



D4.14.2 Definition of indicators/metrics providing information on air quality in relation to the atmospheric stratification and dynamics. [B15]



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1 INTRODUCTION

Atmospheric aerosols and gas, originating from both natural and anthropogenic sources, play a crucial role in Earth's climate, air quality, and human health. They influence the planetary energy balance by scattering and absorbing solar and infrared radiation and have significant implications for air quality, with direct health effects. Despite extensive research, major uncertainties remain regarding the factors controlling the concentration and distribution of aerosol and gas across the atmospheric layers.

A key factor influencing pollution dispersion is the Planetary Boundary Layer (PBL), the lowest layer of the atmosphere that directly interacts with the Earth's surface. The PBL controls the mixing and vertical transport of pollutants, with its height and structure varying due to meteorological conditions, surface properties, and local emission sources. Seasonal changes in the PBL significantly impact air quality; for example, a shallow PBL during winter can trap pollutants near the surface, while a deeper PBL in summer facilitates their dispersion. Additionally, complex interactions with urban heat islands, wind patterns, and extreme weather events can further modulate pollutant concentrations.

Given these dynamics, improving our ability to characterize the PBL and its role in pollutant dispersion is critical for air quality assessment and mitigation strategies. The ITINERIS project aims to address this challenge by integrating Ceilometer-based remote sensing with in-situ observations and reanalysis data providing a comprehensive dataset to evaluate PBL evolution and its impact on aerosol and trace gas concentrations.

This deliverable focuses on defining key indicators and metrics that quantify air quality in relation to atmospheric stratification and dynamics, structured around three main activities:

- Integration of ceilometer with in-situ observations
- Simultaneous measurements at different altitudes
- Integration of reanalysis data with historical datasets

These activities contribute to improving air quality monitoring strategies, supporting policymakers in developing targeted interventions to mitigate pollutant exposure and its associated health impacts.

2 PILOT STUDIES AND FIELD CAMPAIGNS

Within the framework of the pilot, four field experiments, merging remote-sensing and in-situ measurements, have been conducted: RI-URBANS, GAI_{infra}, AIRPODYNAMICS and WHAFFERS.

2.1 RI-URBANS

A comprehensive one-year measurement campaign (2023) in Milan was conducted within the framework of the RI-URBANS project. Milan is the second-largest city in Italy and, due to the poor air circulation in the Po Valley, is prone to poor air quality. As one of the 13 European pilot cities of RI-URBANS, Milan was chosen for its strategic relevance in understanding urban air pollution dynamics.

The campaign integrated in-situ and remote sensing observations across four key measurement sites, designed to characterize air quality, aerosol properties, and atmospheric stratification (Figure 1). The two primary in-situ sites were:

- Milan-CNR (urban background station) – Representing typical urban pollution levels.
- Milan-Linate airport (urban hotspot site) – A high-emission area near intense traffic and airport operations.

At Milan-Linate, the AEROLAB platform, an ACTRIS-RI exploratory unit, was deployed from January to September 2023. It conducted continuous measurements of Aerosol optical properties (absorption, scattering, backscattering), aerosol size distributions from 10 nm to 20 μm , covering both ultrafine and coarse particles, trace gas concentrations (NO , NO_2 , NO_x) and meteorological parameters, including wind, temperature, pressure, and downwelling radiation. Simultaneously, the Voyager3 laboratory, located at Milan-CNR, provided an advanced suite of instruments for online aerosol chemical composition (ToF-ACSM), volatile organic compounds (VOCs) analysis using a VOCUS CI-ToF (Chemical Ionization Time of Flight Mass Spectrometer equipped with a VOCUS reactor (ion-molecule reaction region where the proton-transfer reaction happens) and greenhouse gas monitoring (CO_2 , CH_4 , H_2O) with a Picarro analyzer. Although most analyses focused on Linate, the CNR site served as a reference for urban background conditions, enabling comparisons between hotspot emissions and typical urban air masses. In addition to in-situ measurements, lidar-based aerosol remote sensing measurements were performed at university of Milan-Bicocca (Remote 1) and Rubattino Station (Remote 2). These sites hosted two ceilometers as part of the ALICENET network: CHM15k (Lufft) at Bicocca, operating January–September 2023, CL61 (Vaisala) at Rubattino, operational since June 2023, with depolarization capability useful for aerosol typing. Ceilometer data provided continuous profiling of aerosol attenuated backscatter, essential for determining the mixed aerosol layer (MAL), a key indicator of planetary boundary layer (PBL) height.

This campaign represents the most extensive and detailed atmospheric observation effort in Milan to date. By integrating in-situ and remote sensing data, it enables a multi-dimensional analysis of urban air pollution, boundary layer dynamics, and aerosol interactions.

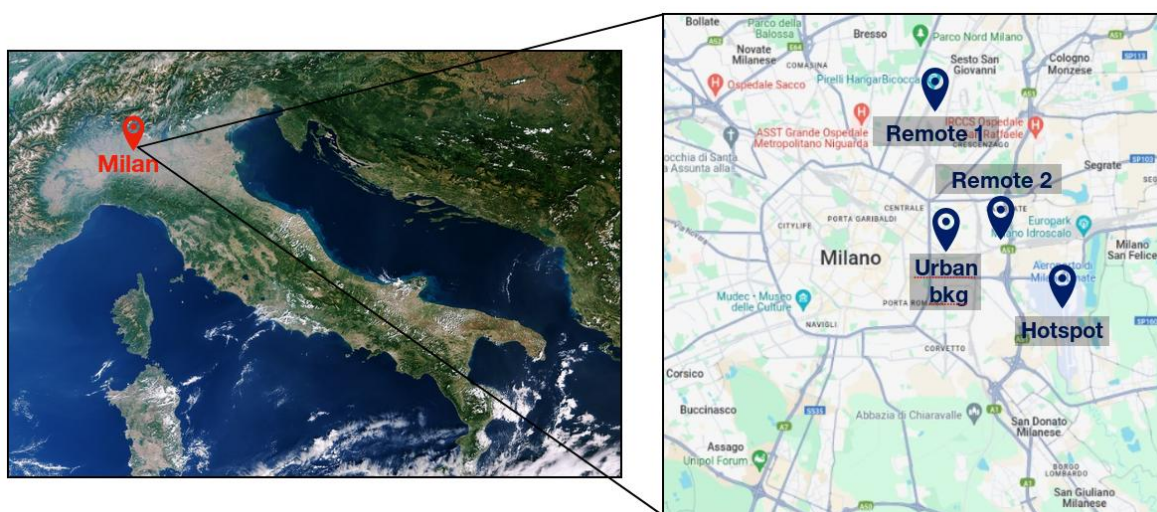


Figure 1 Left panel: location of the city of Milan in Italy; right panel: map of the city with the position of the four measurements stations.

2.2 GAInfrA

Thanks to the synergy with the PRIN GAIA project, a marine version of the AEROLAB, GAInfrA (Figure 2) was developed. GAInfrA was deployed aboard the German research icebreaker Polarstern, managed by AWI, during the 2024 Arctic cruise between June and October. This advanced mobile laboratory incorporated the Lufft-CHM15K ceilometer acquired within ITENERIS project, specifically designed to operate under extreme Arctic marine conditions. Throughout the campaign, GAInfrA's instrumentation continuously collected high-temporal-resolution data on aerosol chemical, physical, and optical properties, broadband and spectrally resolved radiation budgets, as well as aerosol and cloud vertical profiles. The platform demonstrated outstanding reliability, successfully collecting high-quality data for over 90% of the campaign duration, significantly extending observational capabilities over marine environments and providing critical insights into aerosol–radiation interactions and their implications for climate dynamics.



Figure 2 Deployment of the aerosol in-situ and remote sensing on board of the Research Vessel Polarstern. Track of the Polarstern cruise in 2024.

2.3 AIRPODYNAMICS

AirPoDynamics aims to assess the impact of planetary boundary layer (PBL) dynamics on the concentration and properties of aerosol particles in the Po Valley (Figure 3). From August to September 2024, a comprehensive measurement campaign was conducted at two sites within the ACTRIS Po Valley facility: the urban location of Bologna (BO) and the mountain observatory of Monte Cimone (CMN).

At the Bologna site (54 m a.s.l.), remote sensing measurements were conducted using a ceilometer (Lufft CHM15k) to retrieve aerosol backscatter profiles, from which the vertical distribution of aerosols and the height of the mixed aerosol layer (MAL) were derived. For the MAL retrieval, the methodology adopted in the RI-URBANS project was combined with a deep learning-based image segmentation approach (Wijnands et al., 2024). This hybrid method was employed to enhance the robustness and accuracy of MAL estimation from ceilometer measurements. Although BO and CMN are approximately 60 km apart, the tropospheric dynamic conditions observed over BO were considered broadly representative of those at CMN during the campaign period. In situ measurements of aerosols particles and trace gases were performed simultaneously at both sites. This deliverable will focus on the carbonaceous fraction of the aerosol particles: black carbon and organic matter. Equivalent black carbon (eBC) mass concentration was measured with Aethalometer instruments

(AE33, Magee Scientific) at both sites. Aerosol chemical composition was characterized using an Aerosol Chemical Speciation Monitor (ACSM-ToF) equipped with a ToF mass analyzer at CMN and an ACSM-QMS equipped with a quadrupole mass analyzer at BO. Trace gases included measurements of volatile organic compounds performed with a Vocus CI-ToF-MS, installed at BO for measuring gases from anthropogenic as well as biogenic sources.

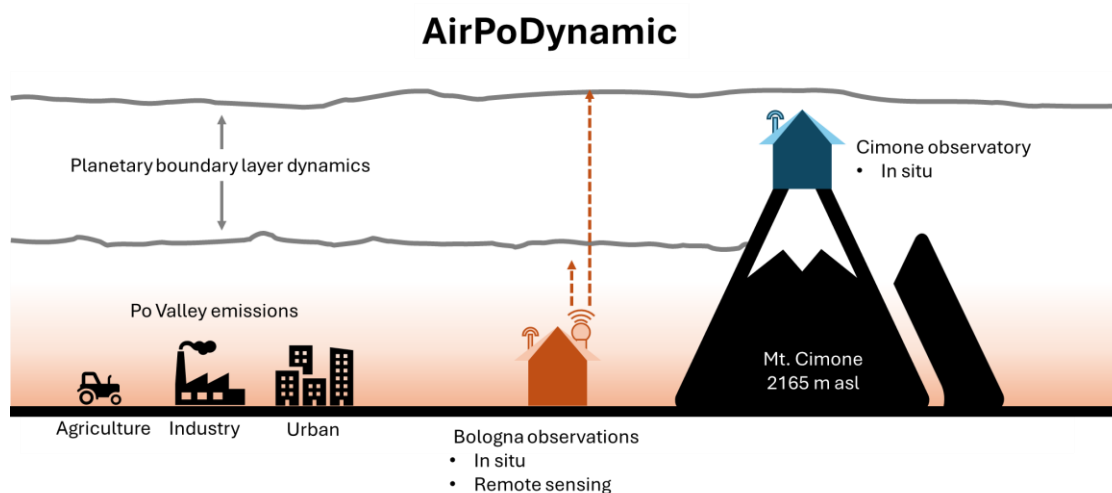


Figure 3 Schematics of the AirPodynamics campaign held in the Po Valley between August and September 2024.

2.4 Mt. Cimone long-term observations

Among the long-term observations, special focus is given to the measurement of aerosol absorption coefficient using the Multi-Angle Absorption Photometer (MAAP). These measurements, covering the period 2007–2023, provide one of the longest continuous time series of aerosol light absorption in Southern Europe. From MAAP data, the equivalent black carbon (eBC) concentrations were derived, offering crucial insights into the variability and long-term trends of light-absorbing aerosols at high altitude. While generally isolated from local emissions, CMN is seasonally affected by upward transport from the planetary boundary layer, including pollution exported from the Po Valley. To understand the seasonal impact of the boundary layer dynamics on BC concentration at CMN, we integrated data from reanalysis and modeling tools with in-situ observations over the period 2007–2023. The ERA5 reanalysis was used to extract the planetary boundary layer (PBL) height, providing insight into the site's coupling with boundary layer dynamics and its exposure to Po Valley emissions. These global georeferenced reanalysis data are available with a $0.25^\circ \times 0.25^\circ$ horizontal resolution and a pressure range of 1000–1 hPa binned on 37 pressure levels. A detailed description of the ERA5 products is provided by Hersbach et al. (2020). CAMS global reanalysis data were employed to retrieve BC concentration at regional scale, enabling the characterization of large-scale patterns and long-range transport events. These global georeferenced reanalysis data (fourth generation ECMWF global reanalysis; EAC5) are available with a $0.75^\circ \times 0.75^\circ$ horizontal resolution and a pressure range of 1000–1 hPa binned on 25 pressure levels. An overview of the CAMS products is provided by Inness et al. (2019), while details on the aerosol schemes are given in Morcrette et al.

(2009) and Bozzo et al. (2017). Additionally, the FLEXPART Lagrangian dispersion model was applied to determine the source region and emission type of the air masses reaching the site, distinguishing between anthropogenic and natural contributions to black carbon aerosol (Pisso et al., 2019). Domestic sources are defined as residential and commercial sector including emissions from combustion in heating and cooking stoves and boilers in households and public and commercial buildings. Transportation includes emissions from all land-based transport of goods, animals and persons on road networks and off-road activities. Forest fire contribution represents open biomass burning (excluding agricultural fires) and accounts, only, for natural emissions. This combined approach allowed for a more robust interpretation of the observed aerosol variability at CMN, particularly regarding the roles of PBL dynamics, free-tropospheric influence, and Po Valley outflow.

Integration of long-term observations with numerical simulation at Mt.Cimone

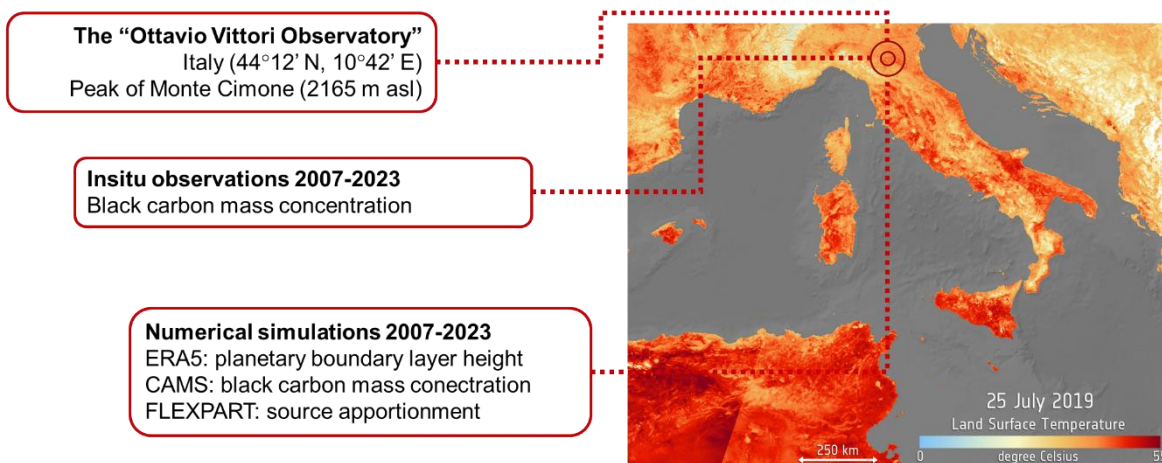


Figure 4 Integration of long-term observations performed at Cimone with Copernicus and FLEXPART products

2.5 WHAFFERS campaign

In the frame of the ITINERIS project, the Fourier Transform Spectrometer (FTS) IFS 125HR, produced by Bruker, is expected to be installed at the CNR-ISAC of Bologna during the next months. This instrument will acquire ground-based Infra-Red atmospheric spectra with a high spectral resolution (0.0036 cm^{-1}) suitable to retrieve the concentration of several atmospheric trace gases (such as: O_3 , HCl , HF , ClONO_2 , HNO_3 , N_2O , CH_4 , CO , C_2H_6 , HCN , CO_2 , H_2O , O_2 , HDO) present in the PBL. These measurements will provide further useful information to investigate the role of the PBL height in the dispersion of the pollutants. However, since the IFS 125HR instrument is not already present at the institute, to acquire expertise on a similar instrument (FIRMOS), we participated to the measurement campaign WHAFFERS, organized by ESA. The aim of this campaign was to exploit the ground-based measurements acquired by FIRMOS, a ground-based FTS developed by the CNR-INO of Florence, capable to measure up to the Far IR (FIR) spectral region. WHAFFERS started at the beginning of January 2025 and continued up to the 14th of February 2025. It took place in Canada, at two different sites at the same time: Ottawa, where FIRMOS was installed and Gault, a natural reserve close to Montreal.

For the first month, FIRMOS measured the zenith atmospheric IR spectra at the Ottawa airport. During specific periods, FIRMOS' measurements were integrated with correlative measurements of chemical and physical atmospheric parameters and microphysical cloud properties measured from aircraft by both in-situ and remote instruments. Moreover, dedicated radiosoundings have been also performed from the Ottawa airport. During the last week, FIRMOS was moved to Gault to measure in synergy with two other similar ground-based spectrometers, a LIDAR and still supported by correlative measurements from radiosoundings and aircraft flights. Moreover, a particular attention to the measurements acquired during the PREFIRE satellite overpass was given.

The primary objective of this campaign is to scientifically support the future ESA satellite mission FORUM and to help to define the strategy for its in-orbit validation. However, the large amount of collected data together with the IR spectra acquired by FIRMOS, represents a unique opportunity to assess the quality of the chemical compounds' information retrieved from ground-based IR spectra. This first experiment is hence preparatory to the acquisition and processing procedures of the FTS IFS125HR, that will be installed at CNR-ISAC of Bologna and provides important hints on how it can be managed to study the trace gases concentrations in relation to the PBL.



Figure 5 FIRMOS measuring atmospheric zenith-sky IR spectra at Ottawa airport.

3 INDICATORS AND METRICS

3.1 Collocated remote sensing and in-situ observations

In this part of the deliverable, we address the metrics derived by directly combining the height of the Mixing Layer (MAL), observed with remote sensing, with the concentration of pollution tracers at the ground. In the current status, we focused on anthropogenic primary emitted aerosol particles such as black carbon, greenhouse gases (CO_2 and CH_4) and volatile organic carbon (VOC).

3.1.1 Determination of the Mixed Aerosol Layer from Ceilometer Data

The height of Mixed Layer Height (MAL) is a key parameter for assessing and managing air pollution, as it defines the vertical extent of the atmosphere where aerosols and trace gases are mixed

by turbulence. Its height strongly influences surface pollutant concentrations, especially in urban areas, by determining the volume available for dilution. Accurate MAL estimation is therefore essential for both atmospheric research and operational applications, including air quality forecasting and health risk assessment. Understanding its temporal and vertical evolution also provides insights into the roles of local sources, long-range transport, and secondary aerosol formation making high-resolution, continuous observations of MAL increasingly vital. In recent years, the deployment of large-scale ceilometer networks, such as the European EUMETNET E-PROFILE and the Italian ALICENET has enabled continuous, high-resolution monitoring of aerosol profiles across vast geographical areas. Ceilometers, originally designed for cloud base detection, are now widely used for tracking the evolution of aerosol layers and boundary layer dynamics, thanks to improvements in signal processing and interpretation techniques. Within ALICENET, a two-step approach based on physical principles is used to retrieve the MAL height from ceilometer data (Bellini et al., 2024, 2025). First, the temporal evolution of the aerosol backscatter signal is analyzed using a Dynamic Time Warping (DTW) algorithm, which quantifies the local displacement between consecutive profiles and highlights vertical motion due to turbulence. This output serves as a proxy for vertical aerosol fluxes. Second, a statistical analysis of the variability in this signal over 30-minute time windows is performed. The altitude at which this variability rapidly decreases is identified as the top of the Mixed Aerosol Layer, corresponding to the height where turbulent mixing becomes inefficient. This method, fully automated, has been successfully applied in the RI-URBANS campaign in Milan. A different approach was adopted in the AirPoDynamics campaign, where the DeepPathFinder algorithm was used. This method relies on deep learning and image segmentation to detect atmospheric layers directly from ceilometer backscatter data. The algorithm was adapted and modified for compatibility with the CHM15K ceilometer settings used in the campaign. Input samples for the determination of the MAL consisted of 224×224 pixel plots extracted from the full 24-hour Range-Corrected Signal (RCS), each covering a 56-minute observation period and a maximum height of 3360 meters.

The results for the AirPoDynamics campaign are reported in Figure 6. For this analysis, days affected by precipitation were excluded, as the MAL is undefined during precipitation events.

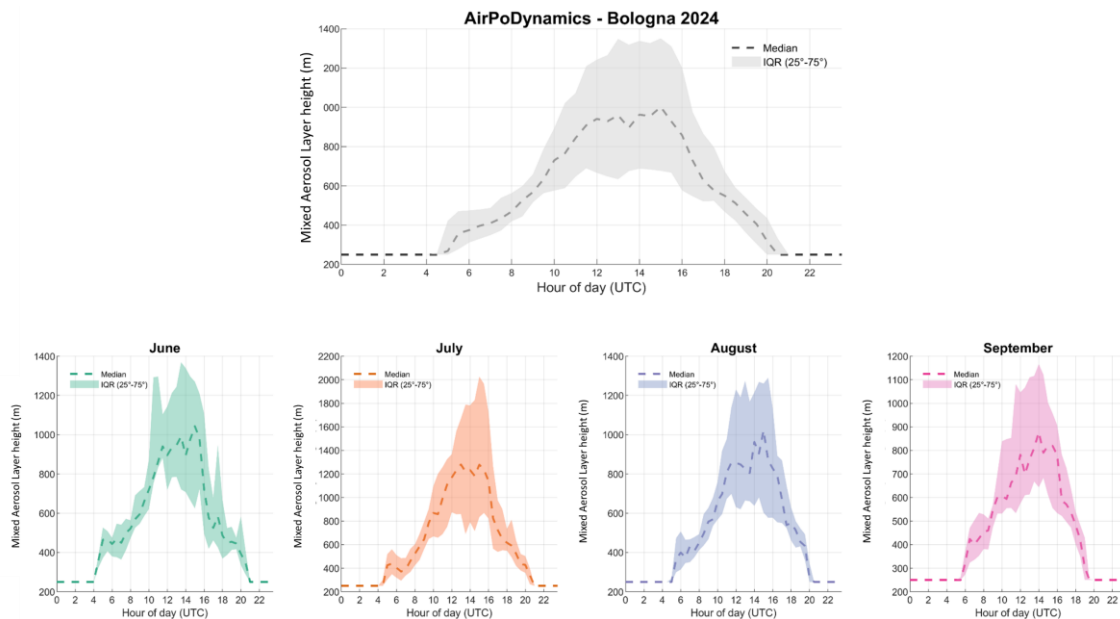


Figure 6 - Diurnal evolution of the height of the mixed aerosol layer (MAL) during the AirPoDynamics campaign in Bologna (2024)

The figure shows the median diurnal cycle of the MAL derived from ceilometer observations using the adapted DeepPathFinder algorithm. The top panel reports the overall median and interquartile range (25°–75° percentile) for the entire campaign. The bottom four panels show the same statistics for each month from June to September.

The MAL exhibits a typical summertime pattern, with a rapid growth starting at sunrise, reaching its maximum in the early afternoon (between 13:00 and 15:00 UTC), and then decreasing sharply after sunset.

- June and August show relatively similar behavior, with median MAL peaking around 1200–1300 m.
- July displays the highest values, with median peaks exceeding 1500 m, likely due to stronger surface heating and increased convective activity.
- September presents lower MAL values, with the median peaking just below 1000 m, reflecting the seasonal transition to cooler conditions and reduced solar input.

The interquartile range remains narrow during nighttime and early morning hours, when the boundary layer is shallow and stable, and widens significantly in the afternoon, indicating greater variability in turbulent mixing and vertical development under convective conditions.

3.1.2 Definition of the ventilation index

The ventilation index (VI) was derived to quantify the efficiency of ventilation in dispersing pollutants at ground level (Murthy et al., 2020). It is defined as the product of horizontal wind speed and the height of the PBL. Since wind data in our dataset are available only from weather stations, this index is based on surface wind measurements. Typically, high values of the VI indicate good ventilation, which is expected to correspond to improved air quality, as pollutants are dispersed more

effectively. On the other hand, low VI values reflect poor ventilation, suggesting limited pollutant dispersion and potentially higher concentrations at the surface, which may lead to worse air quality. To support this interpretation, we computed the daily evolution of the VI for both February and August. During August, typical daytime VI values exceeded 3100 m²/s, while in February they rarely surpassed 1900 m²/s. The monthly averages confirm this difference, with a mean VI of approximately 2120 m²/s in August and only 1320 m²/s in February. This contrast reflects both the higher PBL heights and stronger surface winds typically observed during summer months. The seasonal and diurnal variability of the VI further supports the observed differences in BC concentrations and their relationship with boundary-layer dynamics. High VI values during summer, specifically during afternoons, facilitate pollutant dispersion and are associated with lower surface BC levels. In contrast, persistently low wintertime VI confirms that stagnant conditions dominate, limiting dilution and promoting accumulation of pollutants near the surface.

3.1.3 Diurnal variability of greenhouse gases with planetary boundary layer.

During the RI-URBANS experiment, the diel variabilities of CO₂ and CH₄ were characterized by evident cycles in all seasons, characterized by an increment of hourly values during early morning and evening/night. These cycles were consistent with those reported in other urban areas. Both the CO₂ and CH₄ diurnal amplitudes were larger in winter (73.8 ppm and 302.8 ppb, respectively) than in summer (38.1 ppm and 176.5 ppb respectively). In the morning, as a function of the different months, CO₂ peaked at 5:00 – 6:00 UTC (July – October) and 6:00 - 8:00 UTC (November – March) clearly pointing out the impact of the adoption of the daylight saving time (DST, from April to October) which led to a shift of anthropogenic emissions 1 hour earlier when solar time (ST) is adopted on the last Sunday of October. The evening peaks in CO₂ was not visible in July and August, probably due to the combined decrease of vehicular traffic loading and domestic heating together with the relatively high MAL at 18:00 UTC. This observed variability is the result of several factors: the seasonal activity of the biosphere (including vegetation and microbial activities), the temporal variability of anthropogenic emissions (including domestic heating, vehicular traffic, energy production, industry, waste management), as well as the seasonal cycle of the MAL, which influence the dilution and the mixing of local GHG and pollutant emissions.

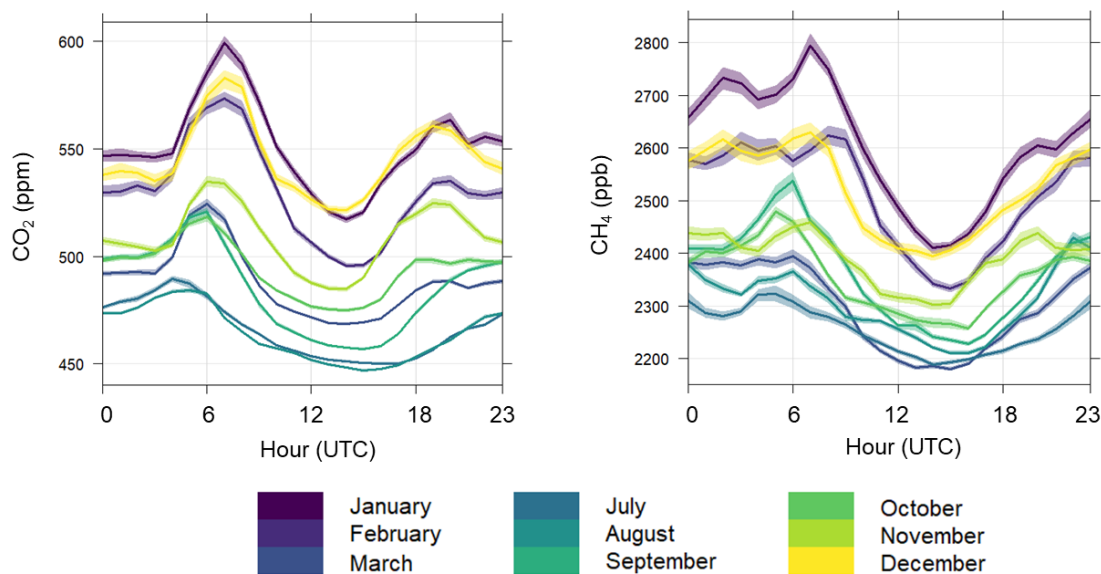


Figure 7 Mean hourly values of CO_2 and CH_4 at Milan during the RI-URBANS experiment. Shaded areas denote the 95% confidence level while the color code denotes the months of observations from July 2023 to March 2024.

Wind speed is a key factor in modulating the dispersion of CO_2 and CH_4 emissions in urban areas (e.g. Xueref-Remy et al., 2018) and it can be considered as proxy for dilution and ventilation within the atmospheric boundary layer. For all the seasons, the absolute values as well as the range of CO_2 and CH_4 mole fractions decreased with the increase of wind speed. At low wind speed, the relatively high level of variability can be associated with the impact of fresh and local/regional anthropogenic CO_2 emissions. For high wind speeds, typically associated with northerly winds, the hourly averaged mole fractions tended to converge towards background values.

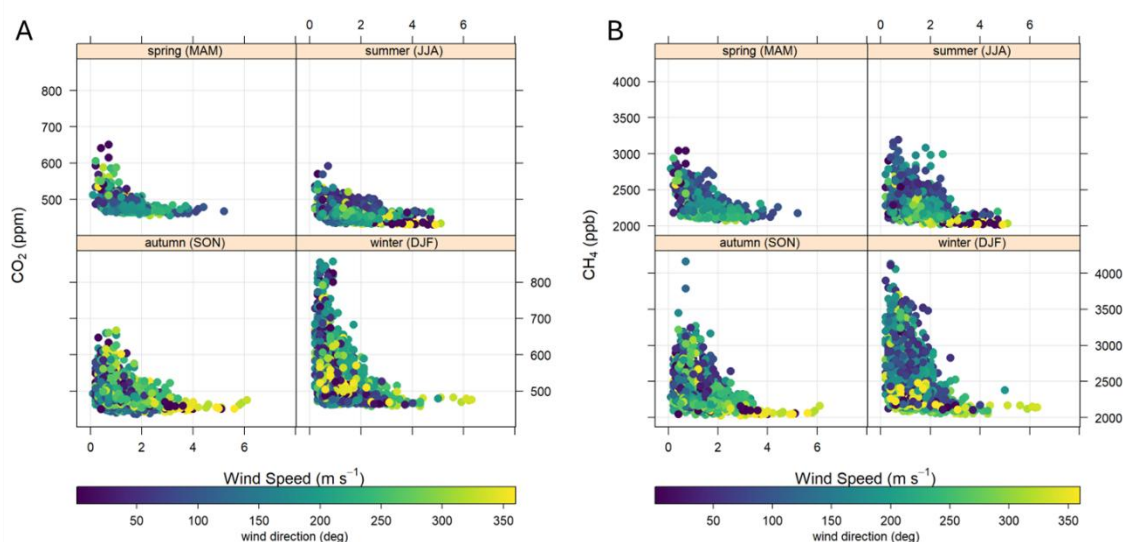


Figure 8 CO_2 (A) and CH_4 (B) hourly means at Milano as a function of the wind speed (m s^{-1}) and colored by wind direction (degrees).

3.1.4 Diurnal variability of volatile organic carbon with planetary boundary layer.

Volatile organic compounds (VOCs) are reactive trace gases emitted in the atmosphere from natural and anthropogenic sources.

In order to investigate the main removal mechanisms influencing VOC atmospheric concentrations in Milan and in Bologna we focused on six different VOCs having remarkably different atmospheric lifetimes and reported their diel variability together with the mixed aerosol layer. Figure 9 shows measurements from wintertime in 2023 in Milan (Figure 9b) and from summertime in 2023 in Milan (Figure 9b), while Figure 10 shows measurements from September 2024 in Bologna.

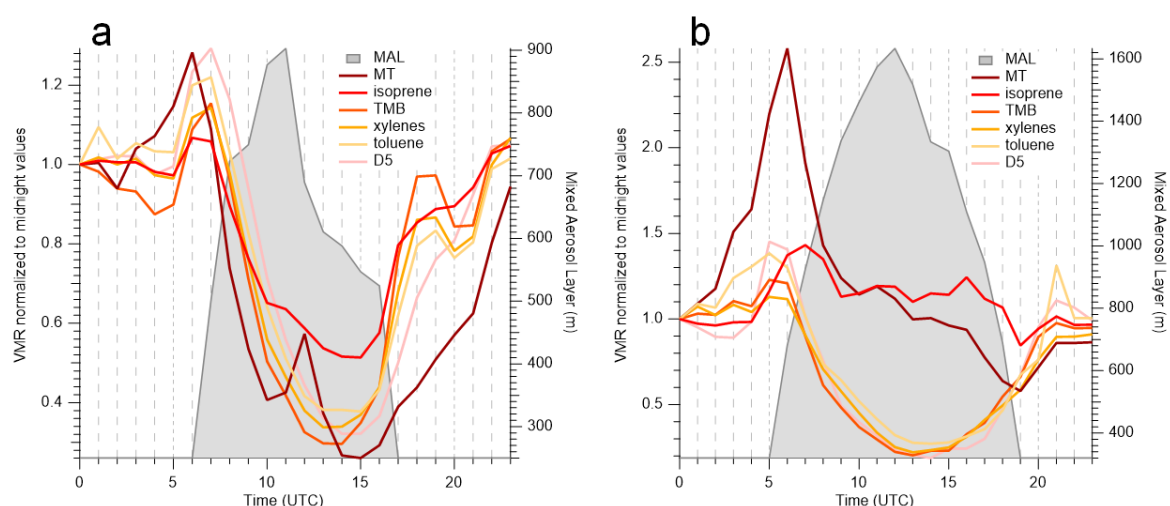


Figure 9 Diel profiles of normalized to midnight values volume mixing ratios of six VOCs having different atmospheric lifetimes with median diel values of mixed aerosol layer height retrieved from ceilometer measurements. VOCs are sorted in the legend from the most reactive one to the least reactive one. MT stands for monoterpenes while TMB stands for trimethylbenzenes. a) shows values measured during winter 2023, while b) shows values measured during summer 2023. Measurements were performed in Milan during the 2023 RI-URBANS campaign.

All compounds have larger concentrations during the night than during the day in winter (Figure 9a) and show two simultaneous peaks in the morning and in the evening, suggesting that most of these compounds are emitted from traffic with the two peaks representing the traffic rush hours in Milan. Interestingly, both isoprene and MT, mainly emitted from biogenic sources, show some differences when compared with the other VOCs. Monoterpenes (MT) have a distinct profile characterized by a morning peak occurring earlier in the day, a midday peak possibly resulting from local cooking activities, and lower concentration during the evening. Isoprene has larger concentration during the day suggesting continuous emissions from local biogenic sources. During summertime (Figure 9b), the majority of VOCs show a similar pattern: they have larger mixing ratios during the night and smaller mixing ratios during the day. Morning and evening peaks are shifted compared with wintertime data, due to differences in winter and summer times as well as duration of sunlight. Again, MT and isoprene have a distinct pattern, with larger concentrations during daytime reflecting photosynthetic activity from vegetation.

In winter and in summer, the dominant removal mechanism during daytime is atmospheric dilution, due to the increased PBL height as reflected in the MAL measurements. This is noticeable in both the mirrored profiles of VOCs and MAL, as well as the similar normalized concentrations of VOCs during the day. Indeed, if chemical loss was the dominant removal mechanism during the day, a resulting distinct normalized volume mixing ratio of the six VOC would be observed. Particularly, MT, having the shortest lifetime, would have had the lowest VMR, while D5, having the longest lifetime, would have had the largest VMR. Such differences should be larger than the measurement uncertainties as differences in rate constants of the reactions between VOCs and OH span two order of magnitudes across the six selected compounds.

Similarly, in Bologna, VMR differences during the day do not point at chemical reactions as the main removal mechanism of the measured VOC during daytime (Figure 10). Like in Milan, most of the measured VOC have mirrored diel profiles with MAL, and show a morning and an evening peak corresponding to anthropogenic emissions. Similarly to summertime in Milan, isoprene and MT show a different diel profile, with larger concentrations during the day for isoprene, and larger concentrations during the afternoon for MT. Interestingly, biogenic emissions in Bologna are 2x larger than in Milan.

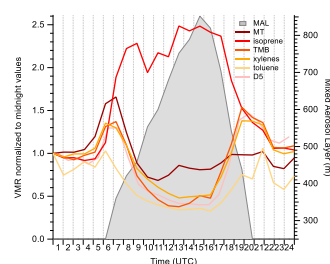


Figure 10 Diel profiles of normalized to midnight values volume mixing ratios of six VOCs having different atmospheric lifetimes with median diel values of mixed aerosol layer height retrieved from ceilometer measurements. VOCs are sorted in the legend from the most reactive one to the least reactive one. MT stands for monoterpenes while TMB stands for trimethylbenzenes. Measurements were performed in Bologna during the 2024 September EMEP-VOC campaign, to which AirPODynamics connected to.

3.1.5 Diurnal variability of primary aerosol pollutant with planetary boundary layer

The concentration of black carbon (BC) near the surface is strongly influenced by the height of the planetary boundary layer (PBL), which determines the atmospheric volume available for the dilution of emitted pollutants. Shallow PBLs, typically occurring at night or under stable meteorological conditions, limit vertical mixing and trap pollutants near the surface, resulting in elevated BC concentrations. In contrast, deeper boundary layers associated with convective mixing during daytime or warmer seasons enhance vertical dispersion, leading to lower surface BC levels (Engeln

and Teixeira, 2013; Seibert et al., 2000). This daily and seasonal modulation was clearly observed in Milan during the RI-URBANS campaign. In winter, equivalent BC (eBC) concentrations exhibited a distinct diurnal pattern, with a pronounced morning peak occurring before the full development of the PBL. As the boundary layer grew vertically through the day, BC concentrations decreased due to enhanced dilution, until convection weakened in the afternoon, reducing mixing and allowing BC to accumulate again near the surface. Although a similar diurnal cycle was observed during summer, key differences emerged compared to winter conditions. Higher temperatures in summer promoted more efficient vertical development of the PBL, with daily maximum heights often exceeding 1500 m asl, compared to less than 1000 m asl in winter. Moreover, lower emissions in summer, particularly during nighttime, contributed to an overall reduction in BC concentrations. During the day, efficient vertical dilution further decreased surface-level BC, resulting in significantly lower concentrations in summer compared to the winter (Figure 11).

3.1.6 Correlation of primary aerosol pollutants with planetary boundary layer

In light of the observed diurnal and seasonal modulation of black carbon (BC) concentrations by the planetary boundary layer (PBL) dynamics, we further investigated their statistical relationship through a linear regression analysis. This analysis aimed to quantify how variations in PBL height influence near-surface BC concentrations under contrasting seasonal conditions. Two representative months were selected: February, characterized by shallow boundary layers and high BC emissions, and August, marked by deeper boundary layers and generally lower BC concentrations. During winter (February, Figure 11c), the relationship between PBL height and BC concentration was negligible, with an R^2 value approaching zero, indicating no significant linear dependence. The absence of correlation suggests that other factors, such as thermal inversions, weak winds, and variable emission sources, play a dominant role in controlling pollutant accumulation under wintertime conditions. Under stable meteorological conditions, the PBL tends to develop poorly, further trapping pollutants near the surface. Additionally, generally higher emission levels during winter intensify this effect, making PBL height a less reliable predictor of BC variability. During summer (August, Figure 11d), the negative correlation between PBL height and surface BC concentration was strong ($R^2 = 0.81$), highlighting the dominant role of vertical mixing in modulating pollutant levels in summer. This result clearly indicates that atmospheric dilution, driven by enhanced PBL development, is a key mechanism controlling the concentration of aerosol primary emissions near the surface. Nevertheless, persistently shallow boundary layers still contribute significantly to elevated surface concentrations, by limiting vertical dispersion and enhancing the trapping of emissions near the ground.

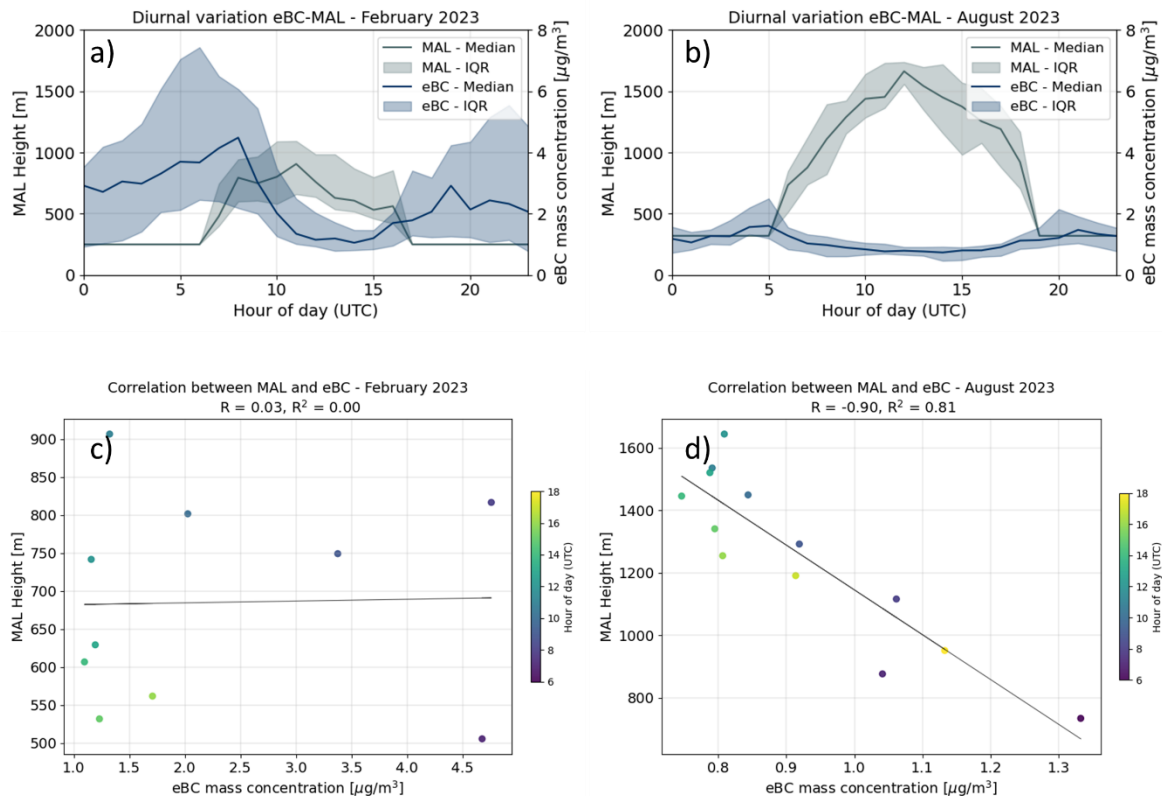


Figure 11 Diurnal evolution of equivalent black carbon mass concentration (eBC) and height of the mixed atmospheric layer (MAL) in February (a) and August (b) 2023. Correlation plot between MAL and eBC in February (a) and August (b) 2023. Data representative of the RI-URBANS Milan campaign.

3.2 Tracing boundary layer dynamics with simultaneous observations of carbonaceous particles at different altitudes

To address the influence of the boundary layer on the distribution of concentrations, we monitored simultaneously the concentration of carbonaceous aerosol particles in two locations at different altitudes, one mostly representative of the free troposphere (Mt. cimone, CMN) and one, representative of the mixing layer (Bologna, BO)

3.2.1 Organic matter and black carbon diurnal variability across the mixing layer

The diurnal variability of the mass concentration of black carbon (BC) and organic matter (OM) at CMN and BO is shown in Figure 12. BC and OM exhibit distinct diurnal variability, shaped by the dynamics of the planetary boundary layer (PBL) at both sites.

At CMN, the lowest BC and OM concentrations are recorded at night, under stable meteorological conditions, with pollutants concentrated in a thin layer near the ground. In the morning and throughout the day, vertical mixing is enhanced by convection, which facilitates the upward transport of pollutants by mountain breezes. This process, confirmed by the diurnal variability of the mixing layer high, leads to higher concentrations during the

day, peaking in the afternoon, with concentrations of BC and OM above $0.2 \mu\text{g}/\text{m}^3$. In Bologna, the daily concentrations of BC and OM were more than a factor of two higher than CMN due to the vicinity of sources.

Moreover, the diurnal profile for OM and BC is clearly different in the urban site and primarily influenced by anthropogenic emissions and the evolution of atmospheric mixing layer. Morning peaks in BC and OM concentrations are driven by increased emissions especially traffic, while enhanced photochemical reactions typical of summertime contributed to OM concentration increase. Despite a time-delay, both carbonaceous particles decreased during daytime until an evening peak. It is important to note a time delay between the two components, which offsets the time occurrence of both the maximum and minimum.

This analysis indicates a good agreement between OM and BC in the remote mountain site, indicating that both variables may be used to trace pollution injection at high altitude from the boundary layer. However, this univocal phenomenology was not observed at the urban site, where sources and photochemistry may represent a non-negligible driving force of OM next to PBL dilution.

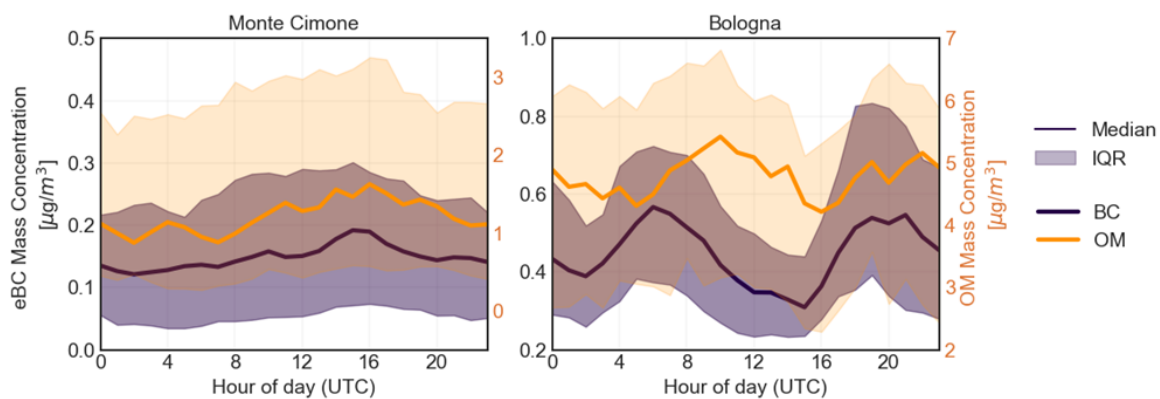


Figure 12 Diurnal variability of BC and OM.

Variability of OM and BC mass concentration at Monte Cimone and Bologna sites from August to September 2024. OM measured by ToF- and Q-ACSM. BC measured by the aethalometer at a wavelength of 880 nm.

3.2.2 Definition of good tracers of PBL dynamics with source apportionment

To assess in more detail the role of different sources, we proceeded with the source apportionment of both BC and OM.

Source Apportionment (SA) via Positive Matrix Factorization (PMF) identified three main contributors to OM, both primary organic aerosol (POA) and secondary organic aerosols (SOA)

- Hydrocarbon-like Organic Aerosol (HOA) is a POA from traffic emissions.
- Less Oxidized – Oxygenated Organic Aerosol (LO-OOA), represents a fresher SOA fraction.

- More Oxidized – Oxygenated OOA (MO-OOA) represents the more aged component, resulting from the transformation of LO-OOA through photochemical and oxidation processes.

The wavelength dependency of the absorption coefficient measured with the Aethalometer was used to identify the contribution of two sources to the observed BC concentration following the method Sandradewi et al (2008) method:

- BC associated with combustion of liquid fuels and thus traffic emission (BC_{TR})
- BC associated with combustion of solid fuels and thus wood-burning emission (BC_{WB})

Organic matter at CMN was dominated by secondary organic aerosol, with no detectable primary hydrocarbon-like aerosol. LO-OOA represents a fresher SOA fraction and closely mirrors the diurnal evolution of total OM, supporting its dependence on PBL-driven transport from the lower Po Valley. MO-OOA represents the more aged component displays a less distinct diurnal pattern consistent with its nature as a regional or background component, less affected by short-term boundary layer dynamics. The contribution of these two components to OM is basically the same, with slightly more LO-OOA (around 55%).

Source Apportionment at BO identifies both primary and secondary contributors to OM. LO-OOA in Bologna exhibits higher concentrations at night and a sharp decline during the warmest part of the day, likely due to the expanding PBL (Figure 13). In contrast, MO-OOA shows a clear dependence on daily hours, with concentrations steadily increasing during daylight hours, in contrast with the potential dilution induced by the deepening of the mixing layer.

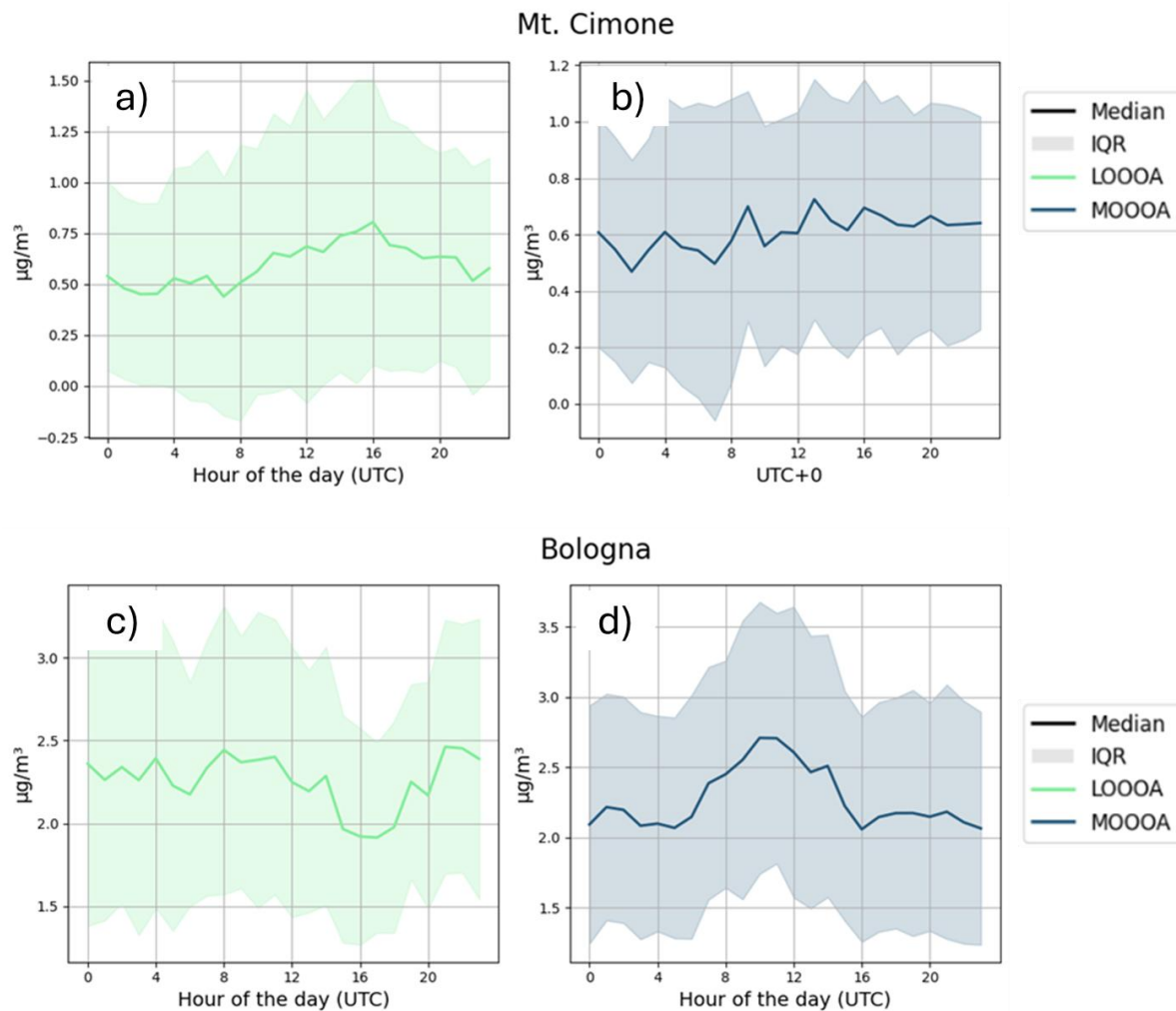


Figure 13 Diurnal variability of SOA mass concentration. OM was measured by ToF- and Q-ACSM at Mt. Cimone and Bologna, respectively, from August to September 2024 and source apportionment (seasonal PMF) was performed, distinguishing SOA in LO-OOA (a and c) and MO-OOA (b and d). Median and interquartile range (IQR; 25th – 75th percentile) are shown, while mass concentrations from each site are displayed on both y axes.

The diurnal behavior of HOA (Figure 14) is influenced by both human activity and PBL dynamics. HOA exhibits two distinct peaks during morning and evening traffic rush hours, with the second peak intensified by the evening PBL contraction, which reduces atmospheric volume and increases pollutant accumulation near the surface. Despite its clear diurnal variation, HOA contributes only about 6% to total OM, with LO-OOA and MO-OOA each contributing around 47%. It is interesting to note how both tracer for traffic emissions, HOA and BC_{TR} , followed the same diurnal variability, without any time-offset as observed between BC and OM. This diurnal is in clear anti correlation with the growth of the mixing layer, indicating a clear and direct influence of atmospheric dynamics on primary traffic emission in urban areas.

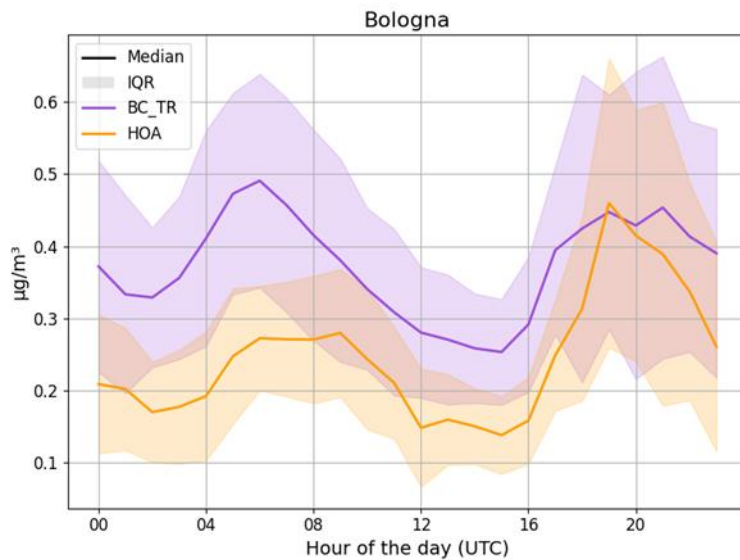


Figure 14 Diurnal variability of HOA and BC_{TR} mass concentration in Bologna. OM was measured by Q-ACSM in Bologna from August to September 2024 and source apportionment (seasonal PMF) was performed, identifying only HOA as POA. BC was measured by aethalometer at a wavelength of 880 nm in Bologna and BC_{TR} derived applying the aethalometer source apportionment method. Median and interquartile range (IQR; 25th – 75th percentile) are shown, while mass concentrations from each site are displayed on both y axes.

3.3 Integration of high-altitude measurements with reanalysis data

The objective of this work is to identify suitable products to investigate the influence of vertical export of pollution to mid-altitudes, modulated by atmospheric dynamics, on long-term historical observations. As potential tracers for vertical export and exchange of air masses we identified black carbon aerosol (BC), which is measured at Monte Cimone since 2007.

As a first step, we evaluated the representativeness of CAMS (Copernicus Atmosphere Monitoring Service) reanalysis products by comparing them with in-situ observations Figure 15. CAMS BC concentrations were extracted at 2300 m a.s.l. at the grid point closest to CMN (approx. 32 km distance). Both datasets show a consistent decreasing trend a marked seasonality and a high correlation (Pearson's $r = 0.82$). Despite a recurring underestimation of 20% CAMS data nicely reproduce the observed ambient variability of BC particles. Using ERA5 data from 2007 to 2023, we explore the potential dependence of observed BC concentrations on height of the planetary boundary layer (PBL). The seasonal cycle of BC mirrors that of the PBL height, suggesting a greater vertical export of pollutants from the Po Valley during summer, when the boundary layer is deeper (Figure 16). However, no clear long-term trend was observed in PBL height, suggesting that vertical transport is not the sole driver of the observed BC decrease at CMN. Preliminary results from FLEXPART simulations for the 2007–2023 period show a clear seasonality in source contributions, with an increased influence of traffic emissions during summer months (Figure 17), further supporting the hypothesis of enhanced vertical transport from the Po Valley.

Overall, reanalysis and numerical modeling provide essential tools to assess the role of atmospheric dynamics on air pollution variability in the absence of continuous remote sensing data over historical time series. The public availability of products such as CAMS (<https://ads.atmosphere.copernicus.eu/datasets>), ERA5 (<https://cds.climate.copernicus.eu/datasets>)

and FLEXPART (<https://flexpart-request.nilu.no/data-access>) represents a valuable resource to investigate the interaction between pollution and meteorological processes, particularly for long-term, monitoring sites diffused within the ITINERIS network.

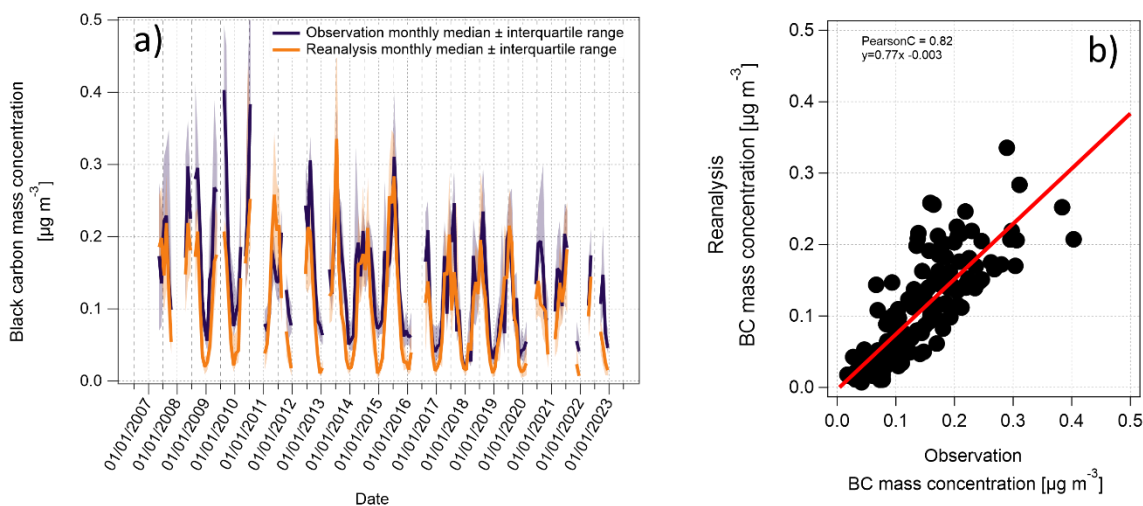


Figure 15 Correlation study between monthly mean black carbon mass concentration observed at Mt. Cimone and black carbon mass concentration derived from reanalysis data (CAM5) between 2007 and 2023.

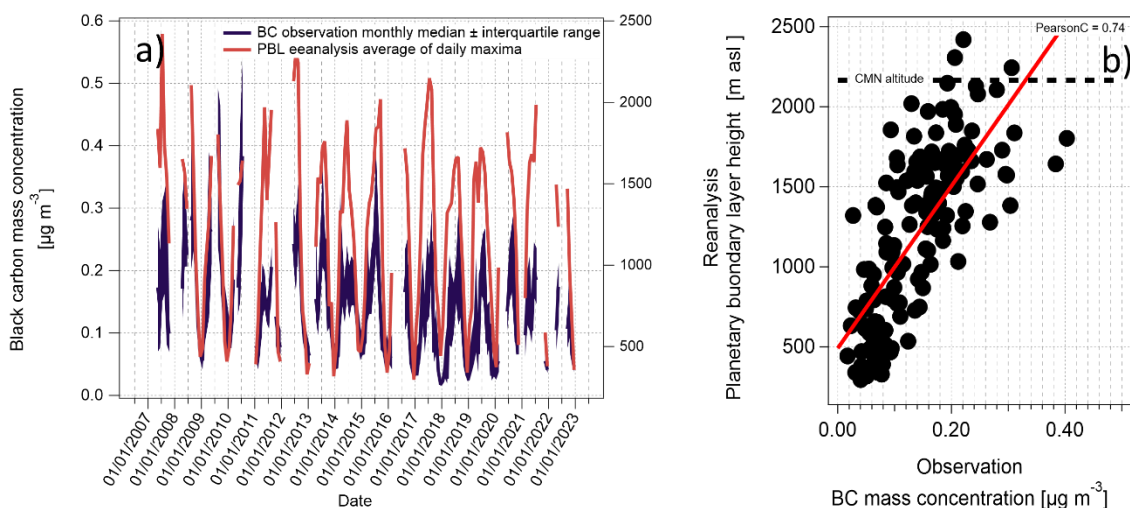


Figure 16 Correlation study between black carbon mass concentration observed at Mt. Cimone and the height of the planetary boundary layer derived from reanalysis data (ERA-5) between 2007 and 2023.

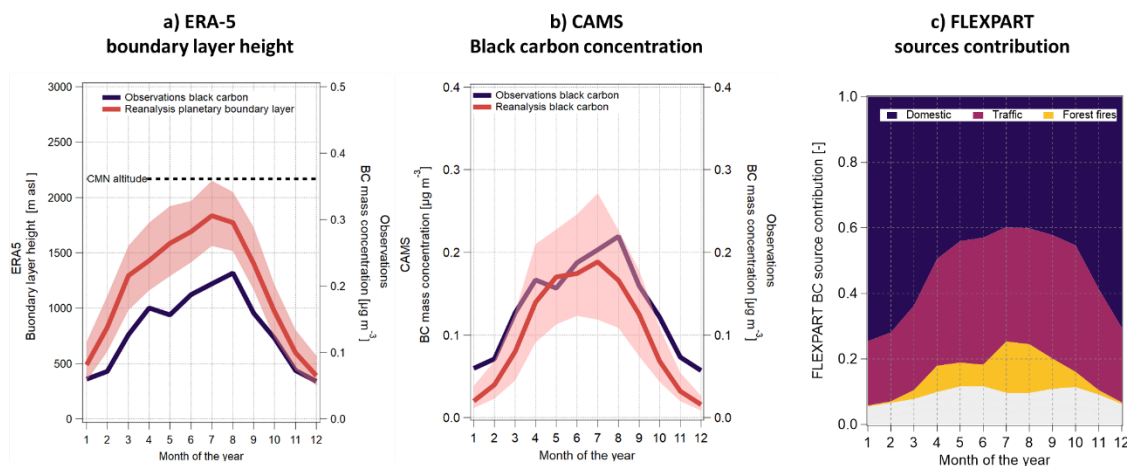


Figure 17 Correlation study of seasonal variability between boundary layer, black carbon mass concentration and black carbon source contribution at Monte Cimone. Data covering the period 2007-2023.

4 FUTURE APPLICATIONS AND PERSPECTIVES

The ITINERIS project granted the reinforcement of the atmospheric observational capability of ISAC-CNR, setting a solid foundation for scientific research. Here we provide a short summary of expected application and synergies with the pilot.

The observational activities carried out within the GAInfra and WAFFERS initiatives marked an important step forward in advancing scientific understanding of atmospheric dynamics and air pollution. These campaigns also reaffirmed the role of ISAC-CNR as a key partner in various European research consortia and provided a valuable opportunity to promote the ITINERIS scientific agenda at the international level.

GAInfra represented the sole observational infrastructure deployed on board the AWI icebreaker Polarstern during the summer 2024 cruise for the in situ and remote sensing characterization of atmospheric aerosol at high latitudes. The campaign offered a rare opportunity to collect data on aerosol particles in a climatically sensitive and under-monitored region. Next to its scientific relevance, this activity significantly fosters national and international collaborations. The deployment of GAInfra enhanced internal synergies within the GAIA project (funded under the MUR-PRIN 2022 program), fostering integrated approaches to aerosol monitoring and data analysis. Building on these achievements, the activity fostered international collaborations developed within the framework of the MI-TRAP project, supported by the European research community, positioning GAInfra and its partner institutions at the forefront of European efforts to advance our understanding of atmospheric processes. The outcomes are expected to contribute valuable insights to environmental policy and air quality management.

Next to the international experience and multi-infrastructure synergy represented by the WAFFERS campaign, shortcoming national developments are expected in the field of trace gases observations. Upon the installation of the Fourier Transform InfraRed Spectrometer (FT-IR-S) at the urban site of Bologna, CNR-ISAC will be capable of quantify the vertical distribution of atmospheric trace gases with the final goal of quantifying the dilution effect on the concentration of gases within the PBL of the Po Valley. The integration of this vertical resolved observations with the continuous in-situ observations at CMN will allow quantifying the vertical export of pollution from the Po Valley emissions towards the free troposphere.

The activity of ISAC-CNR during the RI-URBANS campaign in Milan and the AirPoDynamics in Bologna represents one of the most significant efforts to assess the role of planetary boundary layer (PBL) dynamics on air quality in the Po-Valley. The resulting datasets, collected from multiple monitoring sites and including both in situ and remote sensing observations, will be harmonized and integrated to support a comprehensive analysis. This unified study will aim to characterize the seasonal influence of atmospheric dynamics—particularly vertical mixing and horizontal ventilation—on pollutant concentrations at the ground level, in an European AQ hot spot. By combining measurements of aerosol particles, greenhouse gases, and reactive gases with meteorological data and PBL observations, it will be possible to identify which pollutants are more sensitive to atmospheric ventilation processes and which are not. These findings will demonstrate that relying solely on indicators such as PBL height and wind speed may not be sufficient to fully assess urban air quality, especially for secondary pollutants less influenced by ventilation. Differently, the integration of reanalysis PBL data with historical observations at Cimone will allow identifying anomalies in pollutants concentrations at high altitude caused by climate-change driven feedbacks on atmospheric dynamics in the Po Valley.

5 CONCLUSION

The activity of the PBL-Pilot aimed to identify the impact of planetary boundary layer on concentration of pollutants at ground level. Several field activities have been conducted on national and international level, combining intense observation periods and long-term observations. Overall, the ITINERIS campaign allowed identifying several metrics to investigate the impact of atmospheric dynamics on air quality at the ground.

By multiple inversion algorithms, the height of the mixed aerosol layer (MAL) was derived from ceilometer observations of aerosol backscattering coefficient. The MAL may be used as a proxy for the planetary boundary layer, being representative of atmospheric dynamics in the first kilometers from the surface and impacting the concentration of pollutants at ground level.

By combining in-situ aerosol and gas observations with remote sensing measurement of the mixed aerosol layer (MAL), we identified an anticorrelation of the depth of the MAL with the concentration of primary aerosol species (black carbon) and greenhouse gases (carbon dioxide and methane), volatile organic carbon (traffic tracers) suggesting an efficient dilution induced by the vertical dynamic of the atmosphere. Other sources, associated with biogenic emissions, were found to be less prone to ventilation driven by the PBL dynamics. Concentration of gases also showed a decrease with wind speed, indicating a non-negligible anti correlation between concentration of pollutants at the ground and horizontal ventilation. By combining the horizontal and vertical air motion the ventilation index was derived. High ventilation indices indicate the presence of a deep boundary layer and string wind, causing a substantial decrease in aerosol concentration at ground.

Simultaneous observations of carbonaceous aerosol particles were used to investigate the vertical variability aerosol distribution at different altitudes. Despite both organic matter and black carbon concentration appeared to undergo a clear diurnal cycle controlled by the depth of the boundary layer, source apportionment indicated specific tracers for boundary layer dynamics. Less oxides secondary organic aerosol appeared to be good tracers for injection of pollution from the boundary layer into higher altitudes. On the other side, Hydrocarbon-like Organic Aerosol and traffic emitted BC appeared to be strongly affected by vertical dilution caused by growth of the boundary layer. With the finalization of the inversion of ceilometer data, the role of these tracers will be confirmed for the Po Valley (AirPoDynamics).

In absence of remote sensing observations, we demonstrated that reanalysis data may be successfully used to infer the long-term variability of the planetary boundary height and its impact on BC

concentration. Opposite to low altitude observations conducted in Milan, the concentration of black carbon at high altitude was positively correlated with the height of the PBL. We show that this positive correlation contributes to the seasonal BC variability and may be connected with multi-year tendency of long-term time series. One of the forthcoming objectives of the PBL-pilot will be to verify the representativity of PBL height with MAL observations performed during the pilot.

Task 4.14 identified the metrics needed to quantify: i) the dynamics of the PBL - height of the aerosol mixed layer, ii) combined horizontal and vertical dilution - ventilation index, iii) the pollution and sources tracers - carbonaceous aerosol / greenhouse gases / volatile organic carbon, iv) reanalysis products (height of the planetary boundary layer from ERA-5). Finally, Task 4.14 will aim to provide a harmonized dataset including the here identified metrics needed understand the variability associated with pollution and atmospheric dynamic processes.

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