006, the boundary layer wind tunnel facility at the Environmental Wind Tunnel Laboratory of Hamburg University was used for measurements in controlled conditions of a neutrally stratified boundary layer
  - ✓ Flow measurements were carried out with fiber-optic LDA and concentration measurements with FFI detectors
  - ✓ For each test case, the variables were converted from model scale to full scale

- 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
  - ✓ The concentration measurements were positioned in affected areas of various building configurations
  - ✓ Continuous and puff releases were carried out and both non-blind and blind test cases established

- The Complex Urban Terrain Experiment (CUTE) was designed to test dispersion models in real urban areas and 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, SF_6 was released continuously and the samples at 20 measurement points were analyzed after the trial by means of gas chromatography
  - ✓ In the wind tunnel tests, a scaled model of the city was used and both continuous and puff releases considered



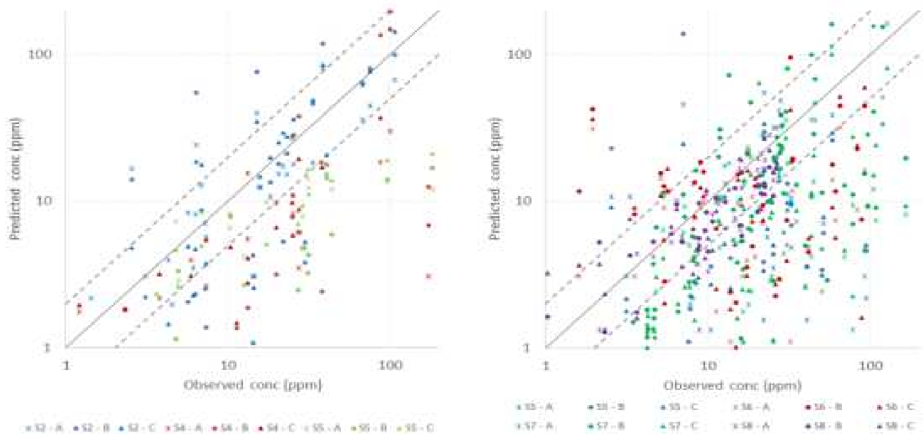
Sketch of Michestadt wind tunnel experiment showing the cross-section of the idealized urban mock-up.
Locations of all sources (left) and examples for source S2 (middle) and source S5 (right)
Sources (red dots), samplers for continuous releases (squares) and puff releases (circles)

Sketch of the Complex Urban Terrain Experiments (CUTE) – Source position (blue squares) and measurement locations (red dots) in the field test site (left) and in the wind tunnel (right)

MICHELSTADT SIMULATION RESULTS (1)

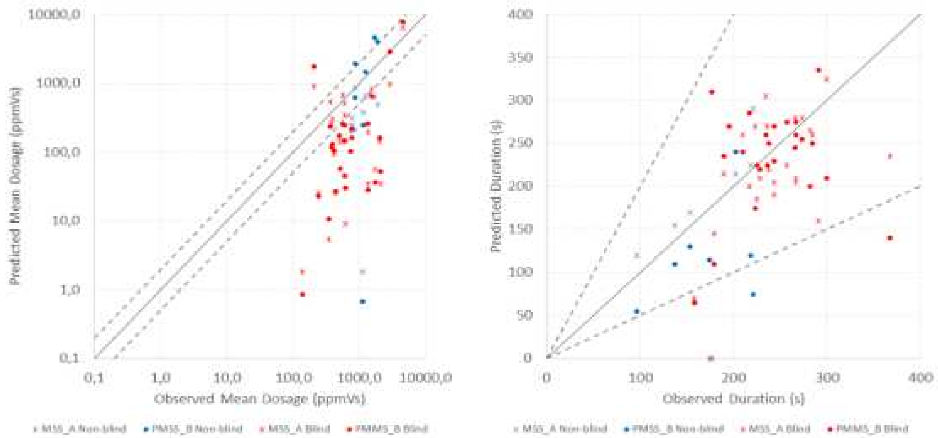
As (P)MSS was run by independent teams of modelers in three configurations, we investigated the sensitivity of (P)MSS results to the version of the model, physical input parameters and numerical parameters

Scatter plots of the predicted and measured mean concentrations for the CONTINUOUS RELEASES 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



- While there is a spread between predictions and observations, a large part of the data lies inside the factor of two area
- The agreement is better for a release taking place in an open square (S2) than in a street-canyon (S4 & S5), at a crossroad (S6 & S7) or inside a courtyard (S8)

Scatter plots of the predicted and measured mean dosages (left) and puff mean durations (right) for the PUFF RELEASES 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



- Given their complexity, the tests show fair enough results, since they timely capture the passage of the puff
- While the simulated mean dosages are under-predicted, quite accurate results are obtained above 10^3 ppmv s
- For the puff duration results, only few points are outside the factor of two area, well within the acceptance range

MICHELSTADT SIMULATION RESULTS (2)

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	MG	VG
Non-blind tests	MSS_A	0.68	4.35	0.46	1.50	4.52
	PMSS_B	0.11	2.15	0.64	1.10	3.94
	PMSS_C	0.73	4.02	0.51	1.96	3.87
Blind tests	MSS_A	0.64	2.07	0.41	2.07	19.15
	PMSS_B	0.36	9.01	0.45	1.71	8.50
	PMSS_C	0.67	11.55	0.38	1.91	9.53

- Regarding FB, the results are mostly acceptable according to the acceptance criterion $|FB| < 0.67$ (as FB > 0, 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 (NMSE is sensitive to far-outliers)
- Regarding FAC2, there is a satisfactory agreement of the model results within the criterion FAC2 > 0.30 applying to this statistical metric for both non-blind and blind tests

MICHELSTADT SIMULATION RESULTS (3)

Michelstadt PUFF RELEASE – 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	MG	VG
Mean dosage	Non-blind tests	MSS_A	1.53	1.04	0.01	14.01	>10^3
		PMSS_B	0.68	6.30	0.38	7.43	>10^3
	Blind tests	MSS_A	1.25	4.94	0.15	10.85	~10^3
		PMSS_B	1.17	3.84	0.08	13.05	~10^3
15-s peak concentration	Non-blind tests	MSS_A	1.25	3.05	0.13	6.25	~10^2
		PMSS_B	-0.40	1.55	0.38	2.78	~10^3
	Blind tests	MSS_A	0.65	2.81	0.31	4.71	~10^2
		PMSS_B	0.35	3.93	0.08	8.49	~10^3
Mean Duration	Non-blind tests	MSS_A	0.09	0.07	0.92	1.09	1.07
		PMSS_B	0.03	0.06	0.96	1.05	1.10
	Blind tests	MSS_A	0.11	0.18	0.86	0.94	1.02
		PMSS_B	0.35	0.27	0.86	1.51	1.35

- The mean dosage tends to be under-estimated with FB exceeding the acceptance limit 0.67 in most of the cases, while the scatter keeps inside the limit of NMSE < 6; FAC2 is acceptable only for PMSS_B in the non-blind case (this poor performance indicates that the model realization does not capture the statistics of this parameter, showing 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 15-s-mean peak conc. results are fair with FAC2 > 0.30 for one of the two models in non-blind and blind tests

CUTE SIMULATION RESULTS (1)

For CUTE, both field and wind tunnel continuous and puff releases experiments were carried out
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

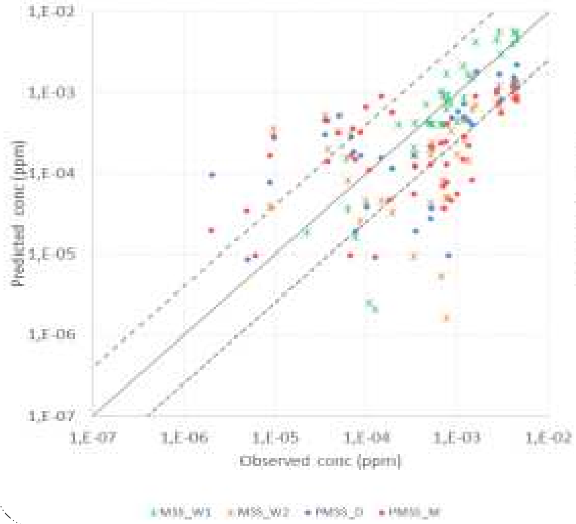
- Sensitivity to the turbulence intensity (two sets of turbulence data for computing the wind field driving PSPRAY)
  - ✓ Evaluating the turbulence intensity is complex due to the heterogeneities in the land-use (river, harbour and urban areas)
  - ✓ A stronger turbulence spreads and dilutes more the plume so that high concentration zones extend less downwind the source
  - ✓ Having information about the variances of the velocities, allows better reproducing the turbulence level in the domain

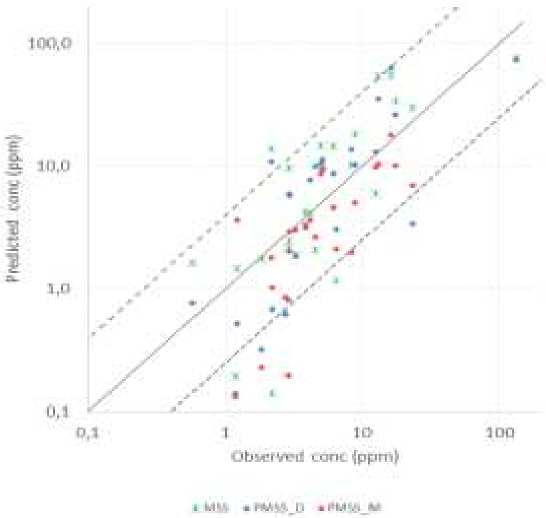
- Sensitivity to the wind direction profile (two simulations of the field experiment using MSS scalar version)
  - ✓ In MSS_W1, a wind profile was calculated with the only available measurement keeping the same direction in the vertical
  - ✓ In MSS_W2, data coming from a weather mast were used to build a wind profile with directions varying in the vertical
  - ✓ The different inputs make the plume deviating in slightly different directions, so that the affected areas are different

- Sensitivity to the flow model (computations 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 and expected to provide a more physically sound and reliable distribution of the tracer gas in a complex geometry
  - Still, in this case, PSPRAY concentration patterns were not drastically different when one wind model or the other was used

CUTE SIMULATION RESULTS (2)

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)

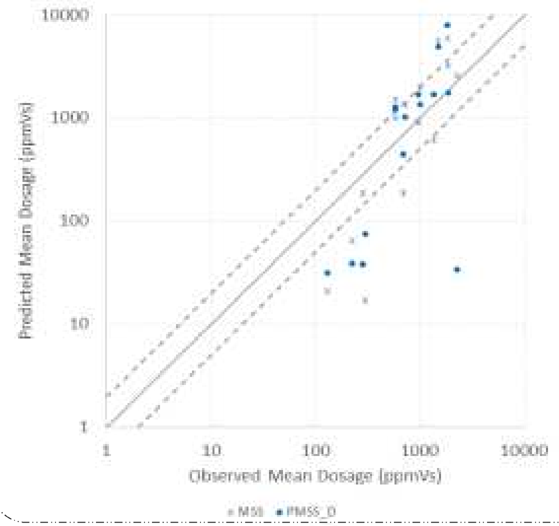


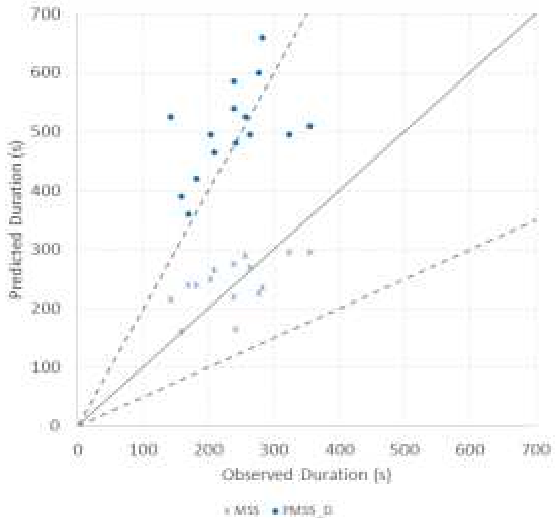


- The scatter plots show a tendency towards underestimation and a high degree of scatter for the weak concentrations while the highest concentrations are more satisfying
- For the field experiment, the best agreement is obtained for MSS_W2 (more relevant wind direction profile)
- For the wind-tunnel experiment, a fair agreement of the predictions with the measurements is obtained in all cases;

(P)MSS PERFORMANCES ARE SIMILAR TO THOSE IN MICHELSTADT WITH THE INFLUENCE OF SOME INPUT CONDITIONS ILLUSTRATED

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)





- 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 mean dosages ranging between 10^2 and 10^3 ppmv s, whereas the highest observed values are well reproduced
- PMSS_D run generates a longer duration than observed while the durations predicted by MSS fits well the observed values

THE RESULTS ARE IN LINE WITH THE FINDINGS IN MICHELSTADT

CUTE SIMULATION RESULTS (3)

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

Statistical metrics			FB	NMSE	FAC2	MG	VG
Field Experiment Cont. release	Mean conc.	PMSS_D	0.03	5.59	0.35	1.03	21.18
		PMSS_M	-1.07	23.01	0.32	2.58	63.45
		MSS_W1	0.96	11.37	0.30	1.89	31.17
		MSS_W2	-0.30	3.01	0.57	1.27	3.98
Wind tunnel Cont. release	Mean conc.	PMSS_D	-0.34	1.75	0.38	1.38	10.13
		PMSS_M	-0.07	2.09	0.47	2.31	9.91
		MSS	-0.21	2.27	0.35	1.15	7.53
Wind tunnel Puff releases	Mean dosage	PMSS_D	-0.47	2.63	0.38	1.46	9.76
		MSS	-0.53	1.67	0.44	1.19	4.14
	15-s peak conc.	PMSS_D	0.77	2.71	0.38	4.21	46.88
		MSS	-0.17	0.44	0.50	0.94	1.64
	Mean duration	PMSS_D	-0.72	0.64	0.27	0.46	1.91
		MSS	-0.03	0.04	1.00	0.96	1.05

- For the field experiment continuous release, the metrics show a variability among the configurations of (P)MSS (half of the results with FB and NMSE larger than the acceptance limits with, in contrast, FAC2 greater than 0.3) (results obtained with the momentum and diagnostic flow models perform equivalently well in terms of FAC2 while concentrations are no more systematically under-predicted when using the momentum flow model)
- For the wind tunnel continuous release, the metrics are better than for the field experiment and all configurations meet the acceptance limits (FB and FAC2 results with PMSS_M improve with respect to results using PMSS_D)
- For the wind tunnel puff releases, the predicted mean dosage, mean peak concentration averaged over 15 s and the mean duration demonstrate predominantly fair performance of the model in both configurations.

CONCLUSIONS

- The validation of (P)MSS has been performed with an increase in the complexity from mock-up scale to full scale, from stationary plumes to puff releases, and from a diagnostic to a momentum equation solving flow model
  - ✓ In most cases, (P)MSS performances are within the acceptance criteria defined for modelling in built-up areas
  - ✓ (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 model
  - ✓ (P)MSS validation addresses the capability and reliability of LPDM in the conditions of an emergency in built-up environment

- 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 and the continuous meteorological monitoring of sensitive industrial sites is recommended

- In real life, first responders and stakeholders are still provided with the results of simplified models, definitely not appropriate in built-up areas, and possibly leading to not effective or even misleading response procedures!
  On the contrary, (P)MSS turns out to be a valuable support to the emergency preparedness and response, what is a real benefit for the atmospheric dispersion field of research!

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Thank you for your attention.

Questions ?

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