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## EXTENDED ABSTRACT

# *Wind tunnel and in-field experimental validation of the recent developments on multi-scale turbulence in the PMSS modelling system*

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**Abstract**: Atmospheric releases can pose a serious risk to human health and the environment. 3D flow and dispersion models realistically account for environmental characteristics, particularly in built environments. They are essential for reliably estimating the consequences of air releases provided they are rigorously validated, such as PMSS. This paper presents simulations performed with the PSPRAY dispersion model using data from the PSWIFT flow model in its current and previous versions. Satistical indicators related to concentrations show a significant improvement thanks to better modelling of both background and obstacle-induced turbulence. Continuous progress of 3D models is crucial to promote their use in high-stakes situations, such as facility licensing or emergency management.

***Key words:*** *PMSS modelling system, experimental validation, Prairie Grass, Michelstadt, CUTE, COST ES1006.*

## INTRODUCTION

Usually, impact and risk studies rely on Gaussian plume or puff dispersion models. However, these models are very limited in accounting for the complexity of the real environment. Lagrangian or Eulerian dispersion models using 3D wind data offer a promising alternative to simulate the distribution of substances released into the air and, ultimately, their consequences on the environment and human health. For these models to emerge, it is crucial that they are rigorously validated based on experimental data.

The PMSS (Parallel-Micro-SWIFT-SPRAY) system combines the 3D diagnostic flow model PSWIFT and the 3D Lagrangian particle dispersion model PSPRAY. Simulations are performed from the mesoscale to the microscale, where buildings are explicitly represented (Tinarelli et al., 2013; Armand et al., 2021). PMSS can handle huge urban areas thanks to highly efficient parallelization (Oldrini et al., 2019; 2021). It aims to provide results close to the accuracy of CFD models with significantly faster computation times.

Over the past years, the PSWIFT model has undergone significant improvements, including adjustment of the flow to respect mass conservation by accounting for topography and obstacles, estimation of turbulent quantities according to Monin-Obukhov theory, and calculation of velocity fluctuations due to background and obstacle-generated turbulence. These developments have been extensively validated and incorporated into PSWIFT version 2.3.1. They were partly presented at the Harmo'22 conference (Ribstein et al., 2024), and further details are given at the Harmo'23 conference in the companion paper (Ribstein et al., 2025).

The present paper focuses on dispersion results obtained from the PSPRAY 4.0.2 model using turbulent flows simulated by PSWIFT 2.3.0 or 2.3.1. Three major experimental campaigns are studied successively: the historical field tests of the Prairie Grass Project, the wind tunnel tests at Hamburg University on the Michelstadt urban mock-up, and the CUTE field campaign in the city of Hamburg.

## PRAIRIE GRASS EXPERIMENTS

### Description of the project

The “Prairie Grass Project” was conducted on a flat prairie in north-central Nebraska (USA), under various weather conditions in July and August 1956. In each of the 70 experiments, $SO_2$ was released continuously for 10 minutes from a source located near the ground. The sensors were distributed in circular arcs centered on the release, and measured concentrations averaged over 10 minutes, 1.5 m above the ground.

Concentration and meteorological measurement data, as well as release rates, can be found in Barad (1958). Based on the measured wind speeds and temperatures, stability conditions were deduced from the literature (Horst *et al.*, 1979). Among the experiments, four were selected to evaluate the performance of the PMSS model in various meteorological situations. Their characteristics are summarized in **Table 1**.

**Table 1.** The four Prairie Grass experiments considered to validate PMSS modelling system

| Experiment | Date and local time | Temp. (°C) at 2 m | Net rad. ($W/m^2$) | u* (m/s) | LMO (m) | Pasquill class |
|---|---|---|---|---|---|---|
| 14 | 7/22/1956 at 22:05 | 16.25 | -41.84 | 0.08 | 7.6 | F |
| 17 | 7/23/1956 at 20:05 | 27.44 | -46.02 | 0.20 | 50 | E |
| 24 | 7/29/1956 at 23:05 | 21.89 | -48.12 | 0.36 | 217 | D |
| 57 | 8/25/1956 at 17:35 | 34.11 | -54.39 | 0.44 | -189 | D |

**PMSS parameterization of the Prairie Grass experiments**

PSWIFT and PSPRAY simulation domains were chosen identically. Horizontally, they were a rectangle of 400 x 220 cells at a resolution of 5 m with a vertical grid of eight levels from the ground to around 50 m.

The terrain was flat with a roughness length $z_0$ equal to 0.006 m. The friction velocity u* and the Monin-Obukhov length LMO were evaluated with Businger-Dyer formulae. A correspondence was used between the Pasquill class and the mixing height $H_{mix}$, and different values of $H_{mix}$ were tested for classes E and F.

The wind speed and temperature profiles measured near the source at the start of the release were used as PSWIFT input data to simulate steady-state flow. We investigated the dispersion of a 30-minute release at the flow rate associated with each experiment. Concentrations were averaged over the last 10 minutes.

**PMSS validation against Prairie Grass experiments**

Simulations were performed for experiments 57 (neutral atmosphere), 24 (neutral), 17 (stable), and 14 (very stable). For the sake of brevity, only a few results are reported for the experiments 57 and 17.

***Evaluation of PMSS in experiment 57 (Pasquill class D)***

**Table 2** presents the seven statistical indicators proposed by Chang & Hanna (2004) calculated for all pairs ($C_{obs}$, $C_{mod}$) in experiment 57. The new version of PSWIFT improves all the indicators, especially FAC2. The systematic bias of the model is also reduced (FB and MG). It should be noted that FAC2 and FAC5 depend on the chosen threshold value for the concentration. With a threshold of 1.0 $mg/m^3$ instead of 0.1 $mg/m^3$ used in the table, FAC2 increases from 0.72 to 0.81, and GV decreases from 10.7 to 2.74.

**Table 2.** Statistical indicators for all pairs ($C_{obs}$, $C_{mod}$) in experiment 57
(FAC2 & FAC5: factor of 2 & 5, FB: fractional bias, NMSE: normalised mean square error, GM: geometric mean, GV: geometric variance, R: correlation coefficient)

| PSWIFT version | FAC2 | FAC5 | FB | NMSE | GM | GV | R |
|---|---|---|---|---|---|---|---|
| Previous | 0.28 | 0.68 | 0.75 | 0.39 | 0.19 | 596 | 0.91 |
| Recent | 0.72 | 0.84 | 0.46 | 0.21 | 2.97 | 10.7 | 0.95 |

**Figure 1** compares the concentrations simulated by PMSS using PSWIFT 2.3.0 or 2.3.1 with observations at four distances from the source. The concentrations are presented along the arc $R\cdot(\theta - \theta_{dir})$, where R is the distance from the source and $\theta_{dir}$ the wind direction in the PSWIFT calculations. $\theta_{dir}$ centers the observations on 0 for distances R = 50, 100, 200, and 400 m. The figure clearly states that the concentration maximum and plume width are better represented by PMSS with the most recent version of PSWIFT.

***Evaluation of PMSS in experiment 17 (Pasquill class E)***

**Table 3** presents the seven statistical indicators proposed by Chang & Hanna (2004) calculated for all pairs ($C_{obs}$, $C_{mod}$) in experiment 17 considering two values of $H_{mix}$. The most recent version of PSWIFT with $H_{mix}$ = 200 m slightly improves FAC2, but deteriorates GV. By choosing $H_{mix}$ = 100 m, the statistical indicators are all equivalent or better with PSWIFT 2.3.1 compared to PSWIFT 2.3.0.

**Table 3.** Statistical indicators for all pairs ($C_{obs}$, $C_{mod}$) in experiment 17

| PSWIFT version | FAC2 | FAC5 | FB | NMSE | GM | GV | R |
|---|---|---|---|---|---|---|---|
| Previous / $H_{mix}$ = 200 m | 0.59 | 0.86 | 0.38 | 0.09 | 0.33 | 15.0 | 0.96 |
| Recent / $H_{mix}$ = 200 m | 0.63 | 0.85 | 0.04 | 0.20 | 0.33 | 55.1 | 0.91 |
| Recent / $H_{mix}$ = 100 m | 0.73 | 0.86 | 0.14 | 0.10 | 0.37 | 24.1 | 0.94 |

**Figure 2** compares the concentrations simulated by PMSS using PSWIFT 2.3.0 or 2.3.1 with observations at four distances from the source. It is important to note that the results were calculated with $H_{mix}$ = 200 m when PSWIFT 2.3.0 was used and $H_{mix}$ = 100 m with PSWIFT 2.3.1. For R ≥ 200 m, the figure shows that the concentrations simulated by PMSS with PSWIFT 2.3.1 are much closer to the observations (with little difference due to the value of $H_{mix}$). For R ≤ 100 m, the most recent version of PSWIFT with $H_{mix}$ = 100 m leads to much lower dispersion, thus higher maximum concentrations and finer plumes (as expected).

| With PSWIFT previous version ($H_{mix}$ = 1,000 m) | With PSWIFT new version ($H_{mix}$ = 1,000 m) | With PSWIFT previous version ($H_{mix}$ = 200 m) | With PSWIFT new version ($H_{mix}$ = 100 m) |
|---|---|---|---|

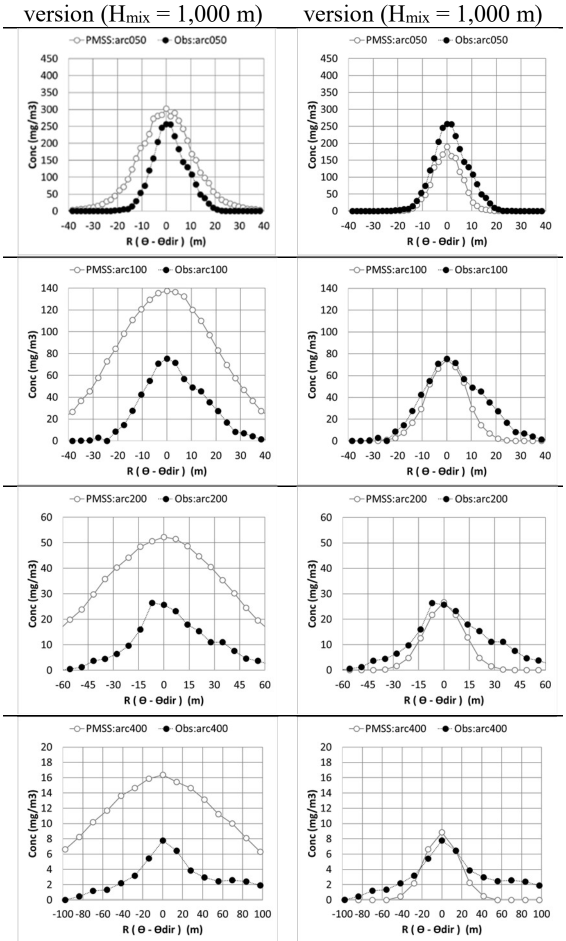


**Figure 1.** Observed and simulated concentrations using PSWIFT 2.3.0 (left) and PSWIFT 2.3.1 (right) in experiment 57

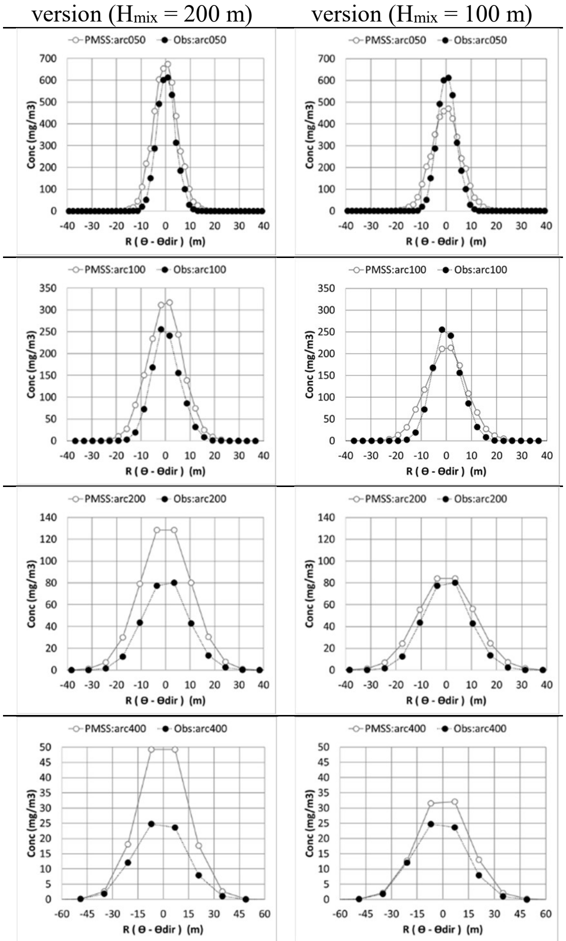


**Figure 2.** Observed and simulated concentrations using PSWIFT 2.3.0 (left) and PSWIFT 2.3.1 (right) in experiment 17

### Conclusions on PMSS validation against Prairie Grass Project

The PMSS modelling system using PSWIFT 2.3.1 versus PSWIFT 2.3.0 improves the agreement between PSPRAY simulated concentrations and observations for all experiments. In a neutral atmosphere, PSWIFT 2.3.1 reduces excessive horizontal turbulence and, conversely, increases the insufficient vertical turbulence of PSWIFT 2.3.0. In a stable atmosphere, PSWIFT 2.3.1 also enhances the too weak vertical turbulence of PSWIFT 2.3.0. To model a stable to very stable atmosphere, the mixing height $H_{mix}$ has a strong influence on the turbulence profiles parameterized by Hanna *et al.* (1982). With the most recent version of PSWIFT, good results are obtained with $H_{mix}$ =100 m in a stable situation and 15 m in a very stable situation.

## MICHELSTADT EXPERIMENTS

### General description

The "Michelstadt" experimental campaign was conducted in the Wotan wind tunnel (Fischer *et al.*, 2010) at the Environmental Laboratory of Hamburg University as part of COST Action ES1006 (COST, 2015). Michelstadt represented the mock-up of an idealized Central European urban district at a scale of 1:255. Transposed to real conditions, the wind speed was 6 m/s at a height of 100 m above the ground and building heights were 15, 18 or 24 m. The mock-up had two orientations with respect to the flow in the wind tunnel.

The wind speed was measured on one profile upstream of the mock-up and on 40 profiles within the mock-up. Ethane was emitted continuously or for a short time from six ground-level sources in an open square, a courtyard, and narrow or wide streets perpendicular or parallel to the wind tunnel flow. The concentrations were measured at 7.5 m above the ground at locations adapted to the area affected by each release.

### PMSS parameterization of the Michelstadt experiments

PSWIFT and PSPRAY simulation domains were a horizontal rectangle of 901 x 601 cells at a resolution of 1.5 m with a vertical grid of uniformly distributed levels from 1 to 28 m, then 11 levels up to 200 m.

The roughness length $z_0$ was equivalent to 3 m at full scale. Neutral stability (Pasquill class D) was imposed, combined with a mixing height $H_{mix}$ of 1,000 m. u* and LMO were evaluated with Businger-Dyer formulae. The velocity standard deviations $\sigma_H$ and $\sigma_z$ and the Lagrangian times $\tau_H$ and $\tau_z$ were evaluated based on the Hanna profiles for background turbulence and a mixing length for obstacle-induced turbulence.

The wind speed and temperature profiles measured upstream of the mock-up were used as PSWIFT input. We considered a one-hour release with a flow rate of 0.5 kg/s. Concentrations were averaged over one hour.

### PMSS validation against Michelstadt experiments

One orientation of the mock-up and continuous releases from three sources were selected to evaluate the performance of PMSS. For the sake of brevity, only a few results are given for sources S2 and S4.

#### *Evaluation of PMSS for source S2 located in an open square*

**Table 4** shows the seven statistical indicators proposed by Chang & Hanna (2004), calculated for all pairs ($C_{obs}$, $C_{mod}$) obtained for the release from S2. The most recent version of PSWIFT improves all indicators.

**Table 4.** Statistical indicators for all pairs ($C_{obs}$, $C_{mod}$) for the release from source S2

| PSWIFT version | FAC2 | FAC5 | FB | NMSE | GM | GV | R |
|---|---|---|---|---|---|---|---|
| Previous | 0.34 | 0.62 | 1.48 | 7.55 | 3.70 | 17.5 | 0.91 |
| Recent | 0.50 | 0.94 | 1.07 | 2.34 | 2.62 | 4.59 | 0.93 |

**Figure 3** compares the cross-section of the concentration field at z = 7.5 m above the ground simulated by PMSS using PSWIFT 2.3.1 versus 2.3.0. The colored squares correspond to the observed concentrations. The most recent version of PSWIFT reduces the velocity standard deviations and the turbulence generated by the obstacles, resulting in less horizontal and vertical diffusion. Thus, steeper concentration gradients are obtained in streets transverse to the plume axis in better agreement with observations.

#### *Evaluation of PMSS for source S4 located in a narrow street parallel to the wind direction*

**Table 5** shows the seven statistical indicators proposed by Chang & Hanna (2004), calculated for all pairs ($C_{obs}$, $C_{mod}$) obtained for the release from S4. The most recent version of PSWIFT slightly improves some of the indicators, in particular FAC5, but deteriorates MG, VG, and R. The release from S4 located into a confined street appears much more complex to simulate than the release from S2 located in an open place.

**Table 5.** Statistical indicators for all pairs ($C_{obs}$, $C_{mod}$) for the release from source S4

| PSWIFT version | FAC2 | FAC5 | FB | NMSE | GM | GV | R |
|---|---|---|---|---|---|---|---|
| Previous | 0.48 | 0.74 | 1.22 | 4.72 | 2.33 | 9.77 | 0.72 |
| Recent | 0.43 | 0.81 | 1.03 | 2.42 | 3.45 | 20.1 | 0.66 |

**Figure 4** compares the cross-section of the concentration field at z = 7.5 m above the ground simulated by PMSS using PSWIFT 2.3.1 versus 2.3.0. The colored squares correspond to the observed concentrations. The reduced velocity standard deviations and turbulence from obstacles in PSWIFT 2.3.1 generate a more compact plume and larger concentration gradients in streets perpendicular to the prevailing horizontal wind.

### Conclusions on PMSS validation against Michelstadt experiments

PSWIFT 2.3.1 decreases turbulence levels compared to PSWIFT 2.3.0, which overestimates it. Above the urban canopy, vertical turbulence is slightly too high and horizontal turbulence is insufficient. In the urban canopy, the mean standard deviation of horizontal velocity is similar to observations. However, obstacle-induced turbulence is added to background turbulence, while measurements suggest a turbulence decrease in the urban canopy. Reduced turbulence induces a more concentrated simulated plume, in better agreement with measurements, particularly vertical profiles for releases over an open space. The reduction in obstacle-induced turbulence induces lower vertical plume spreading. However, PMSS appears to underestimate high concentrations and a notable proportion of concentrations are more than twice lower than observations.

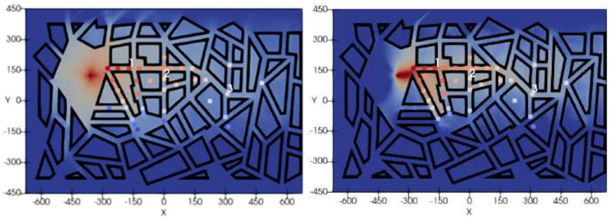

**Figure 3.** Cross-section of the simulated concentration field using PSWIFT 2.3.0 (left) and PSWIFT 2.3.1 (right) and observations for the release from source S2

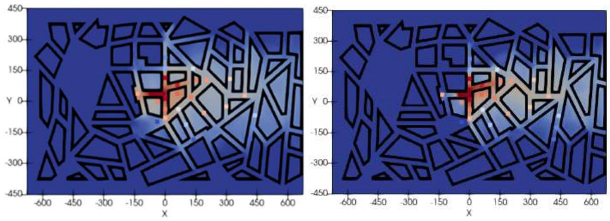

**Figure 4.** Cross-section of the simulated concentration field using PSWIFT 2.3.0 (left) and PSWIFT 2.3.1 (right) and observations for the release from source S4

## COMPLEX URBAN TEST EXPERIMENTS (CUTE)

### General description

The CUTE experimental campaign was conducted to replicate dispersion in the center of Hamburg as part of COST Action ES1006 (COST, 2015). The study area was densely built-up with 25–35 m high buildings. Both wind tunnel and field tests were performed. A 300 m high mast located 8.5 km from the release point was equipped with meteorological instruments. During the field test, a strong southwest wind was observed. The mean speed and direction were 8.9 m/s and 219° at 175 m above ground level. Atmosphere was neutral.

Tracer gas $SF_6$ was released continuously from a boat for 45 minutes at a constant flow rate of 2 g/s. Twenty measuring points were arranged over three arcs with nine bags filled consecutively for 10 minutes at each point. To improve temporal resolution, the bags were filled overlappingly at the points close to the source.

### PMSS parameterization of CUTE

PSWIFT and PSPRAY simulation domains were a horizontal rectangle of 941 x 921 cells at a resolution of 3 m with a vertical grid of uniformly distributed levels from 1 to 28 m, then 14 levels up to 500 m. The topography of the area was extracted from 30 m data obtained from NASA SRTM and interpolated to 3 m.

The roughness length $z_0$ was equal to 0.6 m. Neutral stability (Pasquill class D) was imposed in combination with a mixing height $H_{mix}$ of 1,000 m. u* and LMO were evaluated using Businger-Dyer formulae. The velocity standard deviations $\sigma_H$ and $\sigma_z$ and the Lagrangian times $\tau_H$ and $\tau_z$ were evaluated based on the Hanna profiles for the background turbulence and on a mixing length for obstacle-induced turbulence.

A power-law wind profile was used as PSWIFT input data. While the wind direction measured at 175 m was 219°, the simulation was performed with a slight plume offset and a wind direction of 211.4° to better fit calculated and observed concentrations. Concentrations were averaged over ten minutes.

### PMSS validation against CUTE

The field test 1 was selected to evaluate the performance of the PMSS modeling system. **Table 6** shows the seven statistical indicators proposed by Chang & Hanna (2004), calculated for all pairs ($C_{obs}$, $C_{mod}$) obtained for CUTE field test 1. The most recent version of PSWIFT clearly improves all indicators.

**Table 6.** Statistical indicators for all pairs ($C_{obs}$, $C_{mod}$) for CUTE field test 1

| PSWIFT version | FAC2 | FAC5 | FB | NMSE | GM | GV | R |
|---|---|---|---|---|---|---|---|
| Previous | 0.22 | 0.48 | 1.47 | 4.55 | 6.45 | 57.3 | 0.93 |
| Recent | 0.70 | 1.00 | 0.14 | 0.19 | 1.40 | 1.88 | 0.95 |

**Figure 4** compares the scatter plot of the simulated concentrations versus the observed concentrations using PSWIFT 2.3.0 or PSWIFT 2.3.1. The figure illustrates the significant improvement in the FAC2 and FAC5 ratios as the decrease of the non-systematic errors estimated by NMSE and GV.

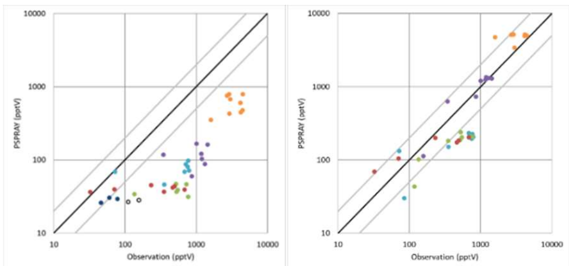

**Figure 5.** Scatter plot of simulated versus observed concentrations using PSWIFT 2.3.0 (left) and PSWIFT 2.3.1 (right) in CUTE field test 1

## GENERAL CONCLUSION AND PERSPECTIVES

The simulations presented in this paper show significant and almost systematic improvement in the results of the PSPRAY 4.0.2 dispersion model, using wind data from PSWIFT 2.3.1 versus 2.3.0. This is explained by a much better assessment of both background and obstacle-induced turbulence. However, progress is possible, particularly with regard to turbulence in urban canyons, which remains overestimated.

Improved 3D models not only brings satisfaction to the modeler, but also contributes to the credibility and growing use of models such as PMSS in high-stakes applications, such as the issuance of operating licenses for industrial plants or the assessment of the consequences of noxious releases in case of emergency.

## REFERENCES


Armand, P., O. Oldrini, C. Duchenne & S. Perdriel (2021) Topical 3D modelling and simulation of air dispersion hazards as a new paradigm to support emergency preparedness and response. *Environmental Modelling and Software*, 143, 105129.

Barad M.L. (1958). Project Prairie Grass, a field program in diffusion. *Geopys. Res. Papers*, vol. I., U.S. Cambridge Research Center.

Chang J.C. & Hanna S.R. (2004) Air quality model performance evaluation. Meteorol. Atmos. Phys., 87, 167-196.

COST ES1006 (2015) Model Evaluation Case-Studies. COST Action ES1006, April 2015, COST Office, ISBN: 987-3-9817334-2-6.

Fischer R., Bastigkeit I., Leitl B., Schatzmann M. (2010) Generation of spatio-temporally high resolved datasets for the validation of LES-models simulating flow and dispersion phenomena within the lower atmospheric boundary layer. *Proc. of the 5th Int. Symp. on Computational Wind Engineering*, Chapel Hill, North Carolina, USA.

Golder D. (1972). Relations among stability parameters in the surface layer. *Boundary-Layer Meteorol*., 3: 56.

Hanna S. R., Briggs G. A., Hosker R. P. (1982) Handbook on atmospheric diffusion. Ed. by J. S. Smith, U.S. Department of Energy.

Horst T. W., Doran J. C., Nickola P. W. (1979). Evaluation of empirical atmospheric diffusion data. Battelle Pacific Northwest Lab.

Oldrini, O., P. Armand, C. Duchenne & S. Perdriel (2019) Parallelization performances of PMSS flow and dispersion modeling system over a huge urban area. *Atmosphere*, 10 (7), 404.

Oldrini, O., P. Armand, C. Duchenne, S. Perdriel & M. Nibart (2021) Accelerated time and high-resolution 3D modeling of the flow and dispersion of noxious substances over a gigantic urban area – EMERGENCIES project. *Atmosphere*, 12 (5), 640-654.

Ribstein, B., Armand, P., Duchenne, C., Yang, X., David, V., Nibart, M., Albergel, A. (2024) Proposals for improving the multi-scale consideration of turbulence in the PMSS diagnostic modelling system. *Proc. of the 22nd Int. Conf. on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes*. 10-14 June 2024, Pärnu, Estonia.

Ribstein, B., Nibart, M., Albergel, A., Armand, P., Duchenne, C. (2025) Improvements in local-scale turbulence modelling in the PMSS flow model with applications to natural and built environments. *Proc. of the 23rd Int. Conf. on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes*. 15-19 September 2025, Hamburg, Germany.

Tinarelli, G., L. Mortarini, S. Trini Castelli, G. Carlino, J. Moussafir, C. Olry, P. Armand & D. Anfossi (2013) Review and validation of Micro-SPRAY, a Lagrangian particle model of turbulent dispersion. In: *Lagrangian Modeling of the Atmosphere*, Geophysical Monograph, American Geophysical Union, 200, 311-327, May 2013, Washington DC.