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D6.2

Inter-comparison between modelled and measured key pollutants concentrations

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EXECUTIVE SUMMARY

A comparison between measurements from the second AVIATOR campaign (October 2021) and simulated data using two different approaches, Lagrangian for LASPORT and Eulerian for CEDRE, was performed for NOx, CO, and the total number non-volatile particles (nvPM) for Madrid Barajas international airport. The maximum hourly NOx concentrations were obtained with the CFD model that simulates concentration's hotspots over the parking areas due strong static point emission sources (APU). In this case, the model overestimates the NOx measurement from low cost sensor (LCS). For CO, some of the values obtained with CEDRE are in the good agreement with the LCS even if on average CEDRE slightly overestimate the concentration. The overestimation of the pollutant concentrations observed with the CFD simulation may be due to the laminar hypothesis made in CEDRE. In the case of LASPORT, the magnitude of high concentration peaks is similar to the measurements although sometimes the measurement shows strong peaks where the model gives none. The agreement between this model-based estimate of total PN and the LCS-based measured values is mostly within a factor of 2. Overall, for some positions (e.g. LCS 14), an interpretation seems straightforward while for others, it is more difficult due to the fact that the statistics rely only on a few data points and that also the occupation of specific runways is not constant but varies with wind direction in a more or less uncorrelated way.

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LIST OF ABBREVIATIONS

APU	Auxiliary Power Unit
CEDRE	Calculs d'Ecoulements Diphasiques Réactifs pour l'Energétique
CFD	Computational Fluid Dynamics
EI	Emission Index
GSE	Ground Support Equipment
HL	High Load (APU mode)
LASAT	LAgrangian Simulation of Aerosol Transport
LASPORT	LASat for airPORTs
MAD	IATA code of Madrid Barajas Airport
nvPM	Non-volatile Particle Mass
nvPN	Non-volatile Particle Number
PM	Particulate Matter
PN	Total Particle Number
SS	Start and Stabilization (APU mode)
UID	Universal Identification
vPN	Volatile Particle Number
WP	Work Package

REPORT ON THE INTER-COMPARISON BETWEEN MODELLED AND MEASURED KEY POLLUTANTS CONCENTRATIONS

1. Introduction

The Deliverable 6.2 (D6.2) is the logical follow up of D6.1 (Emission inventories and time series of modelled concentration distributions). It provides an intercomparison between measured data from WP4 and corresponding model results for two distinct modelling approaches (CEDRE and LASPORT).

The measured data were obtained with a Low Cost Sensor (LCS) network at Madrid Barajas Airport. The advantage of LCS is that many of them can be applied to provide information on concentration gradients at the airport, which can be gained otherwise only by modelling. Hence it is of interest to investigate how well such measured gradients compare with modelled ones.

For the CFD model CEDRE, concentrations of NO, NO_2, and CO were used for comparisons for a specific day in October 2021. A high spatial resolution was applied and different sensitivity studies on plume modelling and assumptions on the running time of auxiliary power units (APU) were performed, see as well D6.1.

The Lagrangian particle model LASPORT was applied for a period of 3 days in October 2021 with a focus on PM number concentration. Here, the modelled concentration of total particle number was estimated from the modelled concentration of non-volatile particle number. The correlation of concentration with wind direction were applied to better understand and interpret the behaviour of measured and modelled concentrations.

The two model comparisons are independent and constitute to some extent distinct approaches towards a better, model-supported understanding of pollutant concentration and concentration gradients at an airport. Possible improvements are briefly discussed at the end of this paper. Further background information on the models and the setup of the dispersion calculations can be found in D6.1. More detailed information on the measurements can be found in the deliverables of WP4.

2. CEDRE simulations

A comparison between those data and the CEDRE results (see D6.1 for the set-up description) is presented in this section. Experimental data obtained during the campaign were provided from W4. The position of the experimental probes (LCS) over the airport used for the experimental campaign is presented in Figure 1.

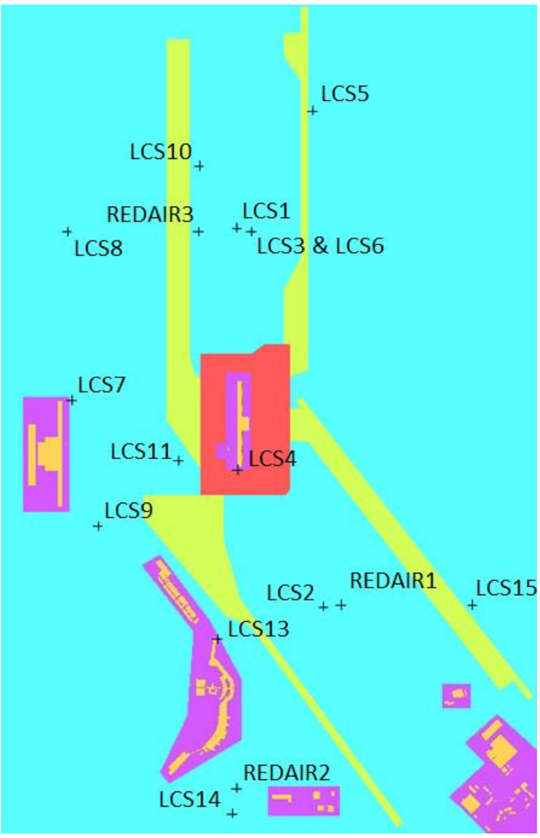

Figure 1: Position of the probes.

A comparison of values between CEDRE model and experimental data for NO, NO_2 and CO concentrations is presented in Figure 2, Figure 3, and Figure 4.

For NO, only a limited amount of values is available from WP4 due to technical difficulties during the campaign, which make the interpretation of the results somehow limited. The data are largely spread with some values obtained with the CFD simulations 100 times higher than for the WP4 values.

For NO_2, good agreement is observed for the low cost censors (LCS) 4, 13, 14, when the measured concentrations are higher than 100 ppbv. Globally, when the measured concentrations are between 1 and 50 ppbv, the CEDRE simulations overestimates NO_2 measured concentrations, which could be explained by the laminar hypothesis made in CEDRE.

For the CO concentrations, a large part of the data from the experimental campaign and the CEDRE simulations results are localized between 50 and 300 ppbv. For some low cost censors (1, 10, 11 and 13), the CEDRE results provide far higher concentrations than the one obtained from WP3.

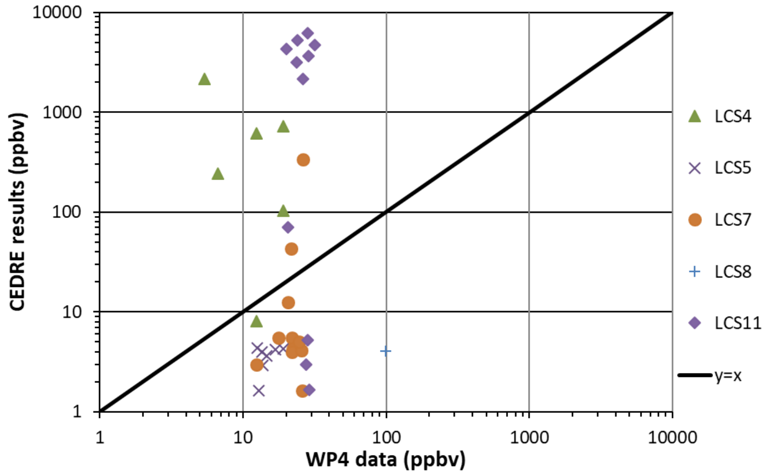

Figure 2: CEDRE results versus WP4 experimental data for NO concentrations (ppbv).

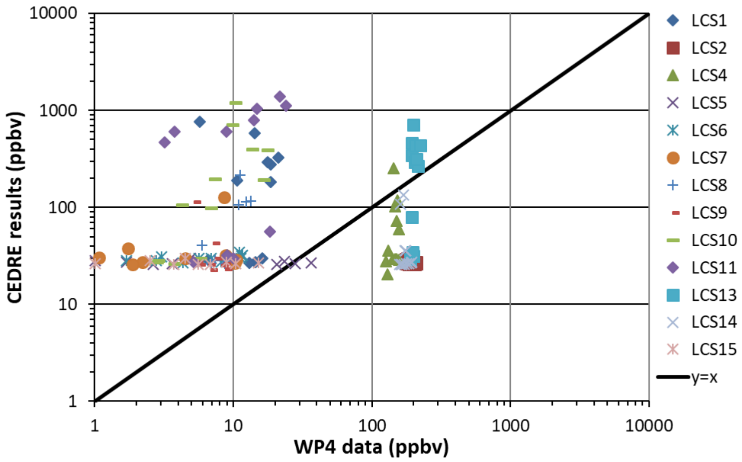

Figure 3: CEDRE results versus WP4 experimental data for NO_2 concentrations (ppbv).

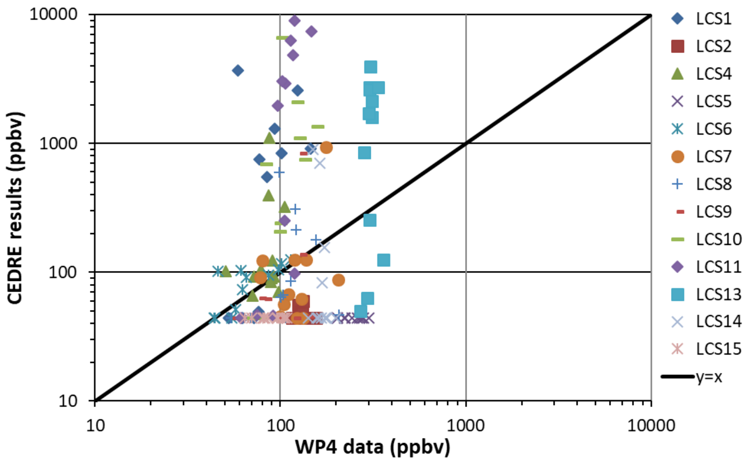

Figure 4: CEDRE results versus WP4 experimental data for CO concentrations (ppbv).

Finally, a comparison of the hourly mean values performed for each LCS and the CEDRE simulations between 0500 LT and 1700 LT for each LCS is presented in Figure 5. For NO, the lowest values measured during the campaign is in very good agreement with the modelled data whereas some values obtained with the CFD simulations can be far higher especially near the parking stations. The simulations tend to overestimate the NO_2 concentrations when the measured data are around 10 ppbv while the data compare well for values greater than 100 ppbv for both NO_2 and CO, even if the simulations tend to overestimate the obtained CO concentrations.

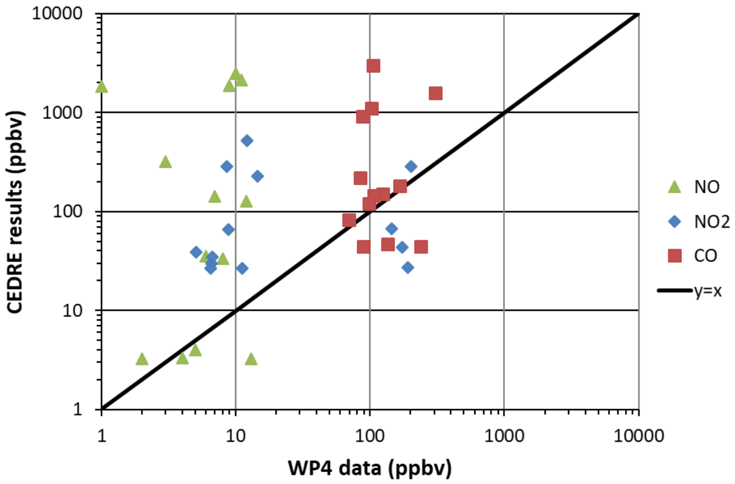

Figure 5: CEDRE results versus WP4 experimental data for each LCS: mean values obtained between 0500 LT and 1700 LT (2021-10-17).

3. LASPORT simulations

In work package (WP) 5 of AVIATOR, an enhanced parametrization of exhaust dynamics was tested and implemented into LASPORT, and near-field comparisons between measured and modelled concentrations behind an aircraft were carried out.

In the subsequent WP6, LASPORT (enhanced version 2.4) was applied to a complete airport scenario for Madrid Barajas (MAD). For the last quarter of 2021, times series of hourly concentrations were calculated. In the following, a comparison and analysis of modelled and measured concentrations is provided.

3.1. Measurements with Low Cost Sensors

In the last quarter of 2021, measurement campaigns were carried out at Madrid Barajas (and other airports) in the context of work package 4. Here we focus on the results from low cost sensors (LCS). The advantage of LCS is that many of them can be applied to provide information on concentration gradients at the airport, which can be gained otherwise only by modelling. Hence it is of interest to investigate how well such measured gradients compare with modelled ones.

A network of LCS was installed at Madrid Barajas with measurements of gaseous species (including NOx and CO) and of total particle number (PN). The locations of the sensors were changed from time to time. A period of 3 days was selected (October 23 to 25) in which a set of 13 sensors was kept at fixed positions at the airport. The positions are shown in Figure 6.

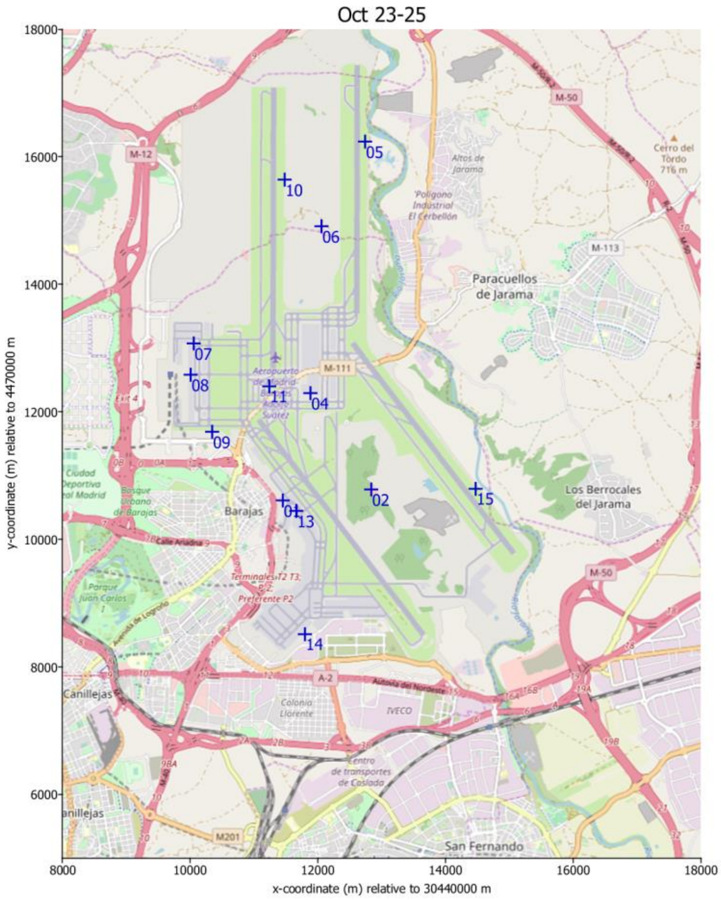

Figure 6: Positions of the low cost sensors (October 23 to 25, 2021) applied in the model comparison.

An analysis of the LCS data and comparisons with high fidelity measurements indicate that the PN results are the most reliable ones, but still with larger uncertainties from a quantitative point of view as compared to high fidelity measurements.

The LCS measurements of PN were provided as series of (approximately) 10-minute means, which were further averaged to hourly means. Table 1 lists the LCS positions, the time period covered, the number hours with valid values and the mean over all valid hours.

Table 1: Low cost sensor positions, number of valid hours, begin and start time, and average total particle number concentration for the study period October 23 to 25 (2021).

POS	*n*	from	to	PN (1/cm³)
01	72	2021-10-23.00:00:00	2021-10-26.00:00:00	6.998e+04
02	58	2021-10-23.00:00:00	2021-10-26.00:00:00	3.173e+04
04	72	2021-10-23.00:00:00	2021-10-26.00:00:00	4.403e+04
05	72	2021-10-23.00:00:00	2021-10-26.00:00:00	5.242e+03
06	72	2021-10-23.00:00:00	2021-10-26.00:00:00	1.755e+04
07	38	2021-10-23.00:00:00	2021-10-24.14:00:00	3.780e+04
09	72	2021-10-23.00:00:00	2021-10-26.00:00:00	3.883e+04
10	72	2021-10-23.00:00:00	2021-10-26.00:00:00	1.795e+04
11	66	2021-10-23.00:00:00	2021-10-26.00:00:00	7.099e+04
13	49	2021-10-23.00:00:00	2021-10-25.01:00:00	5.552e+04
14	72	2021-10-23.00:00:00	2021-10-26.00:00:00	5.021e+04
15	72	2021-10-23.00:00:00	2021-10-26.00:00:00	1.688e+04

3.2. Meteorology and movements

A statistical evaluation of the meteorological data and the 2242 movements in the time period October 23 to 25 are shown in Figure 7 and Figure 8.

As in the whole last quarter of 2021, wind from north is dominant, there was no wind from east during the period of 3 days, which must be later considered when interpreting directional concentration plots. With one exception, all arrivals take place from southeast at runways 32L and 32R, all departures go to north from runways 36L and 36R.

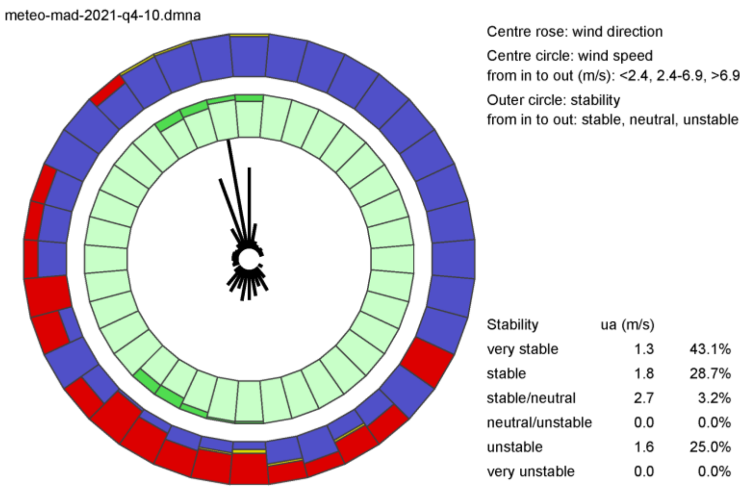

Figure 7: Statistical evaluation of the meteorological time series for the period October 23 to 25 (2021).

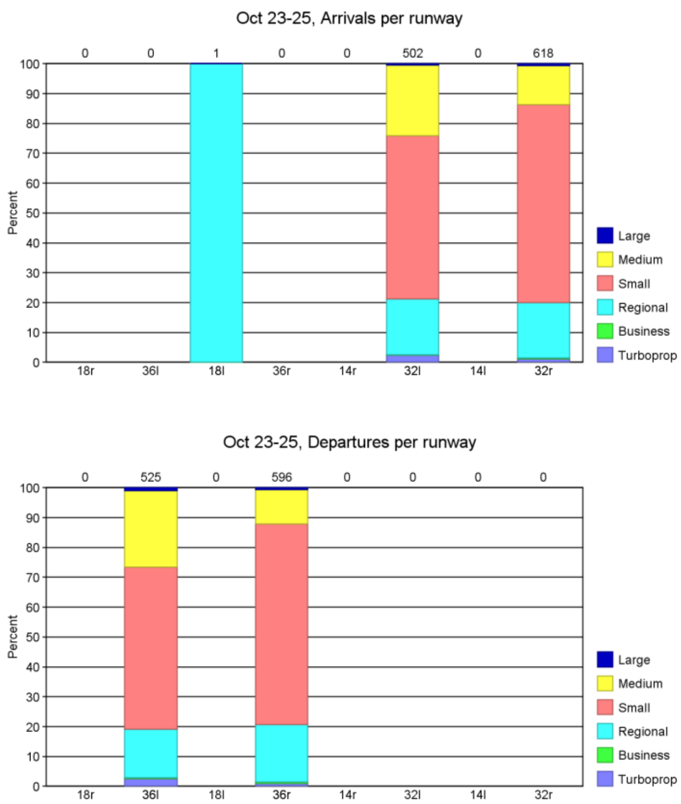

Figure 8: Distribution of arrivals (top) and departures (bottom) over the runways for the period October 23 to 25 (2021).

3.3. Comparisons

The time series of measured hourly mean concentrations of PN were compared to the time series of modelled hourly mean concentrations of nvPN and model-based estimated PN for the period October 23 to 25 (2021).

A problem is that the measured values reflect the contribution from all sources of ultrafine particles, including nearby landside and airside road traffic and contributions from volatile particles, while the modelled results refer to contributions from aircraft and ground support equipment and non-volatile particles only. Hence, some further estimate from the modelling side was required to provide model-based concentrations of PN.

3.3.1. Long-time means

The modelled quantity is nvPN from aircraft and GSE and the measured quantity is total PN from all sources. In addition, the virtue of LCS data consists more in a qualitative description of concentration gradients rather than in a high-fidelity quantitative description.

Therefore, a first comparison between modelled and measured data is made for the relative concentration distribution, where the modelled nvPN data (averages over the 3 days) are divided by the modelled maximum value across the LCS positions (position 13) and likewise the measured PN data (averages over the 3 days) are divided by the maximum measured value (at position 11). The result, shown in Figure 9, indicates that both modelled and measured concentrations gradients at the airport agree quite well in this more qualitative comparison.

For a direct comparison of measured and modelled concentration, an estimate is needed for modelled total PN. Similar to the comparisons in WP5, we take a simple approach and estimate volatile PM number (vPN) by a factor from modelled nvPN and add a constant background. Measurements in WP3 (on-wing measurements) in the winter period (January 2022) yield a factor of about 3 to 20 between vPN and nvPN at distances of a few hundred metres behind an aircraft. We applied a factor of 10 and assumed a constant background of 3000 1/cm³ based on the LCS data. Figure 9 shows the resulting comparison. The agreement between this model-based estimate of total PN and the LCS-based measured value is mostly within a factor of 2.

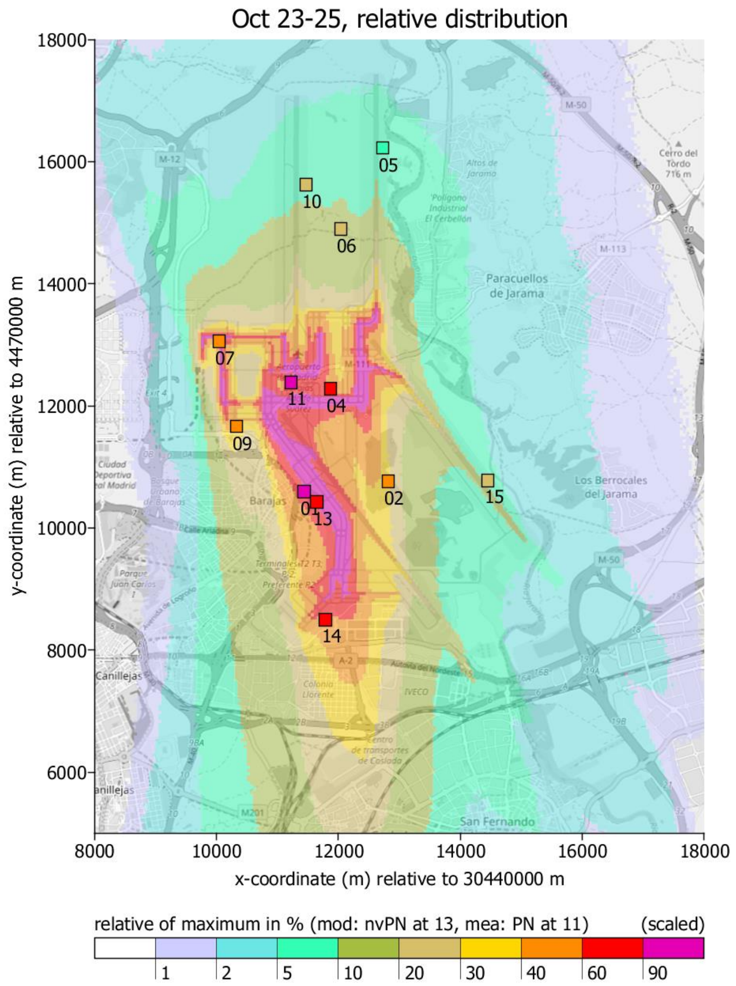

Figure 9: Relative concentration distribution of modelled nvPN (background) and relative concentration distribution of measured PN (squares).

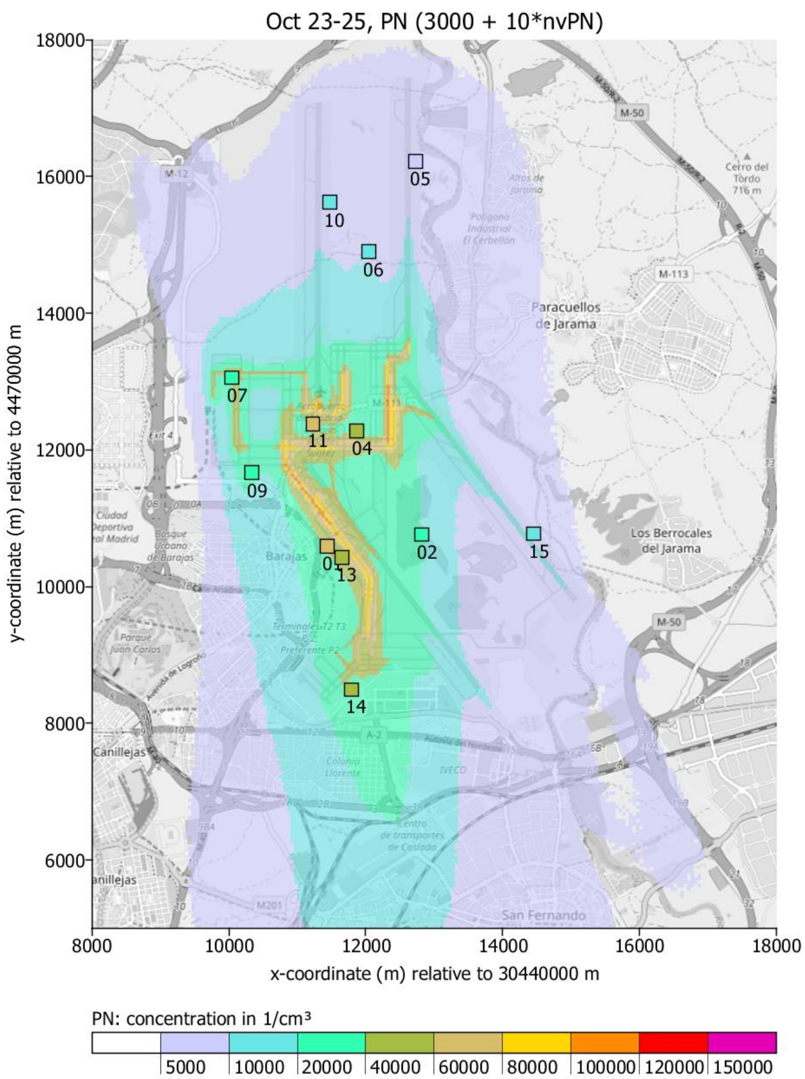

Figure 10: Concentration distribution of model-based PN (background, estimated as 10 times modelled nvPN plus 3000 1/cm³) and measured concentration distribution of total PN (squares).

3.3.2. Hourly means

Further insight is gained by analysing the time series of hourly mean concentrations, where the same estimate of model-based PN is applied as before.

Figure 11 shows the measured (blue) and modelled (red) time series of PN at positions 11 and 14 which is likely dominated by emissions from taxiing and terminal activities. Also indicated is the time series of hourly movements (gray, movements multiplied by 1000).

For an interpretation of such a time series, it must be considered that the local concentration is affected by nearby sources, by strong sources further away and by the current wind direction (and to some extent by current wind speed and atmospheric stratification). Therefore, either a low concentration may be due to low emissions (e.g. little aircraft traffic) or due to unfavorable wind directions that move nearby concentration plumes away from the measurement position.

This may be an indication for local sources that are not accounted for in the modelling and that cannot be approximated by simply up-scaling the modelled nvPN concentration.

Figure 12 shows the time series at position 15, which could be influenced by approach emissions (but, because of wind from north, also by other airport contributions).

Figure 13 shows the time series at the locations 10, 05 and (in between) 06, which are likely affected mainly by departure emissions. The correlation between modelled concentrations (red) and number of departures (gray) is rather week; this indicates that the wind direction has a strong influence on the modelled concentration at these specific positions. The measured peaks are overall less pronounced and appear sometimes when there is no peak predicted by the model. This may be an indication of additional sources, but also of local wind directions that do not coincide with the ones assumed in the modelling, or for effects of exhaust dynamics not covered in the modelling.

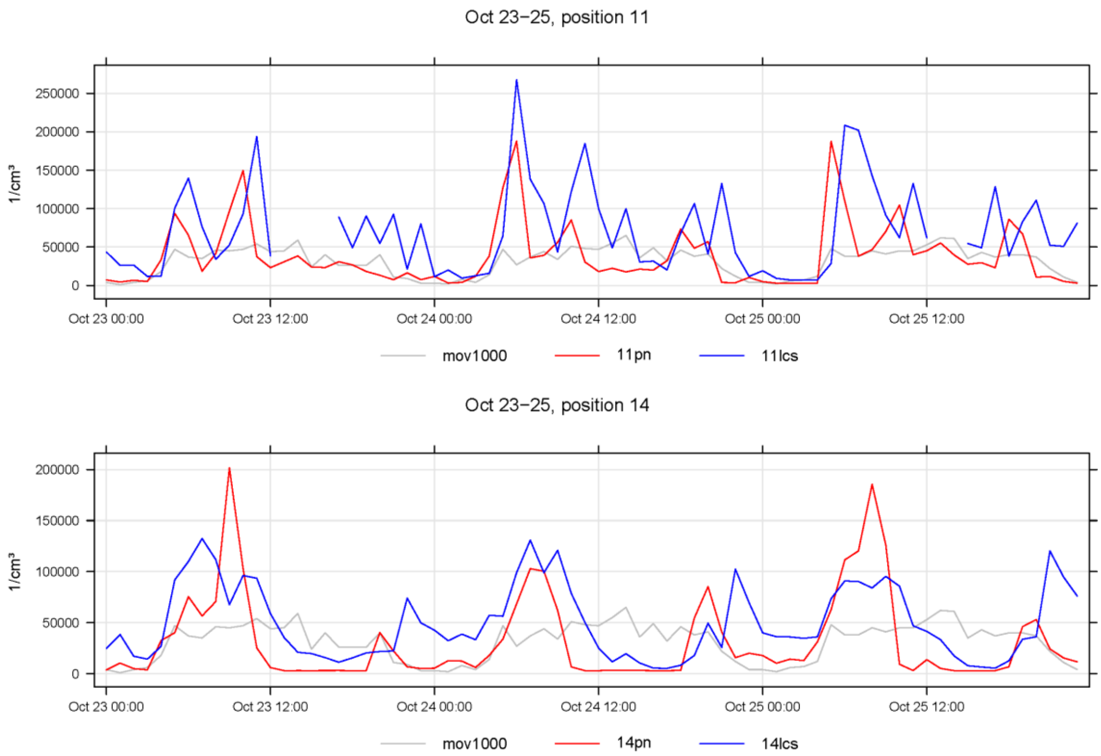

Figure 11: Measured (blue) and model-based (red) time series of PN (hourly means) at positions 11 and 14. The gray line denotes the number of movements per hour multiplied by 1000.

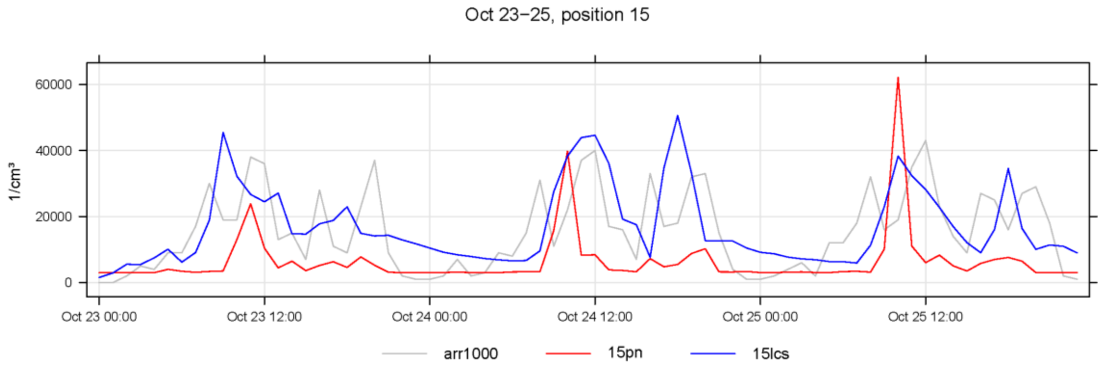

Figure 12: Measured (blue) and model-based (red) time series of PN (hourly means) at position 15. The gray line denotes the number of arrivals per hour multiplied by 1000.

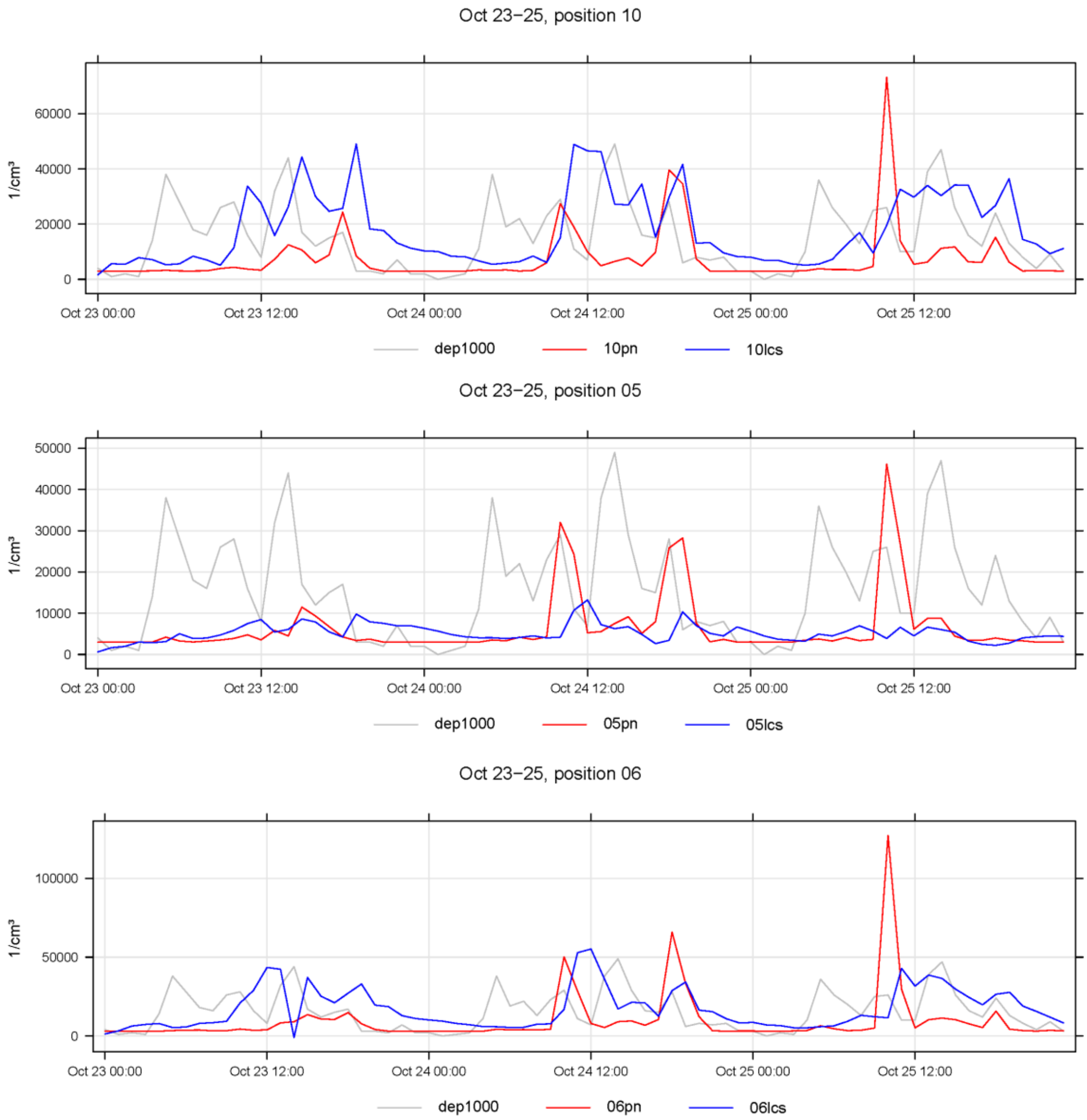

Figure 13: Measured (blue) and model-based (red) time series of PN (hourly means) at position 10 (top), 05 (middle), and 06 (bottom). The gray line denotes the number of departures per hour multiplied by 1000.

Another useful evaluation is the correlation of concentration with wind direction. For wind sectors of for example 30 deg, the concentrations for all hours with a wind direction in a given sector are averaged. Such a concentration is thus the average concentration (sector concentration) that occurs if the wind direction is in that sector.

However, in the present case of a 3-day period with hourly means, there are only 72 hourly means for 12 sectors, which gives 6 values per sector on average. With the strong dominance of wind from north, the statistics is even worse with often only 2 or 3 values per sector or even none (no wind from east).

Nevertheless, Figure 14 shows such a sector plot for position 11. The concentration is plotted in the middle of a sector and the points are connected by lines. The gray bars in the background indicate the frequencies of wind directions, the symbols at the left-hand side the average concentration over the whole time period (weighted average of the sector concentrations). Note that for wind directions around 90 deg, the concentration drops to zero because there was no wind direction in that sector, not because the measured or modelled concentration was zero.

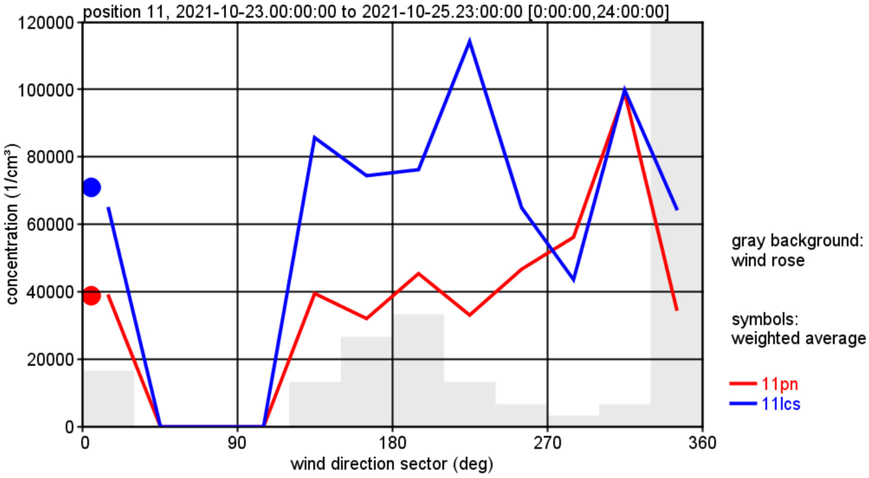

Figure 14: Average concentration as a function of wind direction sector for position 11. The gray bars in the background indicate the frequencies of wind directions, the symbols at the left-hand side the average concentration over the whole time period (weighted average of the sector concentrations).

Figure 15 shows the airport map with the sector plots (note: the vertical axes have different ranges and were omitted for easier reading) at several LCS positions. The individual sector plots are listed in Figure 16. For some positions like position 14, an interpretation seems straightforward. But for others, it is more difficult because the statistics rely on only a few data points and that also the occupation of specific runways is not constant but varies with wind direction in a more or less uncorrelated way.

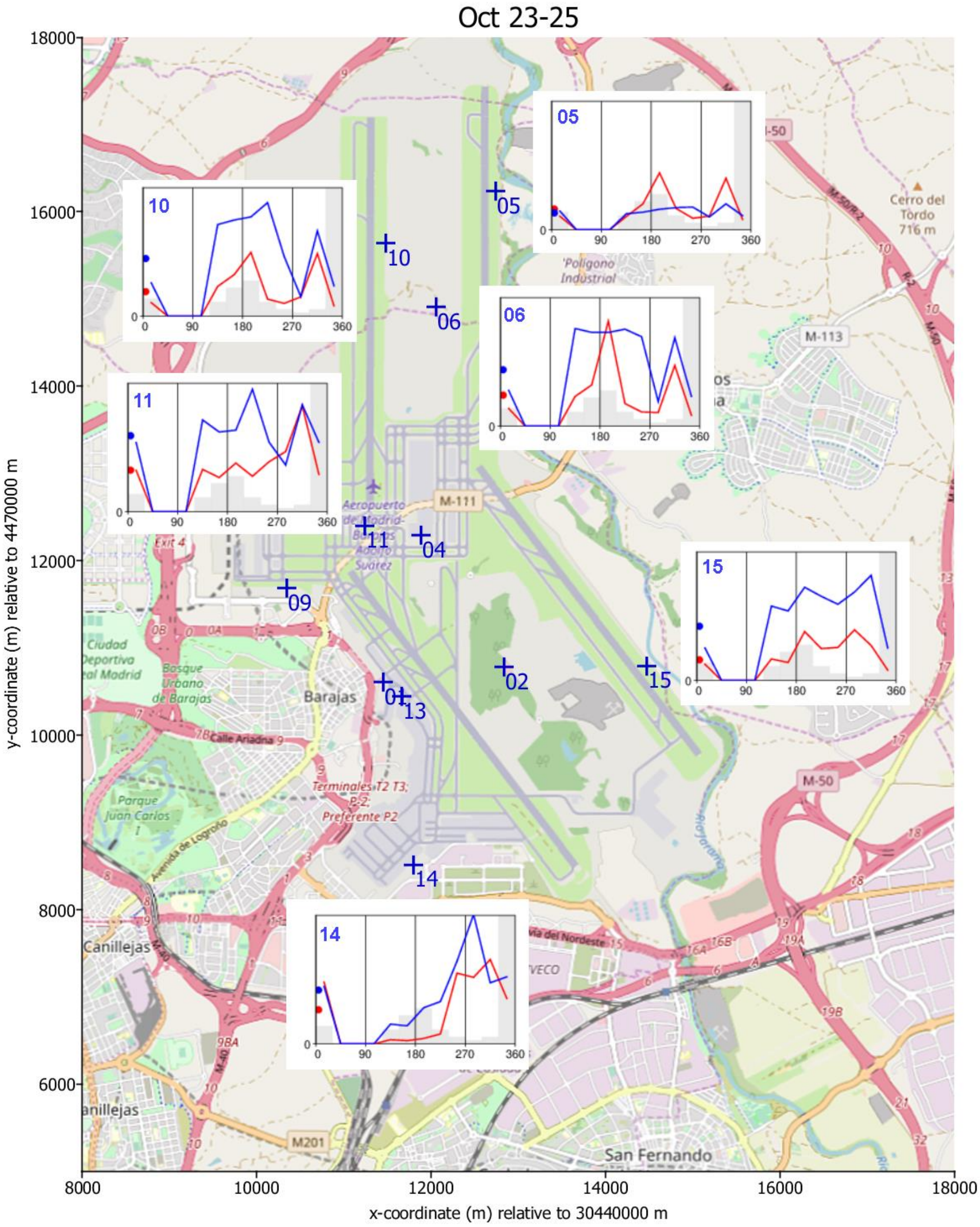

Figure 15: Airport map with the simplified sector plots at several LCS positions.

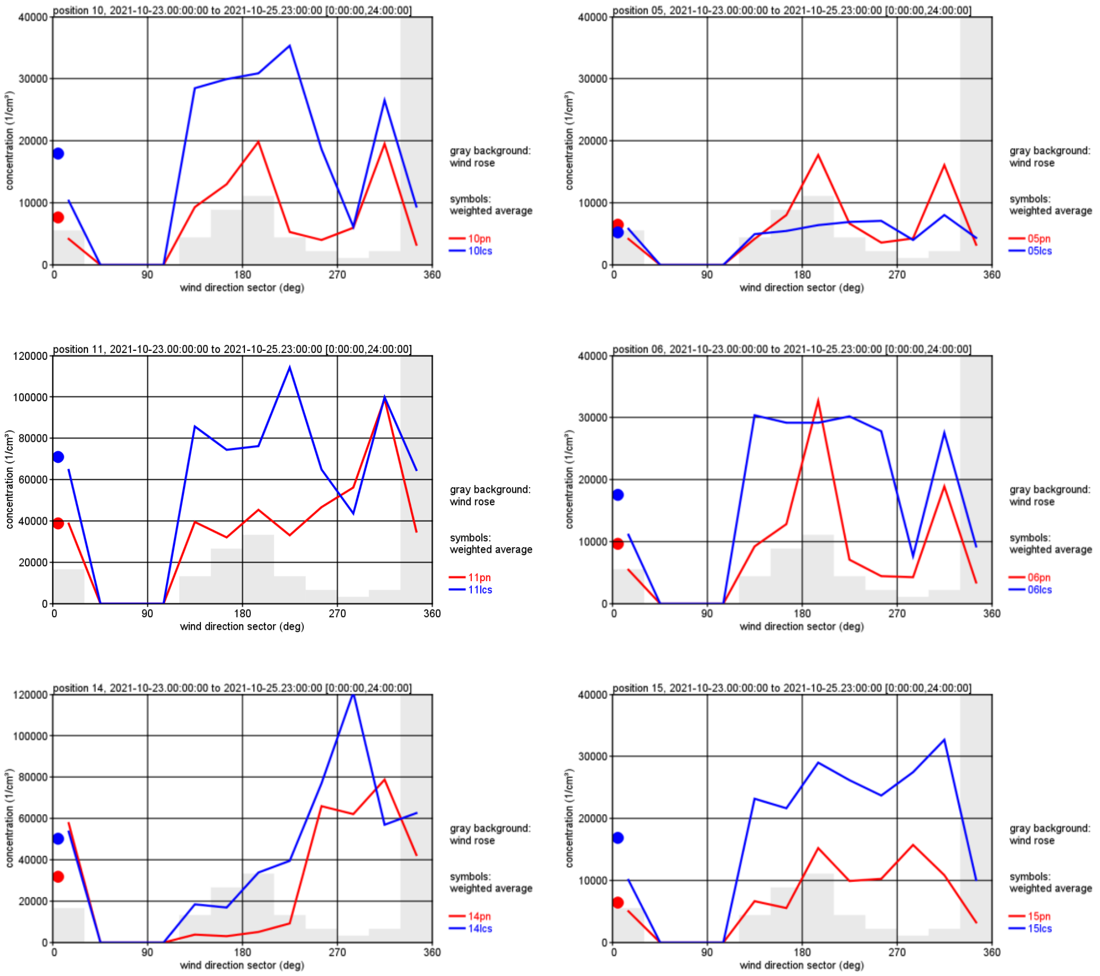

Figure 16: Sector plots at several LCS positions.

4. Discussion and Conclusions

A comparison between modelled data from two distinct modelling approaches and experimental data obtained from WP4 during the campaign was performed WP6.

4.1. CEDRE

Using CEDRE, the hourly NOx modelled concentrations obtained with the CFD approach are overestimating the measurements from LCS network. Indeed, past measurements realized for different airports (Schürmann et al., 2007; Valotto and Varin, 2016) provide maximum NOx concentrations around a few 100 µg/m^3, which is coherent with the values obtained during the AVIATOR campaign whereas the simulation provide larger concentrations near the terminals where strong static emission sources occur (APU) as well as downstream from the buildings. For CO, some of the values obtained with the CEDRE simulations are in the good agreement with the low cost censors' data, even if CEDRE overestimate the concentrations overall.

The overestimation of the pollutant concentrations observed with the CFD simulation may be due to a low representativeness of the LCS network as strong horizontal variation of the concentration are reported especially for NOx as well as the to the hypothesis made in the model concerning the aerodynamic coupling. Indeed, as the flow is assumed laminar, the vertical and horizontal diffusion is likely to be underestimated. Future work should focus on the turbulent aspect of the atmospheric boundary layer with the introduction of wind speed and turbulence.

Another path for further research would be to develop an alternative meshing procedure to better introduce the wind speed and turbulent kinetic energy vertical profiles, given that their conservation seems difficult within the current full tetrahedron grid. Finally, high-quality sets of trajectory locations and associated emissions are essential to avoid an unrealistic reconstruction of the emission location and intensity for taxiing; otherwise, this would introduce potentially a strong source of uncertainties into the modelled concentrations over the airport, especially near the terminals where the parking are located.

4.2. LASPORT

The times series of modelled number concentrations of non-volatile particles (nvPN) were used for a detailed comparison with data measured by a network of low cost sensors (LCS) for the 3-day period October 23 to 25 (2021). An estimate of total number concentration (PN) based on modelled nvPN was applied.

The evaluation for the 3-day average concentration showed that measured and modelled concentration gradients at the airport are quite similar, also the absolute values are the same, mostly within a factor of 2. An analysis of the time series at different LCS positions showed greater variations. These may be due to additional sources not accounted for in the modelling (like motor traffic at the major roads around the airport) or not captured by the simple estimate of PN, or due to local variations of wind direction not accounted for in the modelling, or due to effects of exhaust dynamics not covered in the modelling.

Further insight could be gained by enhancing the time resolution and investigating for example 10-minute averages instead of hourly means. In addition, varying wind directions across the airport area could be accounted for in LASPORT by using a complex wind field model that applies the wind data at several stations at the airport for initialization. These considerably more elaborate modelling approaches were beyond the time scope of the present project.

5. References

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Valotto, G., Varin, C., 2016. Characterization of hourly NOx atmospheric concentrations near the Venice International Airport with additive semi-parametric statistical models. Atmospheric Research 167, 216–223. https://doi.org/10.1016/j.atmosres.2015.07.023