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**COMPARISON OF DIFFERENT DISPERSION MODELLING APPROACHES IN THE
SURROUNDINGS OF LEGEROVA STREET CANYON IN THE CITY OF PRAGUE**

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Abstract: The dispersion of particulate matter (PM₁₀) was studied in the vicinity of one of the main boulevards connecting the north and south of Prague, Czech Republic. A wintertime episode characterized by a strong temperature inversion was selected to perform the intercomparison of three models with varying degree of complexity: the Gaussian dispersion model ATEM, the Graz Lagrangian model (GRAL), and the Large-eddy simulation model PALM. Results highlight the importance of implementing a thorough validation of the models including a temporal and spatial analysis of the outputs. While statistical metrics indicated that ATEM could reasonably predict measurements in the domain, further examination led to conclude that relevant information on the dispersion of pollutants along street canyons was overlooked. GRAL, on the other hand, provided a better representation of circulation patterns in built-up areas, but generally overpredicted concentrations. Although PALM offered the most accurate results, high-resolution input data and high computational costs may limit the practical application of the model.

Key words: *urban pollution, dispersion modelling, particulate matter, wintertime inversion, low-cost sensors.*

INTRODUCTION

The complexity of urban modelling has pushed forward the development of advanced algorithms to be able to simulate the effect of dense street networks, high-rise buildings, and challenging meteorological conditions. Gaussian and Lagrangian models have been widely used and validated for different purposes, while more sophisticated CFD models are still under development, but promise advantages capturing atmospheric processes within densely built and complex urban areas. Street canyons are of special concern due to the confinement of pollutants and channelization effect. Hence, it is essential to use the right tools to predict the turbulent flow inside the canyon. In this context, it is still unclear the level of complexity required to obtain reasonable estimations balanced with an appropriate computational effort.

The north-south oriented one-way boulevards of Sokolská and Legerova in Prague are loaded with a daily traffic intensity over 35 thousands cars. The surrounding area is characterized by compact mid-rise buildings, which favours a poor circulation of air, strengthening the stagnation of air pollutants. Episodes with higher concentrations of PM₁₀ are more intensive during inversion situations typical for wintertime due to higher emissions and low wind speeds. Nevertheless, there is limited research on the simulation and accurate prediction of dispersion features during such stable conditions. Consequently, this research aimed to: 1) compare selected models against air quality measurements; 2) analyse the spatial variability of model outputs; and 3) evaluate the suitability of models for air quality assessment.

METHODS

Experiment design

This study was focused on the temperature inversion formed between 13 and 15 February 2023. The modelling domain covered an extension of 1,200 m × 1,600 m close to the city centre. A dedicated campaign was carried out to collect relevant data for model input and validation. Pollutant concentrations in the area were measured using a network of low-cost air quality sensor (LCS) units, supplemented by permanent stations operated by the Czech Hydrometeorological Institute (CHMI). Most LCSs were located directly in the streets with the highest traffic pollution load: three were placed along Sokolská Street (S10, S11, and S12), two in Rumunská Street (S13 and S20), and four along Legerova Street (S2, S5, S14, and S15). Others were installed in ‘background areas’, such as the PVK garden (S19), and a School Courtyard (S7 and S9). The remaining two were located at considerable distances from the pollution hotspots and at increased heights: in Karlov (S3) and at the Hotel Le Palais (S16). Some sensors were put in pairs at different heights on the facades of the buildings (Fig. 1). A detailed description of the equipment implemented, collected data and post-processing are available in Bauerová et al. (2024).

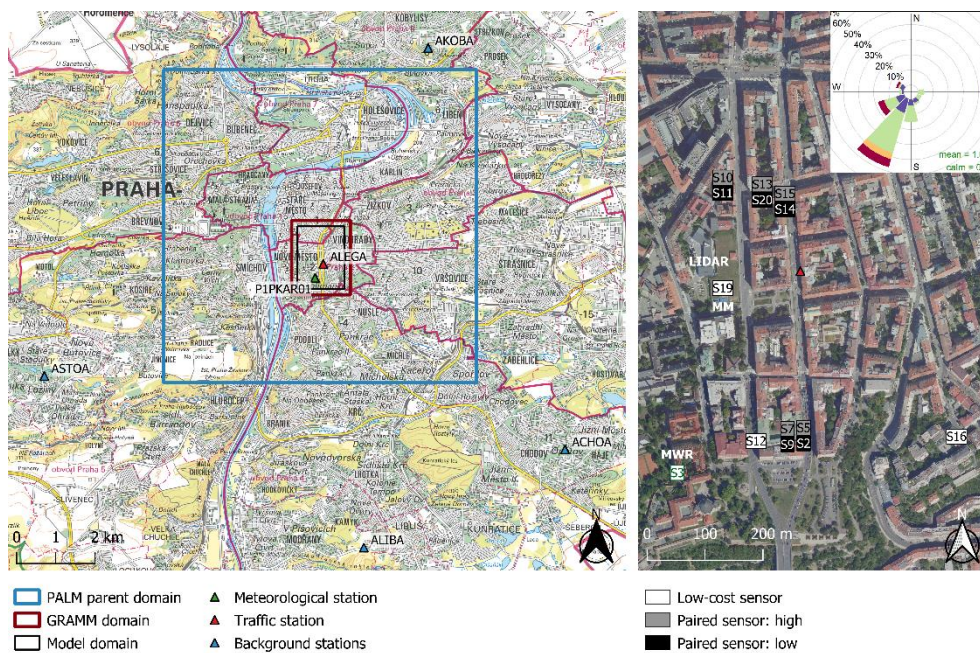


Figure 1. (a) Extent of the domain common for all models (black), location of meteorological and air quality stations. (b) Location of low-cost sensors (LCS), Doppler LIDAR, meteorological mast (MM) and microwave radiometer (MWR). Wind rose of measured meteorology at Karlov station (green) for Feb. 13–15, 2023.

Description of model configuration and input

GRAL system is coupled with a non-hydrostatic mesoscale model (GRAMM) and a prognostic microscale module to handle the effects of obstacles. Dispersion simulations were computed in transient mode, in which released particles remain in the model area and are further tracked in subsequent weather situations. PALM was configured in two nested domains (‘parent’ and ‘child/model’ domain) to simulate all mixing layer processes properly, with the full 3D geometry that allows modelling objects such as bridges and multilevel crossroads. Detailed model settings can be found in Patiño et al. (2024) and Resler et al. (2024).

ATEM and GRAL meteorological input is composed of a time series of wind speed, wind direction, and temperature gradient obtained from measurements at Karlov station and MWR profiles. On the other hand, the meteorological data needed to run PALM include the detailed structure of all wind components, potential temperature, air moisture, pressure and incoming short-wave and long-wave radiation. Thus, PALM is typically driven by a mesoscale Numerical Weather Prediction model (NWP) simulation, in this case, ALADIN model. Further discussion on the sensitivity of microscale simulations to meteorological boundary conditions is found in Resler et al. (2024).

The initial and boundary conditions of pollutants were calculated as the median value of measurements from background air quality stations in the surroundings of the PALM parent domain. ATEM and GRAL do not allow the inclusion of these data as input, therefore, computed values were post-processed to add boundary concentrations. PALM used the aforementioned conditions complemented by CAMS model based vertical profiles scaled to observed near-surface value.

The emission sources in the domain were constituted by mobile sources (road traffic, railways, river ships) and residential heating. Road traffic accounted for 90.7% of PM₁₀ emissions. A complete report on the acquisition of data is available in Resler et al. (2024).

A square grid of computational points with 24 m spacing was implemented for ATEM due to the resulting amount of grid cells and computational demand (the model allows only for the calculation of annual time series). Along the major roads in the domain, a 20 m buffer zone with a 6 m spacing was used. In order to capture the complexity of the processes of dispersion and mixing within the street canyon, it was decided to run GRAL and PALM in a resolution of 2 m horizontally and vertically.

RESULTS AND DISCUSSION

The model performance was judged using common statistical metrics described by Chang and Hanna (2004), Legates and McCabe (2012), and Willmott et al. (2011). A perfect model would have FAC2, r, COE, IOA = 1, and FB, NMSE, RMSE = 0. The type of environment that characterized the location of the measurement points was used to classify the results, i.e., background, roof, and traffic. As a reference, all statistics were calculated for boundary concentrations as well.

Table 1. Statistical performance metrics. Values in bold are within the recommended range according to Chang and Hanna (2004). The best resulting statistics for each group are highlighted in blue.

Type*	Model	n	$\overline{C_{obs}}$	$\overline{C_{mod}}$	FAC2	r	COE	IOA	FB	NMSE	RMSE
Back-ground	ATEM			29.19	0.95	0.50	-0.50	0.25	0.27	0.15	12.78
	GRAL	216	38.31	30.82	0.87	0.21	-0.92	0.04	0.22	0.25	17.10
	PALM			25.57	0.86	0.60	-0.85	0.07	0.40	0.23	14.98
	Boundary			24.51	0.85	0.61	-1.01	-0.01	0.44	0.27	15.83
Roof	ATEM			27.85	0.99	0.56	0.03	0.51	0.10	0.09	8.56
	GRAL	144	30.72	27.37	0.98	0.51	-0.14	0.43	0.12	0.12	9.93
	PALM			26.12	0.94	0.51	-0.10	0.45	0.16	0.12	9.64
	Boundary			24.51	0.97	0.53	-0.21	0.40	0.22	0.14	10.22
Traffic	ATEM			30.86	0.89	0.56	-0.62	0.19	0.37	0.22	17.23
	GRAL	720	44.64	62.55	0.76	0.23	-2.15	-0.37	-0.33	0.67	43.38
	PALM			41.79	0.88	0.24	-0.63	0.18	0.07	0.18	18.28
	Boundary			24.51	0.63	0.60	-1.31	-0.13	0.58	0.46	22.38

*The stations were grouped as follows: S19 and S9+S7 (background); S3 and S16 (roof); ALEGA station, S12, S11+S10, S20+S13, S14+S15, and S2+S5 (traffic). Sensor pairs are denoted by a plus sign and the lower one is indicated first.

According to the values indicated in Table 1, the models fulfilled the suggested criteria for FAC2 and NMSE, which reflect systematic and random errors. Models were negatively biased and generally brought improvement over the reference boundary, except for GRAL at the traffic locations. ATEM and GRAL would appear to have a reasonable predicting capability, especially considering the LCSs located in background locations and roofs. PALM exhibited the best performance for traffic locations, although the correlation coefficient was exceptionally low because the model was driven by the outputs from ALADIN simulation rather than observed meteorology, and thus it might not reproduce correctly the time variability of measured data. On the other hand, criteria such as COE and IOA revealed that the models were less effective than the observed mean in predicting the observed values due to the large deviation of modelled values compared to measurements, as can be seen from the calculated RMSE.

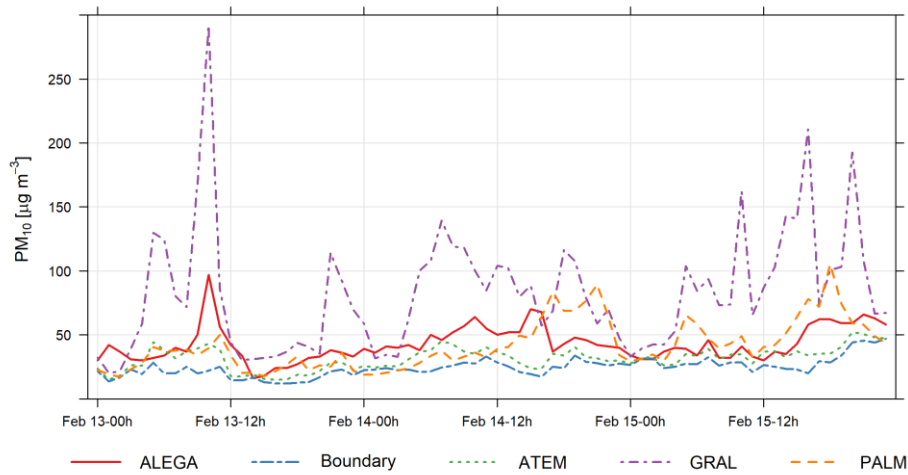


Figure 2. Time series of PM₁₀ concentrations computed using ATEM, GRAL, and PALM compared against ALEGA station measurements.

A closer insight is provided by Fig. 2 and Fig. 3, allowing an evaluation of the temporal and spatial variation of predictions, respectively. The time series of modelled values were compared against measurements at ALEGA station (Fig. 2). An exceptionally high value was recorded on 13 February (Monday) at 10:00 UTC, which coincides with the peak in traffic emissions (Patiño et al., 2024). Simulations indicated that ATEM usually followed the boundary concentration curve and therefore underestimated the measured concentrations, especially in the daytime. Conversely, GRAL systematically overpredicted the measurements, mainly during rush hours. Modelled concentrations were almost 2–3 times larger than observations, sometimes reaching unrealistic values. Predictions using PALM were in accordance with the daily trends of measurements, slightly underestimating concentrations in the first half of the period and overestimating afterwards.

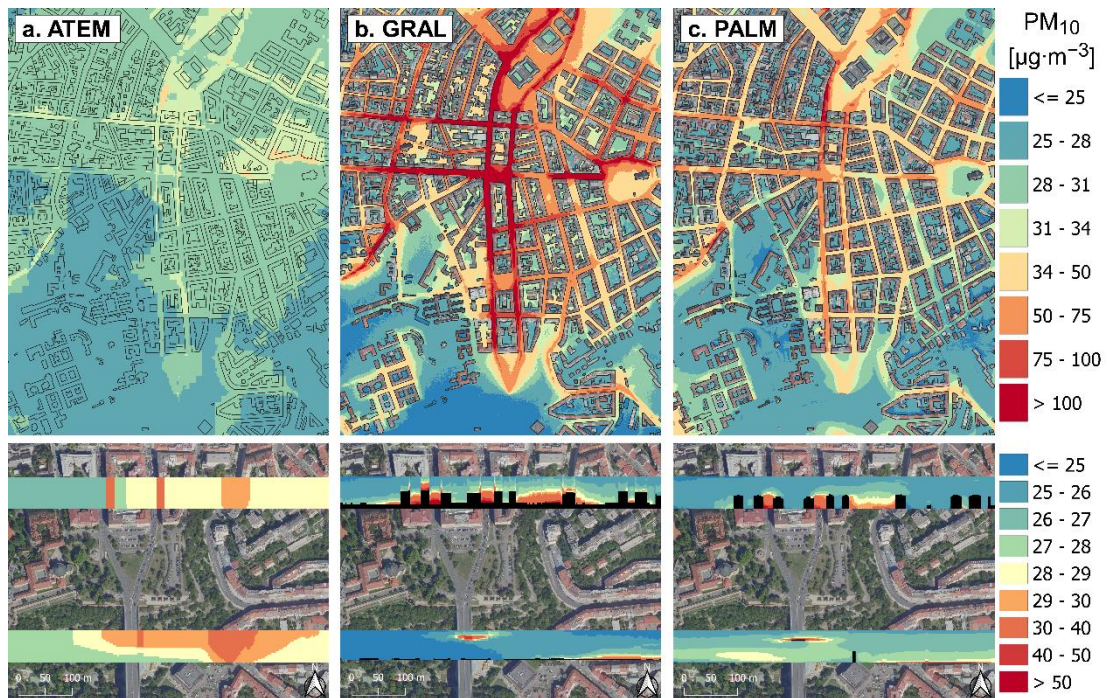


Figure 3. Mean PM₁₀ concentrations at 3 m AGL (upper) and close up of vertical cross-sections (lower) for the period 13–15 February using ATEM (a), GRAL (b), and PALM (c).

Furthermore, maps of average concentrations at 3 m above ground (Fig. 3, upper) illustrated a remarkable difference among the models, i.e., ATEM evidently underrepresented the distinction between hotspots and ‘cleaner areas’ (Patiño et al., 2024). Meanwhile, GRAL and PALM results exhibited high spatial variability, with the highest concentrations corresponding to the streets with the highest traffic loads. It was also crucial to evaluate the spatial pattern of concentrations in the vertical dimension to fully comprehend the behaviour of model algorithms in built-up areas (Fig. 3, lower). The lack of a microscale resolution module in ATEM and underlying simplifications of pollutant dispersion above the plume axis led to a spread of the traffic emissions according to the prevalent wind direction across the streets with uniform (and generally higher) concentrations in the upper levels. On the contrary, GRAL and PALM reflect the influence of obstacles on the ventilation along the street canyon.

Though, GRAL estimated a larger extent of the accumulation of pollution at the street ground level and concentrations increased unrealistically at the facades of buildings. This deficiency stems from the stepped resolution of terrain, as well as the underdevelopment of the reflection and the well-mixed criterion (Oettl et al., 2020). In the case of PALM, pollution stagnation is observed in the leeward ground-level corner of Legerova and Sokolská streets, in agreement with the earlier studies by Gidhagen et al. (2004), Liu et al. (2004), and Park et al. (2015) for regular symmetric street canyons.

CONCLUSIONS

Selecting models for air quality assessment based exclusively on summary statistics might be misleading. In this particular situation, it could be concluded that the simplest of the models, ATEM, would be the most suitable for urban applications since it fulfilled all the acceptance criteria and overall scored the best results. However, the advanced models demonstrated a behaviour that is more coherent with reality, while still complying satisfactorily with statistical metrics. Particularly, PALM obtained the best accuracy for traffic locations and estimated the distribution of concentrations among different urban areas properly.

Nonetheless, in a real application, other factors need to be considered such as time and financial resources, availability of high-resolution data input or the end purpose. For instance, an assessment of annual air quality statistics with ATEM and GRAL is possible even in the presence of limitations, whereas in the case of PALM, further research is needed in this field. Otherwise, when it is necessary to evaluate detailed concentration patterns in the street canyons only the more sophisticated models can be used.

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