

# CARBON ATMOSPHERIC TRACER RESEARCH TO IMPROVE NUMERICAL SCHEMES AND EVALUATION



## CATRINE

Carbon Atmospheric Tracer  
Research to Improve  
Numerics and Evaluation

### D4.2: Report on sensitivity experiments in very high-resolution simulations

|                                         |                              |
|-----------------------------------------|------------------------------|
| Due date of deliverable                 | 30/09/2026                   |
| Submission date                         | 08/10/2026                   |
| File Name                               | CATRINE-D4.2-V2.0            |
| Work Package /Task                      | WP4                          |
| Organisation Responsible of Deliverable | URCA                         |
| Author name(s)                          | Thomas Lauvaux, Maarten Krol |
| Revision number                         | V2.0                         |
| Status                                  | Issued                       |
| Dissemination Level / location          | PUBLIC                       |



Funded by the  
European Union

The CATRINE project (grant agreement No 101135000) is funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Commission. Neither the European Union nor the granting authority can be held responsible for them.

## 1 Executive Summary

This report summarizes the sensitivity experiments of Large-Eddy Simulation (LES) models performed during the CATRINE project. Focusing on the representation of urban plume characteristics, we intended to diagnose the main drivers of plumes' structures, amplitudes, and variations within various modeling systems. Beyond the explicit representation of turbulence, we explored different LES models with various levels of parameterizations, including urban surface schemes, boundary conditions, spatial and temporal resolutions, and the impact of current plume quantification techniques (IME, cross-sectional). For these tests, three LES models were used: MicroHH, WRF-LES, and PALM. We summarize here our main findings for future work on high-fidelity plume simulations.

The accurate representation of the urban surface energy budget was the main driver of meteorological performances in WRF-LES, specifically the use of advanced urban land surface schemes with multiple building levels, and an additional energy model for heating and cooling. By increasing the spatial resolution from 900m to 100m, the amplitude of the variations in hourly CO<sub>2</sub> concentrations increased by two-fold, reaching the observed variations for mid-cost sensors deployed in and around Paris. Additional measurements from Doppler Lidars measuring the Planetary Boundary Layer (PBL) heights across the urban landscape showed an improvement in the modeled PBL heights, with an increase over the Paris city center (Urban Heat Island effect). The hourly variations estimated by correlation coefficients remain unchanged (no significant improvement compared to mesoscale simulations), as rapid plume fluctuations remain nearly impossible to predict. For satellite applications, the urban plume structures evolved from a single broad plume (at 900m) to three smaller plumes corresponding to the main industrial point sources (urban heating systems) at 100m resolution.

When comparing to observed plumes from TROPOMI over Rotterdam, the aggregation (coarsening) from 100 m to 4 km did not modify the plume's centre line but the coarsening of the grid affected its width, its peak concentrations and fluctuations. Beyond 15-20km from the city center, the two resolutions converge to similar plume structures, impossible to distinguish as the diffusion reduces their differences. Overall, the total cross-plume mass applied to different models (IFS at 4km and MHH at 100m) show similar results, despite large variations in width and rapid fluctuations. The near-source meandering of the plume differs from the MicroHH reference run, similar to a satellite snapshot. Representation errors become large in the near-field, due to largely unresolved eddies.

## CATRINE

We note here that the wide IFS plume is not only a grid-resolution effect. Even after coarsening to 4 km and averaging to hourly, both LES plumes from WRF and MicroHH remain narrower than IFS. The extra width in IFS must therefore come from its parametrised mixing, wind turning and coarser resolution inventory (CAMSGLOBANT, Soulie et al, 2024). This is a useful nuance to Brunner et al. (2023), who attribute wide plumes in coarse models mainly to be caused by the low resolution of the model. In addition, output frequency of XCO<sub>2</sub> mole fractions is an important parameter to consider when building hourly means. Six snapshots per hour (WRF) are not sufficient to give a representative hourly-mean plume, while 60 (MHH) are. Hence, we recommend evaluating plume representativeness over a large number of snapshots, even for high resolution models.

Regarding the CO<sub>2</sub> boundary conditions introduced into LES simulation domains, we note that large plumes coming from distant sources are impacting the observed enhancements over Rotterdam and Paris. For such large urban areas, boundary conditions can matter more than resolution. WRF's inflow from the outer nests is of the same order as the Rotterdam signal, and large plumes have been observed over Paris, mainly coming from the Benelux region. For Rotterdam, the signals are so important they inflate the plume width and the integrated mass. When trying to remove these signals, averaging over the simulation domain was not sufficient to remove these artefacts. Setting up the domain so the target plume can be isolated is at least as important as resolution.

## Contents

|          |                                                                                     |           |
|----------|-------------------------------------------------------------------------------------|-----------|
| <b>1</b> | <b>EXECUTIVE SUMMARY .....</b>                                                      | <b>2</b>  |
| <b>2</b> | <b>INTRODUCTION .....</b>                                                           | <b>5</b>  |
| 2.1      | BACKGROUND .....                                                                    | 5         |
| 2.1.1    | <i>Work performed in this deliverable.....</i>                                      | <i>5</i>  |
| 2.1.2    | <i>Deviations and counter measures.....</i>                                         | <i>5</i>  |
| 2.2      | PROJECT PARTNERS:.....                                                              | 5         |
| <b>3</b> | <b>RESULTS .....</b>                                                                | <b>6</b>  |
| 3.1      | SENSITIVITY TO URBAN SURFACE SCHEMES (WRF-CHEM) .....                               | 6         |
| 3.1.1    | ENERGY BUDGET AND PLANETARY BOUNDARY LAYER HEIGHT (PBLH) .....                      | 6         |
| 3.1.2    | METEOROLOGICAL VARIABLES .....                                                      | 9         |
| 3.2      | SENSITIVITY TO SPATIAL RESOLUTION (WRF-CHEM) .....                                  | 10        |
| 3.3      | SENSITIVITY TO BOUNDARY CONDITIONS (MICROHH) .....                                  | 14        |
| 3.4      | PLUME RISE (MICROHH) .....                                                          | 14        |
| 3.5      | EFFECTS OF AVERAGING ON SIMULATED XCO <sub>2</sub> FIELDS (MICROHH, WRF, IFS) ..... | 15        |
| <b>4</b> | <b>CONCLUSIONS AND RECOMMENDATIONS .....</b>                                        | <b>19</b> |
| <b>5</b> | <b>BIBLIOGRAPHY .....</b>                                                           | <b>21</b> |

## 2 Introduction

### 2.1 Background

This report describes the results performed with the different high-resolution modeling systems presented in previous deliverables (e.g. D3.3), including MicroHH, PALM, and WRF-LES. These different Large-Eddy Simulation (LES) models have been tested over the two test cases selected for the CATRINE project, namely Rotterdam and Paris. Rotterdam was selected for its large industrial sources, near the shore and across the city, while Paris presents more concentrated emissions within the metropolitan area. In the project, LES models aim to assess the complexity of urban plumes and the performances of coarser-resolution models, such as the IFS used in CO2MVS. Here, we focus on selected events corresponding to intensive observing periods (January and June 2024, and August-September 2022). Sensitivity experiments are essential to assess high-resolution simulations considering that the direct evaluation of such turbulence representations is limited by the chaotic nature of the atmospheric transport. This well-known limitation in fluid dynamics forces us to consider statistical metrics and indirect diagnostics, rather than direct evaluations of variables.

#### 2.1.1 Work performed in this deliverable

This deliverable includes model simulations with several LES models (WRF-LES, MicroHH, PALM) as described in the initial proposal. The sensitivity experiments covered the most important schemes and parameters influencing the spatial structure and temporal behaviour of urban plumes. Performances were assessed using various data sets in Paris and Rotterdam, over different seasons.

#### 2.1.2 Deviations and counter measures

No deviation was needed during this part of the project.

### 2.2 Project partners:

| Partners                                                       |              |
|----------------------------------------------------------------|--------------|
| EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS             | ECMWF        |
| COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES | CEA          |
| METEO-FRANCE                                                   | METEO-FRANCE |
| WAGENINGEN UNIVERSITY                                          | WU           |
| KARLSRUHER INSTITUT FUER TECHNOLOGIE                           | KIT          |
| HELSINGIN YLIOPISTO                                            | UH           |
| UNIVERSITE DE REIMS CHAMPAGNE-ARDENNE                          | URCA         |
| ALBERT-LUDWIGS-UNIVERSITAET FREIBURG                           | UFR          |

### 3 Results

Sensitivity experiments have been performed using the WRF-LES and MicroHH models. In the following sections, the most important results are presented. Land use and land cover (LULC) came from the hybrid 100 m CGLC-MODIS-LCZ dataset: combining Copernicus Global Land Service Land Cover, Moderate Resolution Imaging Spectroradiometer, and Local Climate Zones (Demuzere et al., 2023). This dataset provides a detailed description of urban and natural surfaces with a total of 61 land cover categories. It incorporates 10 urban built types, capturing the heterogeneity of urban surfaces. This heterogeneity influences roughness length, albedo, heat and moisture fluxes, and biogenic CO<sub>2</sub> exchanges. Accurate LULC input is particularly important in urban LES simulations, where spatial variations in land use strongly affect atmospheric mixing, heat island effects, hence pollutant dispersion.

#### 3.1 Sensitivity to Urban surface schemes (WRF-Chem)

We investigated how different urban surface parameterizations influence boundary-layer dynamics and near-surface CO<sub>2</sub> concentrations over the Paris metropolitan area during winter and summer conditions. Using the Weather Research and Forecasting (WRF) model, four configurations are evaluated: a no-urban representation (No\_URB), a single-layer urban canopy model (SLUCM), and two multi-layer urban schemes (BEP: Building Effect Parameterization and BEP-BEM: Building Energy Model). Model outputs were evaluated against surface observations of energy fluxes, turbulence, planetary boundary layer height (PBLH), and near-surface CO<sub>2</sub> concentrations from dense urban and suburban monitoring networks, as well as meteorological parameters including wind, air temperature, and humidity.

##### 3.1.1 Energy budget and Planetary boundary layer height (PBLH)

We start here with the sensitivity of the main surface energy budget and the Planetary Boundary Layer height (Figure 3.1).

In **winter**, the No\_URB and SLUCM configurations exhibit narrowly distributed sensible heat flux errors centered slightly below zero, together with near neutral or weakly underestimated friction velocity and a pronounced underestimation of turbulent kinetic energy (TKE). This combination systematically limits both buoyancy production and turbulent transport, resulting in consistently shallow boundary layers, as reflected by PBLH error distributions skewed toward negative values. The coherence of these distributions indicates a physically consistent but weakly forced boundary layer that is unable to respond effectively to daytime heating.

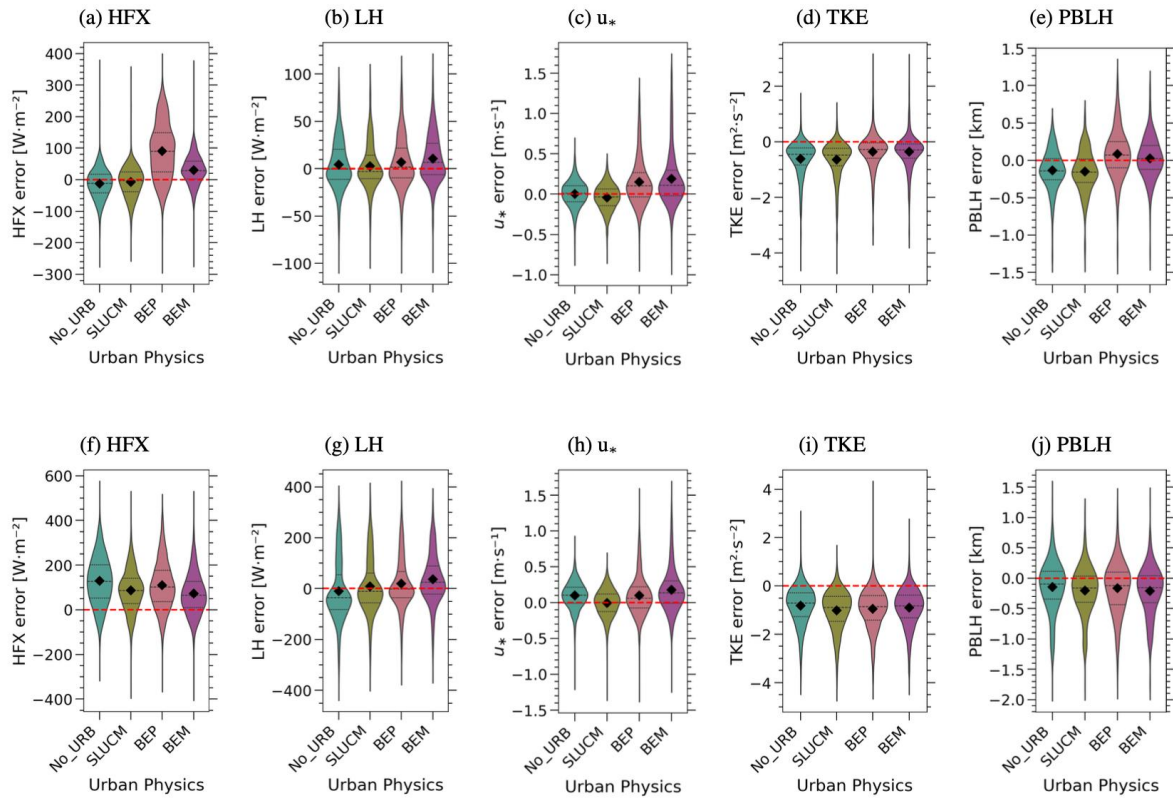


**Figure 3.1:** Distribution of errors (WRF - observations) for near-surface sensible heat flux (HFX), latent heat flux (LH), friction velocity ( $u_*$ ), turbulent kinetic energy (TKE), and planetary boundary layer height (PBLH) during winter (10–31 January, top panels) and summer (1–20 June, bottom panels) 2024. Results compare WRF simulations using different urban parameterization schemes against observations during active daytime conditions. Black points indicate the mean error, dashed black lines represent the inter-quartile range, and the red dashed line denotes zero error.

In contrast, the BEP scheme shows a fundamentally different balance among processes. Its sensible heat flux error distribution is broad and strongly shifted toward positive values, indicating frequent episodes of excessive buoyancy forcing, while latent heat flux errors remain comparatively small and play a secondary role. BEP also exhibits a strong positive bias in friction velocity, reflecting enhanced mechanical forcing by explicit building drag. Despite this, near-surface TKE remains slightly underestimated, suggesting that turbulence production is not fully converted into sustained vertical mixing. Nevertheless, the combined effects of excessive surface heating and strong mechanical forcing are sufficient to offset the TKE deficit, yielding a PBLH distribution centered near zero but with a slight positive bias. This explains why BEP can reproduce near correct mean PBLH while still exhibiting physically imbalanced surface turbulence interactions.

## CATRINE

The BEM scheme achieves a more coherent and physically balanced coupling across all variables. Compared to BEP, its sensible heat flux errors are smaller and more consistent, though not perfectly centered, while friction velocity exhibits a broader distribution with a slightly higher mean than BEP, but its lower quartile remains near zero, supporting effective mechanical mixing. Although TKE is still underestimated on average, the bulk of its distribution is narrower than in No\_URB and SLUCM, with only occasional extreme values, indicating generally improved turbulence representation. This balanced combination of buoyancy and mechanical forcing yields a tightly centered PBLH error distribution with median and mean values close to zero, indicating a realistic boundary layer response without systematic over or under development.

Taken together, the wintertime error distributions demonstrate that PBLH accuracy does not depend on any single process but emerges from the combined regulation of surface heating, momentum exchange, and turbulence generation. Excessive sensible heat and friction velocity can compensate for moderate TKE deficits, as in BEP, while realistic PBLH in BEM arises from a more consistent partitioning of errors across all contributing processes. Conversely, the coherent underestimation of heat flux and turbulence in No\_URB and SLUCM leads inevitably to suppressed boundary-layer growth. This integrated view reinforces the importance of balanced urban physics representations for physically realistic boundary layer development.

In **summer**, the error distributions reveal that all schemes overestimate sensible heat flux, though with varying magnitudes: No\_URB exhibits the largest positive bias, whereas BEM is closest to zero, with its first quartile aligned near zero (Figure 3.1-f). Latent heat flux shows more scheme dependent behaviour: No\_URB slightly underestimates, SLUCM and BEP exhibits a narrow distribution centered around zero, and BEM shows a slight positive bias (Figure 3.1g).

Friction velocity errors largely mirror winter patterns. BEM maintains a similar magnitude of overestimation, BEP and No\_URB show a small positive bias, and SLUCM exhibits a narrow distribution centered around zero (Figure 3.1-h). TKE errors are consistently negative across all schemes, with the zero-line lying above the bulk of the distribution (above the 3rd quartile), indicating persistent underestimation of turbulence (Figure 3.1i). Despite differences in surface and turbulence forcing, the PBLH errors remain broadly comparable across all schemes, with distributions generally centered between approximately -0.1 and -0.2 km (Figure 3.1- j).

These distributions complement the broader result that, in summer, all schemes converge toward a similar boundary layer structure, characterized by an early saturation of convective growth and a limited ability to sustain further afternoon deepening relative to observations.

Even though BEM reduces sensible heat flux errors compared to other schemes and maintains enhanced mechanical forcing, the PBL fails to deepen further in the afternoon. This convergence indicates a seasonal shift in sensitivity: wintertime PBLH strongly depends on the interaction of surface energy partitioning, urban morphology, and turbulence, whereas summertime PBL development appears constrained by more general model limitations, such as entrainment at the PBL top and vertical redistribution of turbulence. Consequently, differences among urban schemes in summer remain relatively small, even when contrasts exist in surface forcing and turbulence production.

### 3.1.2 Meteorological variables

The sensitivity of other meteorological variables is presented in Table 3.1. Overall, the modest inter-scheme differences in near-surface temperature and humidity indicate that these variables are only weakly sensitive to the choice of urban representation. Both variables are constrained by the driver data and the regular re-initialization of the model (every 5 days) which limits the differences among the different configurations. Near-surface wind speed and direction also respond to urban physics, though differences among schemes at the surface are modest (typically  $0.3\text{--}0.6\text{ m s}^{-1}$  in RMSE) compared to the more pronounced contrasts observed in the vertical wind profiles within the lowest few hundred meters of the atmosphere during winter. Multi-layer urban schemes (BEP and BEM) generally improve the representation of vertical momentum distribution relative to simpler configurations, highlighting the height dependent influence of urban physics.

The impact of urban physics on near-surface meteorology occurs primarily through its effect on surface sensible and latent heat fluxes and momentum exchange, rather than through systematic biases in the large scale and mesoscale atmospheric forcing imposed through the boundary conditions. As a result, variables such as HFX, LH,  $u^*$ , TKE, and the vertical structure of wind are more sensitive to urban canopy parameterizations than near-surface temperature and humidity. The relatively small differences in near-surface meteorology suggest that the pronounced variations observed in surface energy fluxes and boundary-layer properties arise mainly from differences in urban energy partitioning and turbulent mixing, rather than from biases in the simulated large scale atmospheric conditions.

| Variable          | Scheme | Winter (January) |      |      |      | Summer (June) |      |      |      |
|-------------------|--------|------------------|------|------|------|---------------|------|------|------|
|                   |        | R                | MBE  | MAE  | RMSE | R             | MBE  | MAE  | RMSE |
| Temperature       | No_URB | 0.97             | -1.1 | 1.4  | 1.7  | 0.88          | 0.0  | 1.2  | 1.7  |
|                   | SLUCM  | 0.95             | -2.0 | 2.2  | 2.6  | 0.87          | -0.4 | 1.4  | 1.8  |
|                   | BEP    | 0.95             | 1.1  | 1.6  | 2.1  | 0.88          | -0.4 | 1.2  | 1.7  |
|                   | BEM    | 0.96             | 0.3  | 1.2  | 1.6  | 0.88          | -0.7 | 1.3  | 1.8  |
| Relative Humidity | No_URB | 0.79             | 2.9  | 6.2  | 7.8  | 0.82          | -3.7 | 7.4  | 9.9  |
|                   | SLUCM  | 0.74             | 7.0  | 8.7  | 10.9 | 0.82          | -2.0 | 7.1  | 9.4  |
|                   | BEP    | 0.72             | -8.9 | 10.0 | 12.4 | 0.82          | -1.9 | 6.8  | 9.1  |
|                   | BEM    | 0.75             | -3.4 | 6.8  | 8.6  | 0.81          | 1.1  | 7.0  | 9.4  |
| Wind Speed        | No_URB | 0.91             | 0.5  | 1.2  | 1.7  | 0.79          | 0.4  | 1.2  | 1.6  |
|                   | SLUCM  | 0.90             | 0.8  | 1.4  | 1.9  | 0.78          | 0.7  | 1.4  | 1.8  |
|                   | BEP    | 0.91             | 0.4  | 1.0  | 1.5  | 0.81          | 0.2  | 1.1  | 1.5  |
|                   | BEM    | 0.92             | 0.0  | 1.0  | 1.4  | 0.80          | -0.2 | 1.1  | 1.5  |
| Wind Direction    | No_URB | 0.82             | 2.8  | 18.4 | 30.3 | 0.82          | 3.7  | 28.2 | 44.9 |
|                   | SLUCM  | 0.82             | 2.2  | 18.9 | 31.2 | 0.82          | 3.2  | 28.2 | 45.0 |
|                   | BEP    | 0.82             | 5.6  | 20.2 | 33.6 | 0.82          | 2.9  | 27.9 | 44.9 |
|                   | BEM    | 0.85             | 3.8  | 18.1 | 30.2 | 0.82          | 2.1  | 27.5 | 44.6 |

**Table 3.1:** Statistical evaluation of near-surface meteorological variables simulated by WRF at 900m resolution for winter (10-31 January) and summer (01-20 June) periods. Results are shown for four urban physics configurations: No\_URB, SLUCM, BEP, and BEM. Statistics include the correlation coefficient (R), mean bias error (MBE), mean absolute error (MAE), and root mean square error (RMSE).

### 3.2 Sensitivity to spatial resolution (WRF-Chem)

The probability density functions (PDFs) of CO<sub>2</sub> concentrations simulated by WRF at horizontal resolutions of 900 m, 300 m, and 100 m are compared with observations in Figure 3.2. The linear scale plots emphasize the central portion of the distributions and allow direct assessment of the dominant concentration ranges. In **winter** (Figures 3.2-a, 3.2-c), the 900 m simulation provides the closest agreement with the observed distributions. Its peak density aligns well with observations, with only a slight overestimation, indicating a realistic

## CATRINE

representation of the most frequently occurring CO<sub>2</sub> levels. In contrast, the 300 m and 100 m LES simulations exhibit higher values for Picarro stations and narrower peaks occurring at lower concentration values (approximately 430 ppmv for Picarro and 435 ppmv for the mid-cost network) compared to the 900 m configuration (around 440–445 ppmv).

In **summer** (Figures 3.2-b, 3.2-d), all three model resolutions produce distributions with higher peaks and slightly narrower shape compared to observations, although the modal concentration remains close to the observed value (around 425 ppmv). This indicates that while the general central tendency is captured across resolutions, the model tends to over-concentrate probability around the mean concentration during convective summer conditions. For the logarithmic plots (Figures 3.2-e to 3.2-h), which emphasize the high-concentration tails, the differences between model resolutions become more pronounced. In winter, the 900 m simulation exhibits a sharp decline in probability density around ~480 ppmv, while in summer the drop occurs near ~450 ppmv, diverging from the observations and failing to reproduce the gradual tail of rare, high-concentration CO<sub>2</sub> events. In contrast, the 300 m and 100 m LES simulations better capture the observed tail behaviour, with the 100 m configuration providing the closest match, although it occasionally produces minor spurious peaks in the tail not present in the measurements. These anomalies occur at very low probability densities (below  $5 \times 10^{-4}$ ) and are consistent with the time series analysis, where fine-resolution simulations sometimes overestimate episodic peaks.

While these artificial fluctuations are minor in terms of overall probability, they highlight the increased sensitivity of fine-resolution LES to localized emissions and turbulent transport, which enhances high-concentration events but can also amplify variability beyond observed levels. These distributional analyses are consistent with the plume, transect, and time series results. In winter, the 300 m and 100 m LES simulations produce narrower central distributions, reflecting high resolution grids' ability to preserve localized emission maxima, whereas the 900 m simulation yields broader distributions due to spatial averaging.

In **summer**, all resolutions show similar linear-scale distributions, indicating that the central tendency is captured regardless of grid spacing. Across both seasons, the logarithmic-scale PDFs reveal that finer resolutions better capture high concentration tails, although the 100 m simulation occasionally introduces minor spurious peaks at very low probabilities. Overall, the PDFs confirm that horizontal resolution strongly influences the representation of extreme concentrations and localized plume structure, complementing the spatial and temporal analyses.

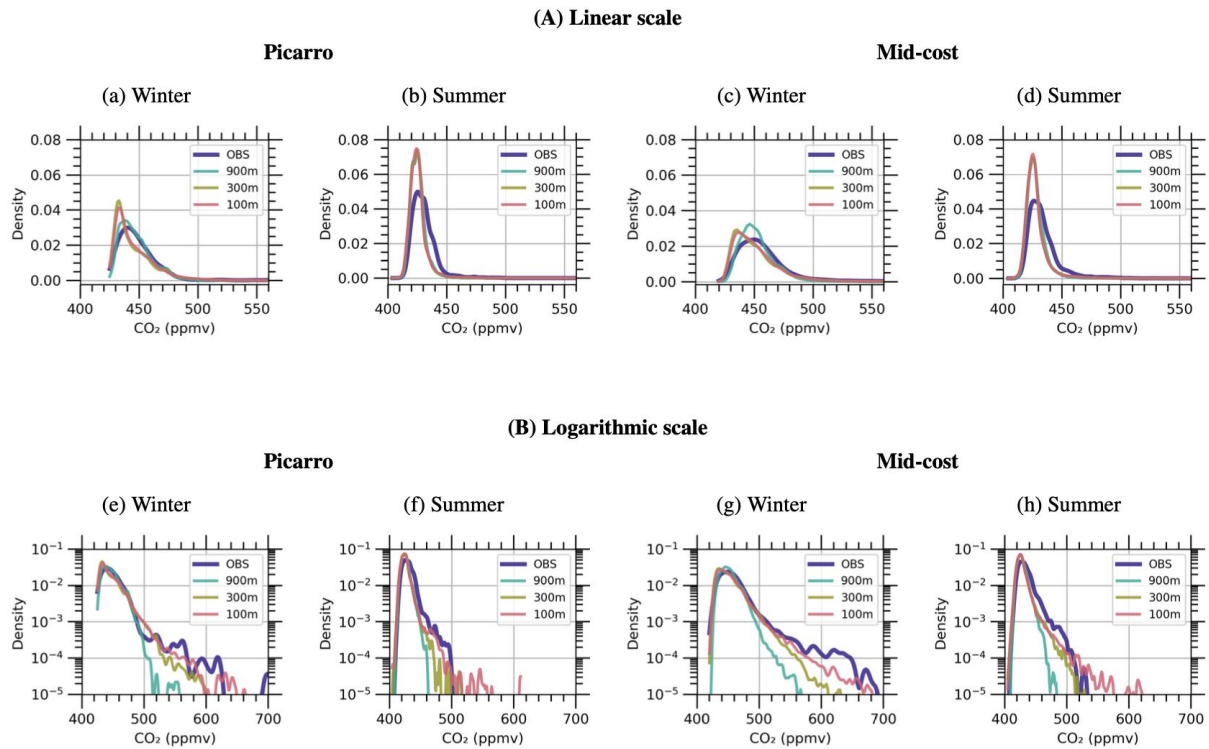


**Figure 3.2:** Probability density functions (PDFs) of  $\text{CO}_2$  concentrations from WRF simulations and in-situ measurements aggregated across all stations. The left panels correspond to Picarro observations and the right panels to Mid-cost sensor measurements. Winter (January) and summer (June) distributions are shown for each instrument type. Panels (A) present PDFs on a linear scale, while panels (B) show the same distributions on a logarithmic scale to better highlight differences in the distribution tails and high concentration events.

Figure 3.3 presents the mean  $\text{CO}_2$  perturbation fields at 35 m above ground level for winter (10–31 January 2024) and summer (01–20 June 2024). This height is sufficiently elevated to avoid near surface numerical noise while remaining within the surface layer, where emission plumes remain clearly expressed. Figure 3.3 (left panels) shows the daytime winter averages. During **summer** daytime, mean concentrations are generally lower and exhibit similar large scale spatial patterns across all three configurations. The aggregated 100 m and 300 m simulations produce slightly higher and more spatially concentrated enhancements near emission hotspots, whereas the native 900 m run displays a broader and more spatially diffused plume structure. This behaviour is consistent with a well-developed and efficiently mixed planetary boundary layer (PBL), as indicated by comparable daytime PBL heights across resolutions, with the 900 m configuration showing a slight overestimation. Under these

convective conditions, enhanced vertical mixing reduces concentration gradients and limits resolution dependent differences.

Figure 3.3 (bottom row) presents the corresponding **summer** daytime and nighttime averages. The overall behaviour is qualitatively similar to winter: aggregated high-resolution simulations maintain more concentrated plume structures and higher local amplitudes compared to the native 900 m configuration. However, absolute concentration enhancements are substantially lower in summer. The winter daytime mean near surface perturbations (averaged over 10–31 January 2024) locally exceed 45 ppmv, whereas summer enhancements are generally below 15 ppmv, reflecting stronger atmospheric mixing and reduced net accumulation during the warmer season. These results demonstrate that spatial aggregation of high-resolution simulations does not fully reproduce the plume structure and magnitude of a native 900 m simulation.

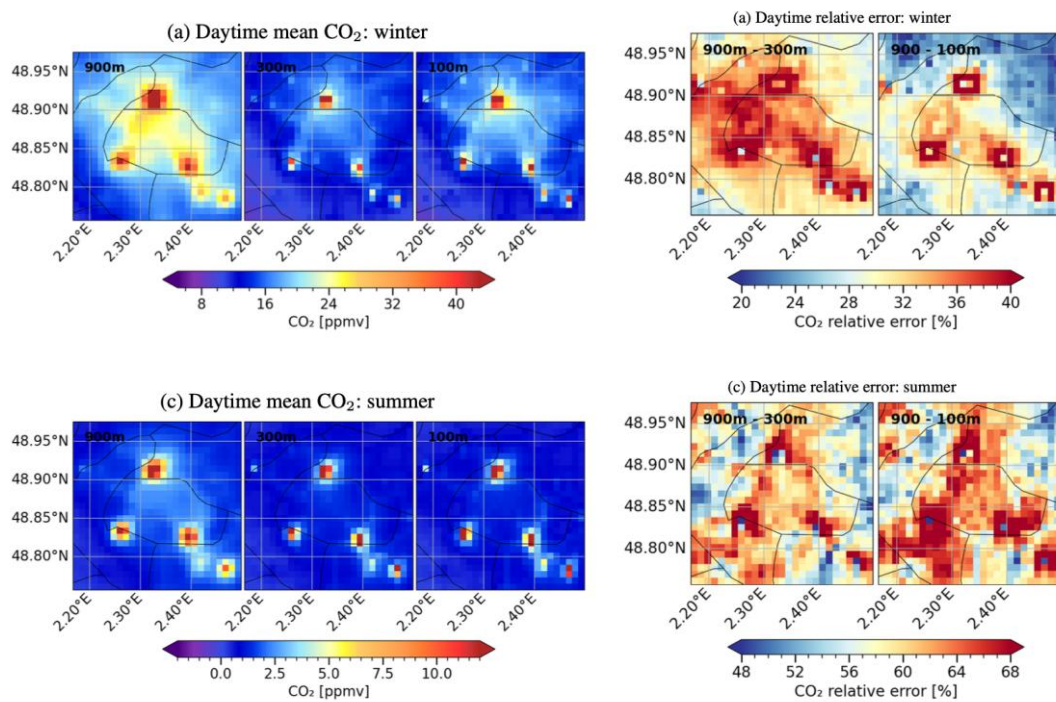


**Figure 3.3:** Mean CO<sub>2</sub> perturbation fields at 35 m above ground level for winter (10–31 January 2024) and summer (01–20 June 2024). Panels show daytime averages for each season. Each map compares the native 900 m simulation with the 100 m and 300 m simulations aggregated to 900 m resolution. The fields represent CO<sub>2</sub> concentration (background subtracted). The figure illustrates how spatial aggregation influences plume magnitude, spatial extent, and concentration gradients under contrasting boundary layer conditions.

### 3.3 Sensitivity to boundary conditions (MicroHH)

In D3.2 the impact of the boundary conditions was assessed. To that end, several MicroHH simulations were performed to test the effects of implementing building drag and meteorological observation nudging on the comparison to observations. Figures 3.4 depicts the *differences* between wind lidar measurements and the simulated winds in the 6 runs.

As described in more detail in D3.2, none of the 6 runs show a clear improvement in their agreement with observations. A too strong drag ( $cd = 5.82$ ) clearly leads to an excessive slowing down of the wind in Rotterdam center.

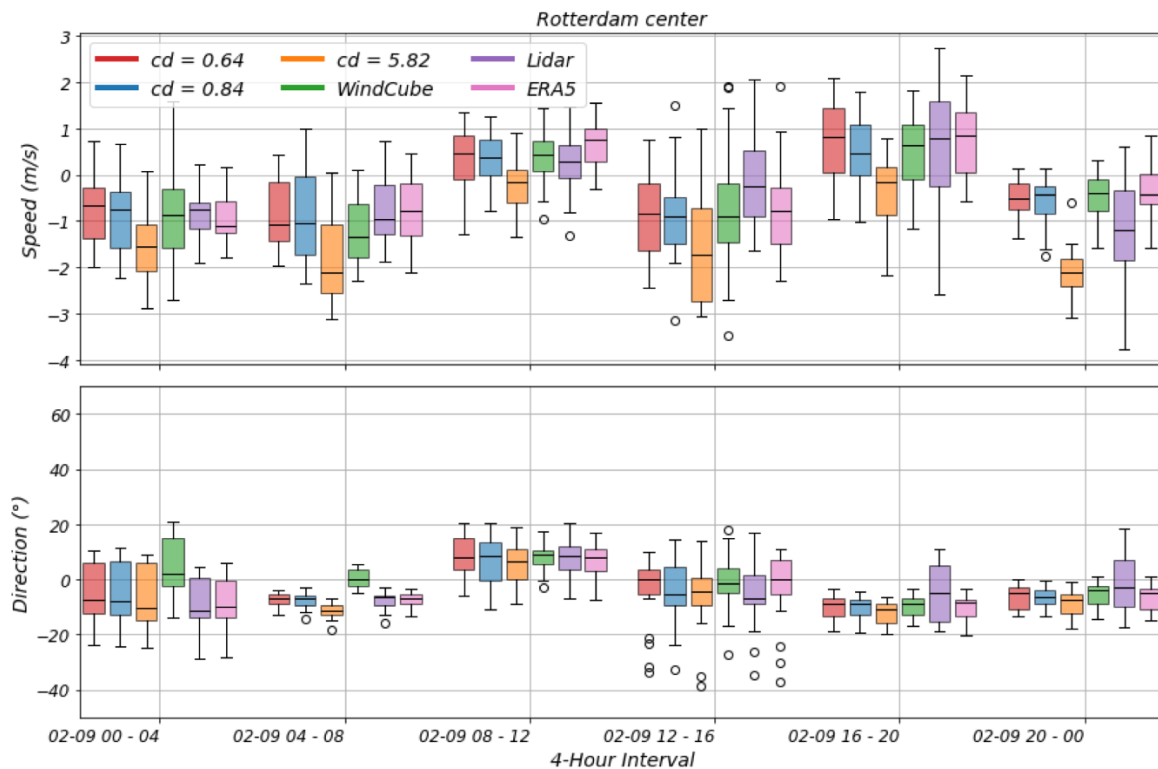


**Figure 3.4:** Wind speed (top) and direction (bottom) differences (simulations - measurements) for the 6 simulations. The simulations are compared to the point wind lidar measurements at Rotterdam centre. Boxplots show interquartile range (IQR), with black line denoting the median, and whiskers showing  $Q1 - 1.5 \cdot IQR$  (bottom) and  $Q3 + 1.5 \cdot IQR$  (top).

### 3.4 Plume rise (MicroHH)

D3.3 reported on the implementation of plume rise in LES (MicroHH). Figure 3.5 shows simulated  $CO_2$  plumes at different resolutions (10, 25, 50, 100, and 200 m) at background winds of  $5 \text{ m s}^{-1}$  (upper panels) and  $10 \text{ m s}^{-1}$  (lower panels) with a plume heat input of 5 MW in a stably stratified atmosphere.

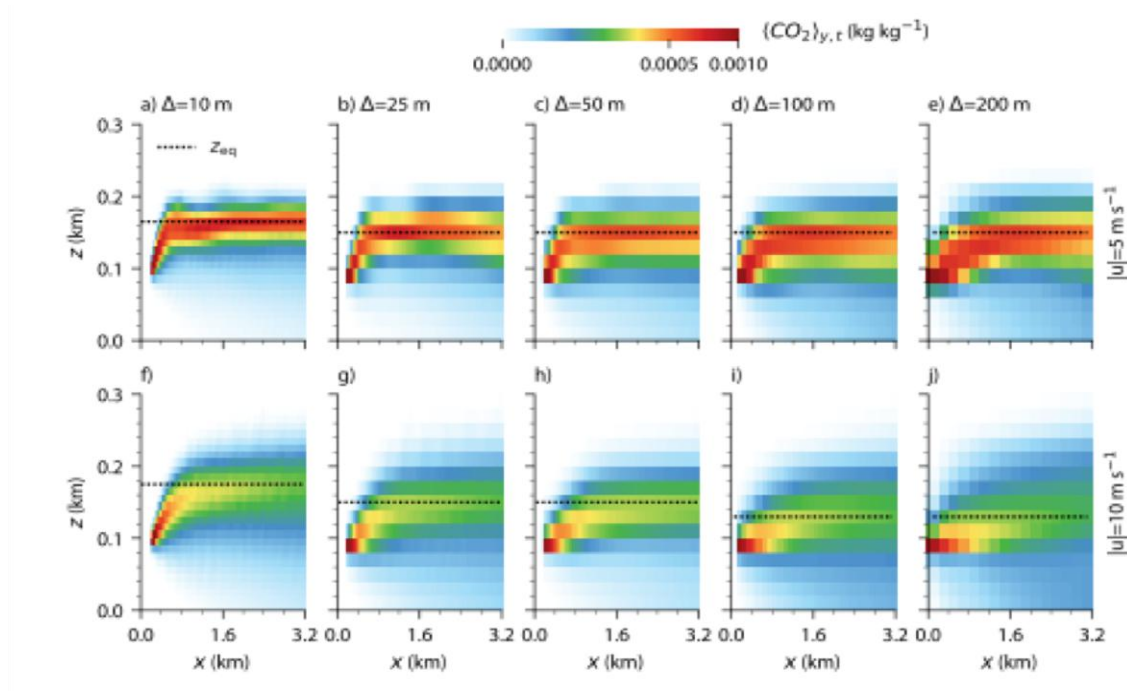


**Figure 3.5.** Spanwise and time averaged cross-section of  $\text{CO}_2$  for the stable case with  $Q=5$  MW. Each row shows a different wind speed, each column a model resolution. The dashed black line indicates the plume equilibrium height.

These plume rise simulations lead to the following recommendations (D3.3):

1. Resolved plume rise in LES remains preferred over parameterisations, despite its resolution sensitivity, as LES simulations outperform any tested parameterization.
2. For large-scale models, Briggs' (1984) method remains a solid choice. The parameterisation gives a reasonable estimation of plume rise under a wide range of conditions. Such method can be implemented without impacting the computational efficiency of large-scale models.

### 3.5 Effects of averaging on simulated XCO2 fields (MicroHH, WRF, IFS)

The very high spatial and temporal resolution LES can be exploited to study the effects of temporal and spatial averaging on the structure of the simulated plume. These averaging effects are important to quantify when, for example, a satellite measured plume snapshot is compared with an IFS modelled plume. The effect of spatial or temporal averaging on a XCO2 plume is illustrated in Figure 3.6 where plumes simulated by MicroHH, WRF and IFS are shown. Since the innermost (D05) WRF domain is smaller than the MicroHH domain, the WRF plumes are shown on latitude and longitude borders of MicroHH for easier visual orientation.

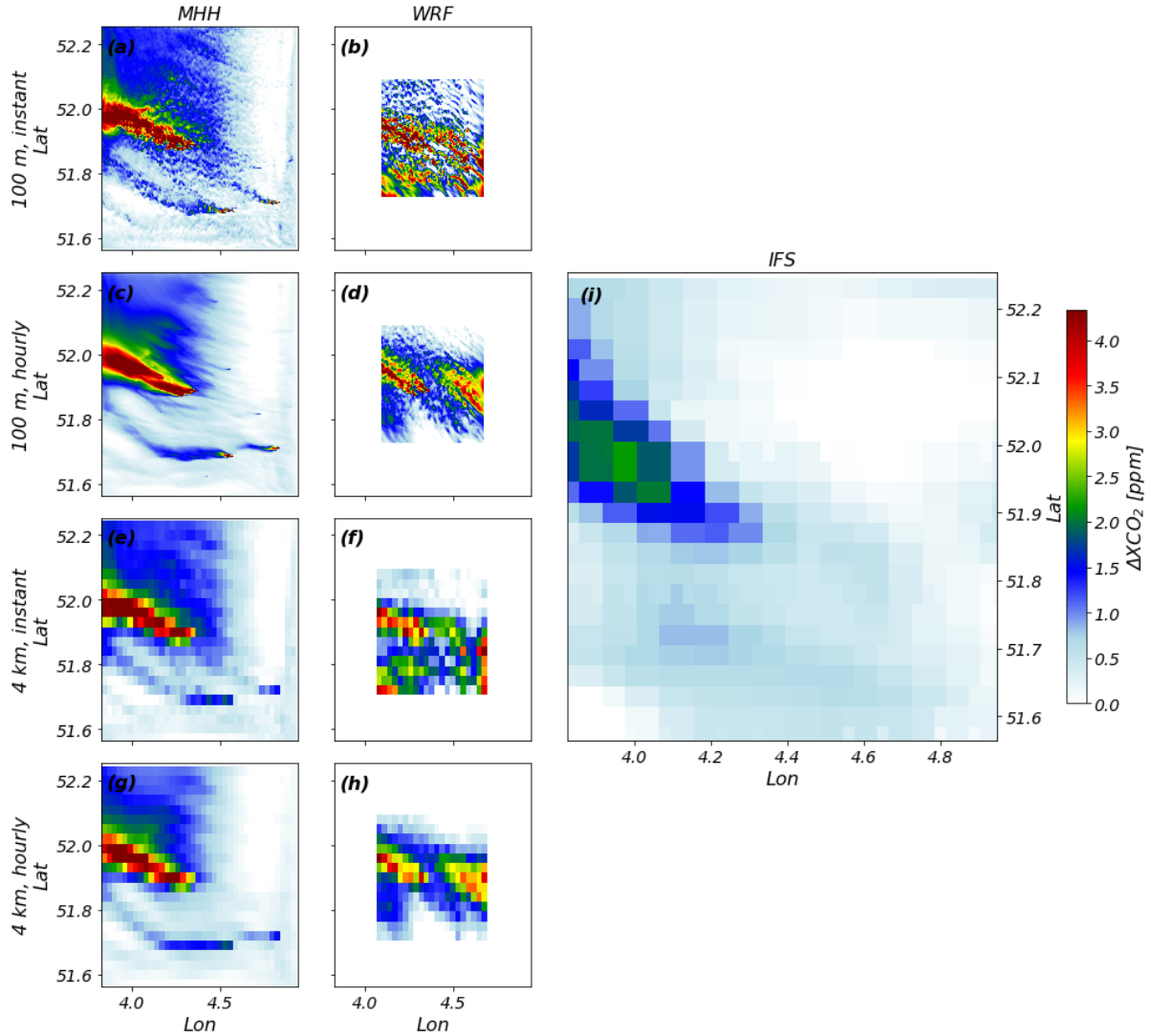


**Figure 3.6:** Rotterdam XCO<sub>2</sub> plume (ppm) as seen in MicroHH (left column), WRF (middle column) and IFS (right). The panels show XCO<sub>2</sub> values with the background subtracted. Panels a) and b) show instantaneous plumes at native (100 m) resolution at 02-09-2022 12 UTC, Panels c) and d) give time averages over one hour (12–13 UTC), and panels e) and f) show instantaneous plumes at 12 UTC coarsened to IFS resolution (4 km). We note here that underlying IFS emissions remain coarser than LES-model emissions (aggregation errors). Finally, panels g) and h) give hourly averages (12–13 UTC) of plumes first averaged to IFS resolution. Panel i) shows the IFS plume in its original resolution at 12 UTC (hourly average, 4 km spatial resolution).

Figure 3.6 panels a) and b) show instantaneous plumes at 12 UTC and with the original model resolution (100 m) as seen in MicroHH and WRF, respectively. In both plumes the high spatial variability and individual plume puffs are clearly visible. This is especially clear in MicroHH, which has only background inflow and all plume structures are generated within the domain. In WRF, for which only the 5th (D05) inside domain is shown in panel b, there is a clear inflow

of plume structures from the outside domain (D04) that interferes with the Rotterdam plume. This hampers the visual separation of Rotterdam plume. Time averages over 12–13 UTC from the two models are shown in panels c) and d). The MicroHH plume is significantly smoothed out without individual puffs visible. The time-averaged WRF plume retains some of the structure, which is a consequence of WRF having only 6 (10 min resolution) instantaneous fields recorded in an hour (MicroHH has 60 with a min resolution). Furthermore, the MicroHH plume retains the maximum concentrations intensity indicating small lateral plume spreading. This is less noticeable in WRF, where the maximum concentrations are slightly smaller after averaging. Panels e) and f) show the same plume snapshot at 12 UTC (as in a) and b)) but now coarsened to the 4 km resolution employed by the IFS model. The individual eddies are now smoothed over the coarser grid in both models. However, the general characteristics of the instantaneous 100 m plume have been retained. The MicroHH and WRF plumes shown in panels g) and h) have been coarsened to 4 km resolution and averaged over 12–13 UTC. They are therefore directly comparable to the IFS plume in panel i). The IFS plume has lower in-plume values of XCO<sub>2</sub> than the WRF and MicroHH plumes. Note here, that IFS uses a different emission inventory than MicroHH and WRF.

To better visualize the differences, Figure 3.7 depicts the calculated plume center, plume width, and cross-plume mass as a function of longitude (wind blows from the east towards the west, note that the longitude axis is reversed with respect to Figure 3.5). The left-hand panels refer to the native resolution, and the right-hand panels to results coarsened to the 4 km IFS resolution (IFS remains identical).

First, coarsening the LES results to 4 km has little impact on the plume position. The IFS plume shows the strongest turning over the domain compared to the un-coarsened and coarsened LES results (upper panels). Averaging LES simulations does affect the plume width and cross-plume mass, however. First, plumes are wider in IFS compared to the coarsened LES results. Second, accumulation of cross-plume integrated mass of the Rotterdam plume is larger in the LES results on the native 100 m resolution, and is closer to the IFS results when coarsened to 4 km. For instance, in the native resolution, MicroHH shows clear point source enhancements in the 100 m simulation, which disappear when coarsened. Currently, we are investigating the impact on source estimation using (synthetic) satellite observations, e.g. from CO<sub>2</sub>M.

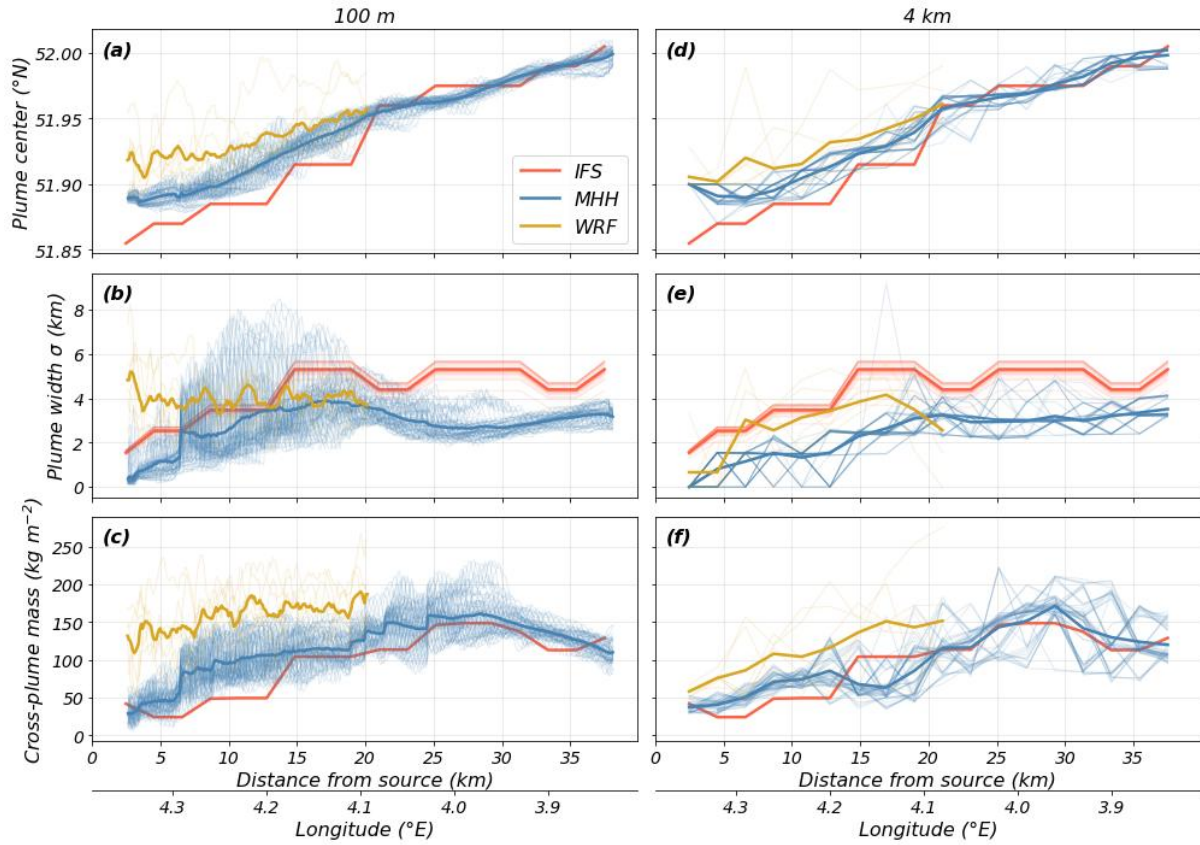


Figure 3.7: Plume center (a,d), plume width (b,e), and cross-plume integrated mass (c, f) for the Rotterdam XCO<sub>2</sub> plume in IFS, MHH and WRF. The left column (a, b, c) shows plume moments calculated from the 100 m resolution fields for WRF and MHH, while the right column (d, e, f) gives the same for fields coarsened to 4 km. In both columns plume moments from IFS 4 km and hourly resolution is overlaid for reference. Bold colours indicate hourly means while lighter colours give moments calculated from instantaneous fields between 12–13 UTC (60 in total for MHH and 6 for WRF).

## 4 Conclusions and recommendations

In this report, we aimed to define the magnitude and the spatial heterogeneity generated by local CO<sub>2</sub> emissions—from both point sources and urban areas—as model resolution increases. While we examined the physical consequences of increasing resolution, we also examined the impact of the representation of urban surface properties, the representation of the turbulence (explicit versus parameterized), and the sensitivity to mass balance techniques. The various sensitivity experiments described here have highlighted the importance of land surface parameterizations, the representation of plumes from distant sources in densely-populated areas, the importance of the high-resolution and the ability to resolve the plume features in the first 15km from the source, and the methodology when comparing plumes at various resolutions. We diagnosed the model performances using a wide array of ground-based sensors, in addition to satellite images which are limited by cloud coverage and by reduced XCO<sub>2</sub> enhancements compared to spatial gradients in near-surface CO<sub>2</sub> concentrations. Our main conclusions are described hereafter, helping to better design future LES simulations needed to quantify uncertainties in CO<sub>2</sub>MVS when applied to urban plumes. While additional work will provide a more complete assessment of representation errors in coarse-resolution inversions, we have determined several major drivers of uncertainties.

The accurate representation of the surface energy budget was the main driver of meteorological performances in WRF-LES, specifically the use of advanced urban land surface schemes with multiple building levels, and an additional energy model (BEM) for heating and cooling from buildings. By increasing the spatial resolution from 900m to 100m, the amplitude of the modeled CO<sub>2</sub> concentrations increased by two-fold, reaching the observed variations at various mid-cost sensors deployed in and around Paris. Additional measurements from Doppler Lidars measuring the Planetary Boundary Layer (PBL) heights across the urban landscape showed an improvement in the modeled PBL heights, with an increase over the Paris city center (UHI effect). The hourly variations represented by correlation coefficients did not show any significant change, as rapid plume fluctuations remain nearly impossible to predict, but are captured statistically over longer time periods. For satellite applications, the urban plume structures evolved from a broad diffuse structure (at 900m) to three smaller plumes corresponding to large point sources (urban heating systems) at 100m resolution.

When comparing to observed plumes from TROPOMI, the aggregation (coarsening) from 100 m to 4 km did not modify the plume's centre line but it affects its width, its peak concentrations and fluctuations. Beyond 15-20km from the city center, the two resolutions converge to similar plume structures, impossible to distinguish as the simulated gradients decrease as a function

of the distance to the source (due to horizontal diffusion). Overall, the total cross-plume mass applied to different models (IFS at 4km and MHH at 100m) show similar results, despite large variations in width and fluctuations. The near-source meandering of the plume differs from the MHH reference run, similar to a satellite snapshot. Representation errors become large in the near-field of large emission hotspots, due to largely unresolved eddies.

We note here that the wide IFS plume is not only a grid-resolution effect. Even after coarsening our original grid to 4 km, and aggregating snapshots to hourly averages, both LES plumes remain narrower than IFS. The extra width in IFS must therefore come from its parametrised mixing, wind turning and emission inventory, which has a different budget and different resolution than the emission inventory used in the LES simulations. This is a useful nuance to Brunner et al. (2023), who attribute wide plumes in coarse models mainly to resolution. In addition, output frequency is an important parameter to consider when building hourly means. Six snapshots per hour (WRF) are not sufficient to give a representative hourly-mean plume, while 60 (MHH) are.

Regarding the CO<sub>2</sub> boundary conditions, we note that large plumes coming from distant sources are impacting the observed enhancements over Rotterdam. For such a large urban area, boundary conditions can matter more than resolution. WRF's inflow from the outer nests is of the same order as the Rotterdam signal. It inflates width and integrated mass, and averaging cannot remove it. Setting up the domain so the target plume can be isolated is at least as important as resolution.

## 5 Bibliography

Brunner, D., Kuhlmann, G., Henne, S., Koene, E., Kern, B., Wolff, S., Voigt, C., Jöckel, P., Kiemle, C., Roiger, A., et al.: Evaluation of simulated CO<sub>2</sub> power plant plumes from six high-resolution atmospheric transport models, *Atmos. Chem. Phys.*, 23, 2699–2728, <https://doi.org/10.5194/acp-23-2699-2023>, 2023.

Lauvaux, T., A. Rafalimanana, A. Raznjevic, and M. Krol: D3.2 Impact of boundary conditions, 20 May 2025, CATRINE-D3.2-V1.0, url : <https://www.catriner-project.eu/sites/default/files/2025-05/CATRINE-D3.2-V1.0.pdf>

Rafalimanana, A., Lauvaux, T., Abdallah, C., Chariot, M., Ramonet, M., Doc, J., Laurent, O., Lopez, M., Raznjevic, A., Krol, M., Järvi, L., Christen, A., Looschelders, D., David, L., Sanchez, O., Bignotti, L., Loubet, B., Grimmond, S., and Morrison, W.: Urban atmospheric CO<sub>2</sub> plumes from space – Part 1: Atmospheric modeling of the urban boundary layer, *EGUsphere* [preprint], <https://doi.org/10.5194/egusphere-2026-2109>, 2026.

Rafalimanana, A., Lauvaux, T., Abdallah, C., Chariot, M., Ramonet, M., Doc, J., Laurent, O., Lopez, M., Raznjevic, A., Krol, M., Järvi, L., Christen, A., Looschelders, D., David, L., Sanchez, O., Bignotti, L., Loubet, B., Grimmond, S., and Morrison, W.: Urban atmospheric CO<sub>2</sub> plumes from space – Part 2: Representation of fine-scale structures, *EGUsphere* [preprint], <https://doi.org/10.5194/egusphere-2026-2581>, 2026.

Soulie, A., Granier, C., Darras, S., Zilbermann, N., Doumbia, T., Guevara, M., Jalkanen, J.-P., Keita, S., Liousse, C., Crippa, M., Guizzardi, D., Hoesly, R., and Smith, S. J.: Global anthropogenic emissions (CAMSGLOB-ANT) for the Copernicus Atmosphere Monitoring Service simulations of air quality forecasts and reanalyses, *Earth Syst. Sci. Data*, 16, 2261–2279, <https://doi.org/10.5194/essd-16-2261-2024>, 2024.

van Stratum, B. and M. Krol: D3.3: Evaluation and Validation of Resolved and Parameterised Plume Rise in Large-Eddy Simulations of Buoyant Emissions. 18-06-2025, CATRINE-D3-3-V1.0, url: <https://www.catriner-project.eu/sites/default/files/2025-06/CATRINE-D3-3-V1.0.pdf>

CATRINE D3.2 Impact of Boundary Conditions <https://www.catriner-project.eu/deliverables>

CATRINE D3.3 Plume Rise and Chemistry <https://www.catriner-project.eu/deliverables>

## Document History

| Version                        | Author(s)                                   | Date       | Changes                                |
|--------------------------------|---------------------------------------------|------------|----------------------------------------|
| 0.1 (Initial document created) | Thomas Lauvaux,<br>Maarten Krol             | 29-09-2026 | None                                   |
| 1.0 (After internal review)    | Thomas Lauvaux,<br>Maarten Krol             | 07-10-2026 | Processed comments internal reviewers. |
| 2.0                            | Thomas Lauvaux,<br>Maarten Krol.<br>RPhipps | 8/10/26    | Minor formatting updates               |
|                                |                                             |            |                                        |
|                                |                                             |            |                                        |

## Internal Review History

| Internal Reviewers   | Date       | Comments |
|----------------------|------------|----------|
| Anna Agusti-Panareda | 05-10-2026 |          |
| Michail Diamantakis  | 05-10-2026 |          |
| Jordi Vila           | 05-10-2026 |          |
|                      |            |          |
|                      |            |          |