MISSIONE 4
ISTRUZIONE
RICERCA

ITINERIS

D4.14.1: Definition of the minimum requirements for a common, matched database of measured/derived variables for both atmospheric composition and atmospheric dynamics [B8]

Finanziato dall'Unione europea
NextGenerationEU

Ministero dell'Università e della Ricerca

Italiadomani
PIANO NAZIONALE DI RIPRESA E RESILIENZA

Deliverable number:	D4.14.1
Work package:	WP4 – Atmosphere
Intermediate Objective:	IO4.4
Deliverable type:	X Document, report
	☐ Websites, patent filings, videos, etc.
	☐ Other: please specify ....
Dissemination level:	☐ Public
	X Restricted
Estimated delivery (bimester):	B8
Actual delivery date:	29/02/2024
Author(s) (Partner-OU):	Francesca Barnaba, AnnaChiara Bellini, Alessandro Bracci, Elisa Castelli, Francesco Cairo, Paolo Cristofanelli, Bianca Maria Dinelli, Luca Di Liberto, Angela Marinoni, Simonetta Montaguti, Enzo Papandrea, Ferdinando Pasqualini, Camilla Perfetti, Paolo Pettinari, Marco Rapuano, Laura Renzi, Marco Zanatta, Nora Zannoni (CNR ISAC)
Reviewed by:	Lucia Mona, Gianluca Di Fiore (CNR-IMAA)
Note:	

IR0000032 – ITINERIS, Italian Integrated Environmental Research Infrastructures System - CUP B53C22002150006 (D.D. n. 130/2022)
Funded by EU - Next Generation EU
Mission 4 "Education and Research" - Component 2: "From research to business" -
Investment 3.1: "Fund for the realisation of an integrated system of research and innovation infrastructures"

Table of contents

Index of tables

Index of figures

INTRODUCTION

To define the minimum requirements for a common database of variables for both atmospheric composition and atmospheric dynamics, we evaluate the CNR-ISAC-BO facilities carrying out simultaneous in-situ and remote sensing observations, following the Research Infrastructure (RI) requirements allowing to study the influence of atmospheric dynamics on the ground pollutants concentration.

1.1 Po Valley Observatories

The "Monte Cimone with Po Valley facilities" observation node (CMN-PV) is an integrated site that provides a three-dimensional observation of one of the most critical hot spots in Europe for climate and air quality. The CMN-PV includes the CNR observatory of Monte Cimone (CMN, 2165 m s.l.m.), the unique Italian global GAW-WMO station and atmospheric class-2 site within ICOS-RI, the urban supersite of Bologna (BOS) and the rural site of San Pietro Capofiume (SPC). GAW is the Global Atmosphere Watch program in the frame of World Meteorological Organization. At these observatories the observation of polluting and climate-altering atmospheric compounds is performed since 20 years by CNR-ISAC in collaboration with other Italian and international institutions.

The three observational sites have been seat of important international field campaigns, including those part of the EU EUCAARI, PEGASOS, ACTRIS-2, FORCeS, QA4EO, RHAPS projects, as well as FRM4DOAS in the next future**.** These experiments have seen the perfect synergy between the observing sites and appropriate mobile platforms (on land and air) offering the opportunity to study different aerosol populations, their horizontal and vertical transport, and the ageing and transformation into the atmosphere. In particular, the AEROLAB ISAC mobile platform have often integrated the Bologna site but is also able to monitor pollution hot spot (e.g. Linate airport, Civitavecchia harbour, Rome DownTown, Bologna) on the national territory, as well as remote environments.

The research work of ISAC-BO focuses on in-situ and ground-based remote sensing measurements of atmospheric properties. By integrating observations with modelling activities, ISAC-BO aims to identify the aerosol and gas sources, long-range transport and their impact on air quality and climate, in particularly vulnerable region to climate change such as in the Mediterranean basin and PoValley

The main competences that will be central to ITINERIS project are summarised in the following:

- Online characterisation of optical properties (scattering and absorption) of atmospheric particles at ground level and over the atmospheric column, separating the planetary boundary layer (PBL) and free troposphere (FT) contribution;
- Characterisation of aerosol size distributions from nanoparticles (0.8 nm) up to the coarse fraction (30µm) to investigate new particle formation (NPF) events, growth processes and identification of processes affecting NPF. Measurements are conducted in the plain and in the mountain site;
- Online and offline determination of aerosol chemical properties;
- Estimate the height of the PBL with different techniques, i.e., by active remote sensing by ceilometers using aerosol as PBL tracer, by radon measurements used as a proxy of the PBL dilution capability;
- Observations of ground level concentrations and vertically resolved/vertically integrated columnar amounts of gaseous main pollutants for air quality applications and characterisation of combustion pollution sources (NO, NO2, NH3, SO2, O3) and GHGs

(N2O, CO2, CH4) and their correlation with aerosol properties and meteorological parameters;

- Analysis of intra-annual and inter-annual long-term trends of atmospheric composition and their correlation with meteorology, evolution of air quality policies, and changes of the main pollution sources;
- Instrumentation operation in remote places, at high altitudes and on balloons or airplanes;
- Evaluation and quality control of dataset of atmospheric climate variables.

1.2 Aerolab

The AERosol mObile LABoratory (AEROLAB) was designed and implemented by CNR-ISAC in 2016 to perform in-depth field characterization of particulate matter in support and/or in the absence of p monitoring stations.

AEROLAB operates on board a motorhome van so to be easily transferred to any destination, to be set-up and operative within 2-3 hours, and run h24 in a comfortable working space. The van has temperature and humidity control systems to make it operable in Mediterranean regimes [approx. from -5°C to 40°C].

Since its development, AEROLAB has been equipped with state-of-the-art instrumentation for the in situ optical (scattering and absorption) and physical (nano to micrometric size) characterization of aerosols, plus ancillary meteorological variables. The aerosol sampling line has a PM10 head with nafion-dryer and an isokinetic splitter that divides the flow to the different analyzers. In situ measurement of trace gases (NO2 - NO- NOx - SO2 - H2S), with a dedicated sampling line, have been recently added.

1.3 Seneca III

CNR-ISAC established an agreement with OGS (Istituto di Oceanografia e Geofisica Sperimentale) for the shared utilization of the Piper Seneca III research aircraft. The access to an airborne platform will allow ISAC-CNR to explore the complex atmospheric processes controlling the vertical transport of pollution from the boundary layer to the free troposphere in synergy with the permanent (Po Valley Observatoris) and mobile (AEROLAB) ground observatories, and other Italian stations being part of European research infrastructures such as ACTRIS and ICOS. OGS owns, maintains and operates the Piper Seneca III aircraft within the European Union as a member of the EUFAR (European Facility for Airborne Research) fleet.

Several European projects, such as CO2GeoNet, have employed the instrumental equipment to conduct remote sensing surveys that enable the identification of CO2 leaks in natural laboratories by combining the data retrieved from the hyperspectral sensor, the Ultraportable Greenhouse Gas Analyzer, the Lidar sensor and digital camera already installed onboard of the Seneca III.CNR-ISAC has decades of experience in conducting measurement campaigns with scientific instrumentation mounted on land, ocean and air platforms. ISAC selected a set of instruments to measure the optical and microphysical properties of aerosol particles with high temporal resolution, essential for airborne observations. The primary objective of the activity within ITINERS is to acquire an instrumental suite for the characterization of atmospheric particulate, mountable on manned aircraft. Following the study of feasibility, the selected instrumentation will be customized for avionic use including the mechanical interfaces, electrical system, thermal conditioning and sampling lines in the cockpit and on the fuselage. The weight of aerosol measuring suit and all needed interfaces will be minimized to increase the operational range (max 1800 km) and prolong the flight time (max 8 hours). Finally, the implementation activity will be finalized by the certification of the instrumental suit for research flights on the Seneca III.

1.4 European Research Infrastructures

Research Infrastructures (RI) are facilities that provide resources and services for research communities to conduct research and foster innovation. They can be used beyond research e.g. for education or public services and they may be single-sited, distributed, or virtual.

The European Strategy Forum on Research Infrastructures (ESFRI) is a strategic instrument coordinating the RI at European level aiming to develop the scientific integration of Europe and to strengthen its international outreach. The competitive and open access to high quality Research Infrastructures supports and benchmarks the quality of the activities of European scientists and attracts the best researchers from around the world. ESFRI operates at the forefront of European and global science policy and contributes to its development translating political objectives into concrete advice for RIs in Europe.

The CNR-ISAC-BO Observatories and facilities are connected with three different European Research Infrastructures: ACTRIS (CMN-PV and Aerolab), ICOS (CMN-PV) and EUFAR (Seneca III). The link with the EU RI is a guarantee for high quality data, homogeneous at European and global level.

IN-SITU VARIABLES

2.1 ACTRIS

2.1.1 Reactive trace gases in-situ

The minimum requirements for NOx (i.e. NO and NO2) measurements are defined by the document “D3.17. Updated Measurement Guideline for NOx and VOCs”(deliverable 3.17 of ACTRIS-2, https://ec.europa.eu/research/participants/documents/downloadPublic?documentIds=080166e5bef908e2&appId=PPGMS) based on the original measurement guidelines for VOCs and NOx, which were produced within the first ACTRIS project (Deliverable D4.9: Final SOPs for VOCs measurements and Deliverable D4.10: SOPs for NOxy measurements). This document defines the minimum requirements in terms of data quality objectives for different measurement purposes and conditions. NOx measurements by chemiluminescence photometry uses either a photolytic or molybdenum converter for transforming NO2 into NO. It is well established that molybdenum converters convert not only NO2, but also other reactive nitrogen species. Please note that at rural and remote sites, only the use of photolytic converters satisfies the recommendations of European Monitoring and Evaluation Programme (EMEP), ACTRIS and GAW.

The document also provides specific information about measurements protocols (air inlet and sample design, instrumentation, calibration strategy) to meet the data quality objectives. A specific focus is devoted to the description of the QA/QC protocols and a list of required metadata variables for the correct implementation of calibrations, suitable corrections of the water vapour and ozone interferences and data quality and flagging of data is provided.

Essential ancillary data are: PMT temperature, reaction cell pressure, ambient ozone concentration, ambient temperature and humidity and other meteorological data. It is also recommended to carefully document useful metadata such as: type of NO2 -> NO converter, time from entry inlet line to entry of NO2 -> NO converter, duration of stay in converter or bypass line, duration of stay in converter, integration time, high voltage of PMT, chamber/instrument temperatures, (all) calibration factors, and length and inner diameter of inlet line (see also https://ebas-submit.nilu.no/templates/NOx/lev0).

Table 1. Requirements defined within ACTRIS for in-situ NOx observations.

Level	**1 (basic)**	**2 (enhanced)**	**3 (high)**[1]
Site characteristics	Continental basic	Continental background	Pristine marine background, free troposphere
Mean mole fraction NOx	> 1 nmol/mol	0.1 – 1 nmol/mol	< 0.1 nmol/mol
Scope (corresponding time resolution)	long term monitoring, trends (1 hour), source-receptor-relationship, transport processes (hour-minute), photochemical process studies (minute)		
Detection Limit (1 hour, 3σ)	NO: 50 pmol/mol NO_2:100 pmol/mol	NO: 10 pmol/mol NO_2:20 pmol/mol	NO: 1 pmol/mol NO_2:5 pmol/mol
uncertainty (1 hour, 2σ)[2]	NO: 40 pmol/mol or 3% NO_2:80 pmol/mol or 5%	NO: 8 pmol/mol or 3% NO_2:15 pmol/mol or 5%	NO: 1 pmol/mol or 3% NO_2:3 pmol/mol or 5%
uncertainty (1 month, 2σ)[3]	NO: 2.5% NO_2: 3%	NO: 2.5% NO_2: 3%	NO: 1 pmol/mol or 2.5% NO_2:3 pmol/mol or 3%
data coverage	66%		
suggested method[4]	CLD / PLC	CLD / PLC	CLD / PLC
Alternative / upcoming methods[5] (backup or QC reasons)	CRDS ; LIF ; DOAS ; TDLAS	CRDS ; LIF ; TDLAS	LIF

[1] in pristine environments with NOx levels below 10 pmol/mol, the required detection limits and uncertainties would be 0.1 pmol/mol for NO and 0.3 pmol/mol for NO_2.

[2] whichever is the larger, e.g. for level 2 "enhanced" at NO_2 of 1 nmol/mol an uncertainty of 50 pmol/mol is required (5% of 1 nmol/mol), at 0.2 nmol/mol an uncertainty of 15 pmol/mol would be required.

[3] assuming that the random uncertainties are negligible compared to the calibration uncertainty

[4] see list of acronyms (Annex 1) for full method names

[5] methods that are either new and not yet fully tested for their long-term applicability or research type instrumentation that is demanding to operate, thus, prone to incorrect handling and therefore not fully suitable for long-term monitoring

Tropospheric ozone measurements have the objectives to (a) detect long-term changes in ozone background concentrations and (b) quantify year-to-year variability in monthly mean background concentrations. To reach these objectives, a combined measurement uncertainty of approximately ± 1 nmol mol-1 (two sigma) should not be exceeded (WMO/GAW, 2019). WMO/GAW (2019) also reports minimum requirements for O3 measurements in terms of completeness (66% for continuous measurements uniformly distributed in time), comparability (i.e. traceability of all measurements to a primary standard), compatibility and representativeness. The same document also reports the minimum requirements in terms of measurement protocols (including station set-up, sampling procedures and materials, calibration and quality assurance protocols) to achieve the defined minimum requirements.

The file template for reporting in-situ near-surface O3 mole fraction data are provided at https://ebas-submit.nilu.no/templates/Ozone/lev2. The following guidelines are indicated:

- Mixing ratio given as [nmol/mol] is the preferred unit. Alternatively [ppb] could be used, assuming this is identical to [nmol/mol]. Data in [proxy ug/m3] = fac × [nmol/mol] is also accepted provided that the fixed values for T and P (typically T=293.15K and P = 1013.25 hPa) used to calculate fac is given in the "Volume std. temperature" and "Volume std. pressure" metadata.

- A default standard value for the absorption cross-section is stated in the "Absorption cross section" element.
- Include information of monitor calibration(s) in the QA metadata.
- Include information on filter test, leak tests, ozone scrubber test etc. in the "Maintenance description" element.
- Include information of any kind if drying in the Temperature/humidity control tab. This is important for the question of whether the values refer to mixing ratio in moist or dry air.
- When calculating average values, e.g. hourly, from measurements with higher time resolution, please disregard any invalid measurements. Any informative flags, e.g. local contamination, occurring at any time during the average period need to be copied to the average value.
- Reference temperature and pressure are only necessary to include when reporting mass concentration.

Due to rigorous emission measures to reduce acid rain formation, sulphur dioxide (SO2) is no longer a major concern in Europe. However, other scientific and air quality issues (i.e. precursor of sulphate aerosol, good tracer for evaluation of air mass origin) justify an interest in better understanding the atmospheric sulphur cycle. Minimum requirements in terms of experimental activities to monitor and investigate atmospheric SO2 variability are reported and described by Schultz et al., 2015 in terms of siting requirements, measurement methods and sampling frequency, QA/QC methods, ancillary variables, archiving procedures.

2.1.2 Aerosol in-situ

Aerosol particles are highly important players in air pollution and climate radiative forcing. Their size and/or shape and/or chemical composition determine their deposition in the respiratory tract, the diseases they trigger, and their impacts on ecosystems (acidification, eutrophication). Moreover, these particle properties determine the ice- or snow-covered area reflectance, the particle interaction with radiation (direct radiative forcing, visibility) and the effect of particles on the formation and microphysical properties of clouds (indirect radiative forcing, precipitation probability). Impacts such as particle light scattering and absorption, cloud formation potential, etc., can be inferred from the particle number size distribution and other independently measured physical variables. Conversely, a detailed knowledge of the chemical composition is essential to determine the sources of aerosol particles, and therefore develop efficient emission abatement measures. All the most relevant variables related to aerosol climate forcing and air pollution shall be measured at ACTRIS Observational Platforms for aerosol in situ observations. This section describes the respective technical concepts and requirements.

2.1.2.1 Observational capabilities

Optimum setup

For the Observational Platforms connected to the Centre for Aerosol In Situ Measurements there is no optimum setup, as each Observational Platform has a specific science case. Instead, minimum requirements are defined below, which account for this broad range of science cases. Therefore, it is distinguished here between mandatory, specializing, added value and auxiliary variables, listed in **Error! Reference source not found.**.

Mandatory and specializing variables

The **minimum requirement** for ACTRIS aerosol *in situ* measurement stations includes measurements of three mandatory variables and at least two free-choice specializing variables. Among the two free-choice variables, at least one must be a chemical variable. The reasons for this concept are: i) the importance of the variables in climate and health issues; ii) the possibility to account for the specific science case of each Observational Platform; and iii) the long-term records for these variables at several sites around Europe using validated standard operation procedures (SOPs) developed by the ACTRIS community and endorsed by the Centre for Aerosol In Situ Measurements.

Added-value variables

Complementary added-value variables permit the full characterization of aerosol particle properties and provide insight to many processes linked to emission, transformation or ageing of particles. Measurements of **trace gases** such as O3 have to be performed in parallel with CO, NO2 and SO2, which are useful tracers for anthropogenic pollution events and therefore parallel measurements of these gases are a clear asset. For the added-value variables, the measurement methodology and the QA/QC procedures are defined outside of ACTRIS. Added-value variables are not mandatory, but very useful to have.

Auxiliary variables

Aerosol *in situ* observations have to be accompanied by measurements of **meteorological parameters** (wind speed, wind direction, temperature, relative humidity) and **radiation** (UV, IR, total radiation) in order to interpret the measured data in an appropriate manner. For the auxiliary variables the measurement methodology and the QA/QC procedures are defined outside ACTRIS. At least the meteorological auxiliary variables must be measured at an Observational Platform connected to the Centre For Aerosol In Situ Measurements.

Instrumentation and calibration

Before describing the requirements in more detail, it is noted that in general the Centre for Aerosol In Situ Measurement sets the quality objectives for the instrument QA, and that the NF is responsible for having instruments quality-assured at the TC at given interval. In addition, the NF is responsible for conducting and documenting QC of both instrument and data, where instrument QC is defined by TC and data QC defined jointly by the TC and DC.

Particle number size distribution mobility diameter (0.01 – 0.8 µm)

A **mobility particle size spectrometer** (MPSS) is used to measure **the particle number size distribution** of the submicrometer size range from approximately 0.010 to 0.8 µm. The technology is well established and is commercially available, but there are also custom-designed models. The MPSS is robust and designed for long-term operations. However, it needs regular checks on-site to quality-assure the measurements. Into the MPSS, a **Condensation Particle Counter** (CPC) is included, which has to undergo also frequent on-site checks. Additionally, MPSS systems must be calibrated every one to two years against a reference instrument at the TC.

Particle light scattering & backscattering coefficients (multi-wavelength)

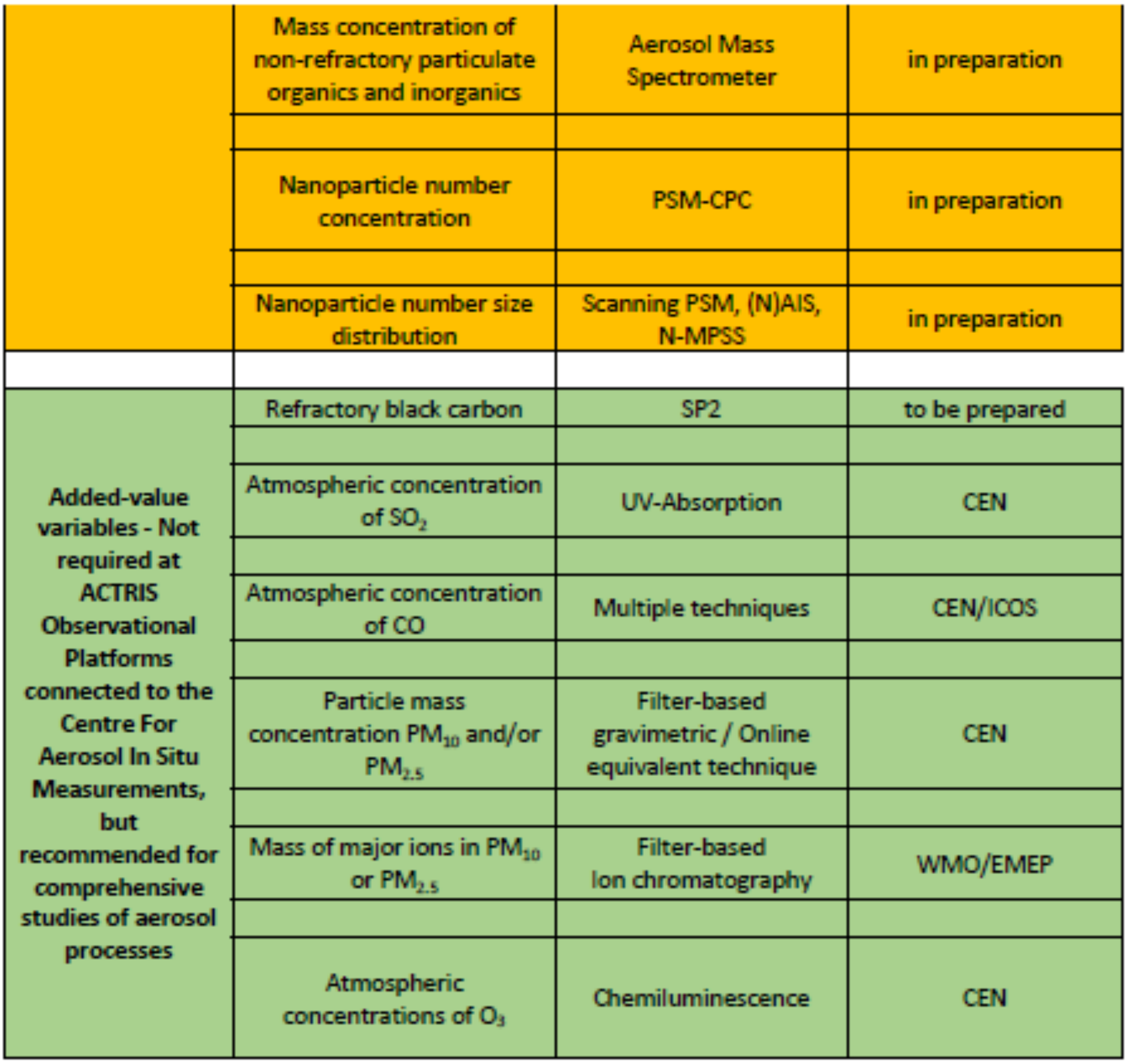
A **multi-wavelength integrating nephelometer** (InNe) is used to measure the **multi-wavelength particle light scattering & backscattering coefficients**. The technology is well established, and a few instruments are commercially available. The InNe is robust and designed for long-term operations. However, it needs regular checks on-site to quality-assure the measurement. Additionally, InNe instruments must be calibrated every one to two years against a reference instrument at the TC.

Particle light absorption coefficient & equivalent black carbon concentration

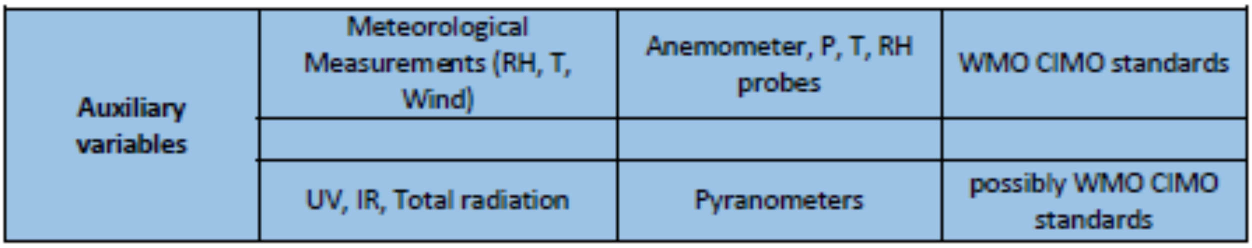
An **absorption photometer** (AP) is used to measure the **particle light absorption coefficient & equivalent black carbon concentration**. The technology is well established and instruments are commercially available. The existing APs are robust and designed for long-term operations. However, they need regular checks on-site to quality-assure the measurement. Additionally, yearly or every two years calibrations against a reference instrument at the TC are required.

Table 2: List of variables for ACTRIS aerosol in situ Observational Platforms.

Variable status	Variable Name	Instrument type	Recommended methodology
Mandatory aerosol variables - Required for an ACTRIS Observational Platform connected to the Centre For Aerosol In Situ Measurements	Particle number size distribution - mobility diameter	Mobility Particle Size Spectrometer	Wiedensohler et al. (2017)
	Particle light scattering & backscattering coefficient	Integrating Nephelometer	GAW report 227
	Particle light absorption coefficient & equivalent black carbon concentration	Absorption Photometer	GAW report 227
Specializing aerosol variables - Provision of at least two specializing variable is mandatory for an ACTRIS Observational Platform connected to the Centre For Aerosol In Situ Measurements	Mass concentration of particulate organic & elemental carbon	Thermo-optical method on quartz filters	EUSAAR-2 / Can be replaced by online OC/EC for specific conditions
	Particle number size distribution – optical and aerodynamic diameter	Aerodynamic & Optical Particle Size Spectrometer	in preparation
	Particle number concentration	Condensation Particle Counter	CEN
	Mass concentration of particulate elements	Filter-based XRF/PIXE/ICP_OES/ICP_MS	in preparation
	Mass concentration of particulate organic tracers	Filter-based IC, GC-MS HPLC-MS, LC/MS	in preparation
	Number concentration of cloud condensation nuclei	Cloud Condensation Nuclei Counter	Rose et al. (2008)



	Mass concentration of non-refractory particulate organics and inorganics	Aerosol Mass Spectrometer	in preparation
	Nanoparticle number concentration	PSM-CPC	in preparation
	Nanoparticle number size distribution	Scanning PSM, (N)AIS, N-MPSS	in preparation
Added-value variables - Not required at ACTRIS Observational Platforms connected to the Centre For Aerosol In Situ Measurements, but recommended for comprehensive studies of aerosol processes	Refractory black carbon	SP2	to be prepared
	Atmospheric concentration of SO_2	UV-Absorption	CEN
	Atmospheric concentration of CO	Multiple techniques	CEN/ICOS
	Particle mass concentration PM_{10} and/or $PM_{2.5}$	Filter-based gravimetric / Online equivalent technique	CEN
	Mass of major ions in PM_{10} or $PM_{2.5}$	Filter-based Ion chromatography	WMO/EMEP
	Atmospheric concentrations of O_3	Chemiluminescence	CEN



Auxiliary variables	Meteorological Measurements (RH, T, Wind)	Anemometer, P, T, RH probes	WMO CIMO standards
	UV, IR, Total radiation	Pyranometers	possibly WMO CIMO standards

Mass concentration of particulate organic & elemental carbon

Thermal-optical analysers are used to determine the amount of **organic carbon** (OC) and **elemental carbon** (EC) deposited on quartz fibre filters after active sampling. Thermal-optical analysers can be calibrated for total carbon measurements by the user, but not for OC and EC due to a lack of suitable commercial standard materials. ACTRIS stations delivering OC and EC concentrations shall participate in Round-Robin inter-laboratory exercises at least once a year.

Particle number size distribution - optical and aerodynamic diameter (0.7 – 10 μm)

Particle number size distribution of particles in the upper accumulation and in the coarse mode range can be measured either by an **optical particle size spectrometer** (OPSS) based on the intensity of particle light scattering (optical diameter) or by **aerodynamic particle size spectrometer** (APSS) based on time-of-flight in an accelerated flow (aerodynamic diameter). Yearly or every two years calibrations of OPSS and APSS against a reference instrument at the TC are required.

Particle number concentration (> 0.010 μm)

The **particle number concentration** can be determined by **CPCs**, which are commercially available. Modern CPCs are based on a continuous aerosol flow, work in a single counting mode, and use most often butanol as working fluid. However, they need regular checks on-site to quality-assure the measurement. Additionally, yearly or every two years calibrations against a reference instrument at the TC are required.

Mass concentration of particulate elements

Mineral dust particles consist of crustal material originating mostly from suspension of wind exposed soil in arid and semi-arid areas such as desert and agricultural regions, but also from re-suspended road dust. Mineral dust particles are primarily in the coarse mode. It is recommended that a **multi-elemental analysis** approach should be used to determine the **mineral dust and associated heavy metal components**, using filter or impactor samples and techniques such PIXE, INAA, XRF, AAS, ICP-MS and ICP-OES. It is also recommended that ISO standard procedures are followed, whenever available when using these techniques.

Mass concentration of particulate organic tracers

Knowledge of specific tracers in aerosol particles provides information on their sources. The ACTRIS measurement program includes the determination of the **mass concentration of specific organic tracers** from **filter samples**. Organic tracers include different type of compounds that can trace biomass-burning activities (levoglucosan), industrial processes or road traffic.

Cloud condensation nuclei number concentration (at various supersaturations)

Cloud Condensation Nuclei (CCN) are particles, which are capable to form cloud droplets at a given supersaturation. The **number concentration of CCN** can be determined by a **Cloud Condensation Nuclei Counter** (CCNC). Commercial CCNC measure the CCN number concentration over a limited range of supersaturations. However, CCNC need regular calibrations and checks on-site to quality-assure the measurement. Additionally, yearly or every two years calibrations against a reference instrument at the TC are required.

Mass concentration of non-refractory organic and inorganic aerosols

Aerosol Mass Spectrometers (AM) measure **concentrations of particulate sulphate, nitrate, ammonium, chloride, and organic mass** at the same time. Upon contact with the heater, the nonrefractory components of the particles are vaporized and ionized by electron impact, resulting in charged mass fragments that are detected either by a quadrupole or a time-of-flight mass spectrometer. Some of the current commercially available AMS are robust and designed for long-term operations.

However, they need regular calibrations and checks on-site to quality-assure the measurement.

Additionally, yearly or every two years calibrations against a reference instrument at the TC are required.

Nanoparticle number concentration (< 0.01 µm)

Nano-CPCs consisting of a Particle Size Magnifier (PSM) and a CPC are designed for nanoscience and nanotechnology and can detect **particles as small as ~1 nm in diameter**. The working principle of a Nano-CPC is to mix turbulently cooled sample flow with heated clean airflow saturated by the working fluid. The resulting supersaturations grow the particles to sizes which can be measured by a standard CPC. Annual or every two years calibrations against a reference instrument at the TC are required.

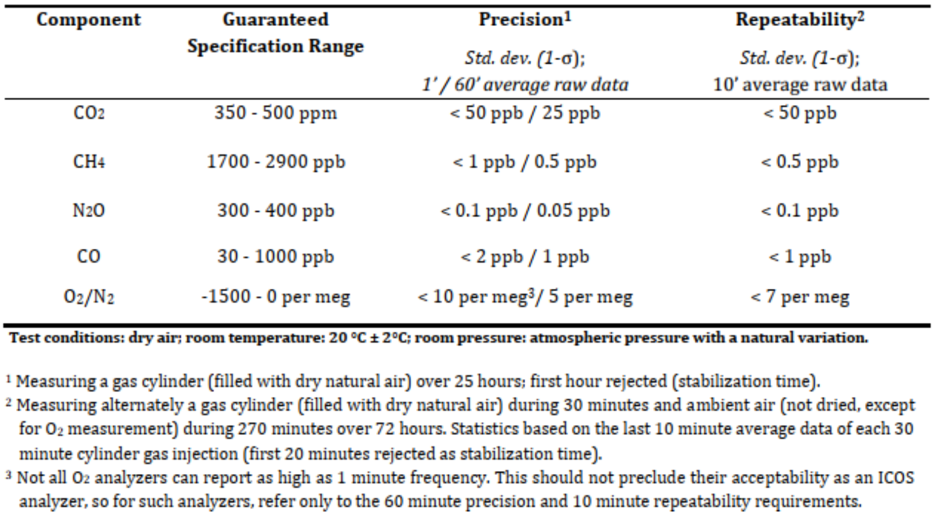
Nanoparticle number size distribution (0.001 – 0.02 µm)

Ion spectrometers (Balanced Scanning Mobility Analyser, BSMA, and Neutral Cluster & Air Ion Spectrometer, NAIS, N-MPSS) can be used to measure **ions down to 0.8 nm in diameter**. NAIS can additionally detect **neutral particles down to ~2 nm**. Annual or every two years calibrations against a reference instrument at the TC are required.

2.2 ICOS

The minimum requirements for measurements of greenhouse gases (CO2, CH4, N2O) and carbon monoxide (CO) have been defined within ICOS. The requirements in terms of analytical performances (i.e. precision, repeatability, measurement ranges) are reported in the document COS RI (2020)to get robust data devoted to the quantification of long-term trends and regional fluxes by means of inversion modelling and meet the WMO compatibility goals (Crotwell et al., 2020).

Table 3. Requirements defined within ICOS for in-situ greenhouse gas observations.



Component	Guaranteed Specification Range	Precision[1] *Std. dev. (1-σ); 1′ / 60′ average raw data*	Repeatability[2] *Std. dev. (1-σ);* 10′ average raw data
CO_2	350 - 500 ppm	< 50 ppb / 25 ppb	< 50 ppb
CH_4	1700 - 2900 ppb	< 1 ppb / 0.5 ppb	< 0.5 ppb
N_2O	300 - 400 ppb	< 0.1 ppb / 0.05 ppb	< 0.1 ppb
CO	30 - 1000 ppb	< 2 ppb / 1 ppb	< 1 ppb
O_2/N_2	-1500 - 0 per meg	< 10 per meg[3]/ 5 per meg	< 7 per meg

Test conditions: dry air; room temperature: 20 °C ± 2°C; room pressure: atmospheric pressure with a natural variation.

[1] Measuring a gas cylinder (filled with dry natural air) over 25 hours; first hour rejected (stabilization time).

[2] Measuring alternately a gas cylinder (filled with dry natural air) during 30 minutes and ambient air (not dried, except for O_2 measurement) during 270 minutes over 72 hours. Statistics based on the last 10 minute average data of each 30 minute cylinder gas injection (first 20 minutes rejected as stabilization time).

[3] Not all O_2 analyzers can report as high as 1 minute frequency. This should not preclude their acceptability as an ICOS analyzer, so for such analyzers, refer only to the 60 minute precision and 10 minute repeatability requirements.

The same document also reports the minimum requirements in terms of measurement protocols (including sampling and calibration protocols) to achieve the defined minimum requirements.

To achieve these targets ICOS implements a quality management plan, which defines quality assurance and quality control measures to be implemented at the measurement facilities. The set of main (e.g. CO2 mole fraction) and ancillary (e.g. H2O mole fraction, internal diagnostic parameters) variables that should be provided to implement the quality management plan for the different model of greenhouse gas analysers currently accepted for the usage in ICOS (i.e. Picarro G1301, G2301, G2401, G5310, LGR 907-0015, LGR 907-0015 (EP)) are described in the document ATC-DU-GN-PR-001 (Ver. 1.5.15, https://icos-atc.lsce.ipsl.fr/documents). As an instance for the greenhouse gas analyser Picarro G2401, the following set of variables must be considered:

"Date,Time,Frac_Days_Since_Jan1,Frac_Hrs_Since_Jan1,Epoch_Time,Alarm_Status,Inst_Status, CavityTemp,CavityPressure,DasTemp,OutletValve,MPVPosition,species,CO2,CO2_dry,CH4,CH4 _dry,h2o_reported,EtalonTemp,co2_base,ch4_base,wlm1_offset,wlm2_offset,co2_pzt_std,ch4_pzt _std,CO,b_h2o_pct,peak_14,peak84_raw,co_pzt_std, final_base84,wlm5_offset".

REMOTE SENSING VARIABLES

3.1 ACTRIS Aerosol Remote sensing

The minimum requirements for the vertical profiles of atmospheric aerosols probed by ground-based instruments are defined by ACTRIS. A site in order to be ACTRIS aerosol remote sensing compliant requires co-located high power lidar (at least 1 Raman and 1 depolarization) and photometer.

In particular, observations of aerosol distribution along vertical paths are covered by two different active remote-sensing instruments: high-power lidar AHL (primary instrument) and automatic low-power lidars (ALC-celiometers) (ancillary instrument). Specifically, AHLs are used to provide profile aerosol optical properties (aerosol backscatter coefficient, aerosol extinction coefficient, and aerosol linear depolarization ratio) at one or more wavelengths, allowing subsequent calculation of several spectral parameters (Ångström exponents, lidar ratios) of the lofted aerosol layers, and therefore aerosol typing.

The minimum setup for aerosol active remote sensing consists of one-wavelength Raman AHL with polarization discrimination capability. The lidar must be operated following the schedule of climatological observations, and measurements of aerosol extinction, backscatter, and depolarization-ratio profiles are to be performed at least at 355 or 532 nm. The minimum requirements for AHLs are the showed in table 4.

Table 4: Minimum requirementsfor AHLs.

Parameter	Minimum requirements
Channels	$1\beta + 1\alpha + 1\delta$ at 355 nm or $1\beta + 1\alpha + 1\delta$ at 532 nm
Height resolution raw (recorded signal)	≤ 15 m
Time resolution raw (recorded signal)	≤ 60 s
Full overlap (m)	≤ 300 1
Minimum altitude range of the 355 raw signal	≥ 15 km
Minimum altitude range of the 532 raw signal	≥ 15 km
Minimum altitude range of the 1064 raw signal	≥ 10 km
Features	Laser alignment (alignment camera) Polarisation calibration Telecover Dark signal measurement Photodetector eye piece

In addition to the AHLs, the ALCs are increasingly providing ancillary measurements useful for the operation of AHLs. Indeed, the temporal coverage and low overlap of low-power lidar instruments are valuable add-ons used to study the diurnal variation of aerosol layers and to trigger advanced measurements performed using high-power lidar instruments. Even single-wavelength low-power lidars are able to detect high-resolution dynamics of aerosol layers.

Guidelines and Standard Operating Procedures (SOP) can be found on the website of the Centre for Aerosol Remote Sensing (CARS), whose mission is to offer operational support to ACTRIS National Facilities operating aerosol remote sensing instrumentation (https://www.actris.eu/topical-centre/cars/announcements-resources/documents)

3.2 NDACC and TCCON

Although CMN-PV does not include the reactive trace gases remote sensing as an component of the ACTRIS national facility, the integration of remote sensing measurements of trace gases concentration is planned for this site because of scientific interest. The standards defined by ACTRIS are taken into account in this integration as guidelines. The minimum requirements for the measurement of trace gases concentrations from ground-based infra-red remote-sensing instruments are defined within the NDACC (Network for the Detection of Atmospheric Composition Change) and TCCON (Total Carbon Column Observing Network) networks. They provide standard practices for the acquisition of high-quality infra-red atmospheric spectra, the calibration procedure and the processing method adopted to retrieve the trace gases concentrations. The minimum requirements for the spectra to be compliant to NDACC and TCCON are:

- Minimum Optical Path Difference (OPD) of 120 cm. 250 cm is recommended for high resolution instruments for optimal profile retrieval.
- Minimum spectral range of 1900-9000 1/cm.
- Continuous spectral coverage in a small number (less than 8) of spectral filter bands.
- Ability to record full-resolution spectrum (in one filter band) in approximately one minute.
- Sun tracker pointing with an accuracy of 0.05°. This accuracy should be routinely monitored.
- Surface pressure measurements with an accuracy of 0.3 mbar.
- Surface temperature measurements with an accuracy of 1 K.
- Accurate knowledge and reporting of the interferogram Zero Path Difference (ZPD) crossing time (within 1 second).
- Routine procedures for monitoring the Instrumental Line Shape (ILS).

More information on the standard calibration procedures, routine validations and processing standard methods can be found in the NDACC (https://ndacc.larc.nasa.gov) and TCCON (https://tccon-wiki.caltech.edu/Main/TCCONRequirements) websites.

The variables that are obtained from the two standard processings of the measured atmospheric spectra are the concentrations of several trace gases. In particular, the NDACC retrieved data include: O3, HNO3, HCl, HF, CO, N2O, CH4, HCN, C2H6, ClONO2 and several other gases that can be detected during episodic events. Due to the high spectral resolution that characterizes the measured spectra, the information is derived on different atmospheric vertical layers, for most of the mentioned gases.

On the other hand, the TCCON retrieved data consist of accurate and precise column-averaged abundances of several atmospheric constituents, including: CO2, CH4, N2O, HF, CO, H2O, O2 and HDO.

CASE STUDIES

4.1 *Example of RI-URBANS / ITINERIS*

One of the objectives of WP4 activity 4.14 is to investigate the impact of the planetary boundary layer (PBL) dynamics on atmospheric pollutants and climate forcers. To achieve this goal, it is important to combine in-situ and remote sensing measurements from different sites (i.e., rural sites, mountain observatories and urban environments). In this way, it is possible to identify the key variables influencing in-situ species concentration and quantify the dilution of pollutions induced by the vertical dynamics of the atmosphere.

During a one-year campaign performed in Milano (2023) within the European project RI-URBANS, it was possible to investigate the impact of PBL on the concentration of various atmospheric pollutants. RI-URBANS involves 13 pilot cities, including Milano, with two main measurement sites for the two main goals: the near real time source apportionment of species (Milano-CNR) and the study of hotspot emissions (Milano-Linate airport). The site Of Milano Linate airport was instrumented with an exploratory platform of ACTRIS RI, which included the full in-situ characterization of optical properties (scattering and absorption coefficients), size distribution (ultrafine, fine and coarse fractions), nitrogen oxides and meteorological variables. The instrumental package included an aethalometer (seven wavelengths), a nephelometer (three wavelengths), a scanning mobility particle sizer, a condensation particle counter, an optical particle counter, an aerodynamic particle sizer, and a NOx gas analyser. The remote sensing included observations from a ceilometer (CHM15k) at Milano Bicocca University. By using aerosols as PBL tracers, it is possible to estimate the PBL height from ceilometer measurements.

As it follows, we report case examples showing the relationship between the height og the PBL and the concentration at the ground of various atmospheric pollutants such as black carbon (BC), NOx and total particles number. For BC and total number of particles, the first four months of the year 2023 are provided, while for NOx, only the months of March and April are included, as the gas analyzer was installed in March. Typical monthly diurnal variations of these variables were derived to compare them with vertical data, particularly with the height of the mixed aerosol layer and the turbulent kinetic energy.

1) Black Carbon (AE33) - solid fuel & liquid fuel (sf & lf)

Source apportionment, using the bilinear model of Sandradewi et al. (2008), was applied to the BC data from the AE33 aethalometer. This approach made it possible to distinguish the two main components of BC: liquid (mainly due to traffic) and solid (mainly due to biomass burning) fuel sources.

The monthly diurnal variations of these components are shown, for the first four months of the year 2023, in the top 4 graphs of the **Error! Reference source not found.**, where the liquid component is in grey and the solid component in orange. The lower graphs show the height of the mixed aerosol layer (MAL), in dark green, and the continuous aerosol layer (CAL), in light green.

It can be observed that the concentrations of both BC components decrease from the winter months towards spring, especially the solid one. Additionally, the peaks due to traffic are more pronounced than others. Besides the typical trend due to the daily variation in concentrations, the depression in the middle hours of the day corresponds to an increase in PBL. Thus, in addition to the daily concentrations trend, there is also dilution due to a higher PBL.

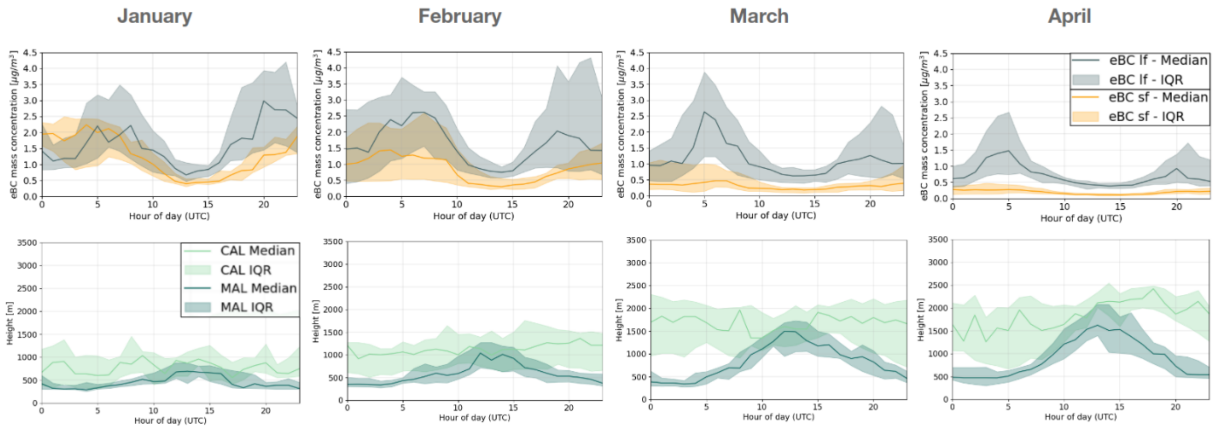


Figure 1: Monthly diurnal variation of BC for year 2023 compared with mixed aerosol layer (MAL) and continuous aerosol layer (CAL).

2) NOx (Gas Analyser)

The monthly diurnal variations of NOx concentrations, obtained with the gas analyser, for the months of March and April in relation to the vertical data are shown in the fig. **Error! Reference source not found.**. The same trend as described above can also be found in this variable. Therefore, in addition to the daily trend, the depression in the middle hours may also be influenced by a higher PBL height.

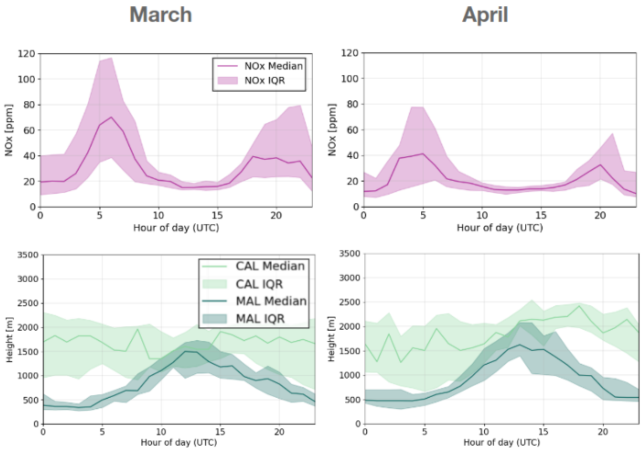


Figure 2: Monthly diurnal variation of NOx for the year 2023 compared with mixed aerosol layer (MAL) and continuous aerosol layer (CAL).

3) Total particles number (SMPS)

The f**Error! Reference source not found.** shows the monthly diurnal variation for the first four months of the year 2023 of the total number of fine particles, obtained from SMPS measurements. Again, the concentrations decrease from the winter months towards the spring months, and the daily trend in concentrations is also linked to a higher PBL height in the middle hours of the day. However, the month of April presents a rather flat trend, unlike what one might expect.

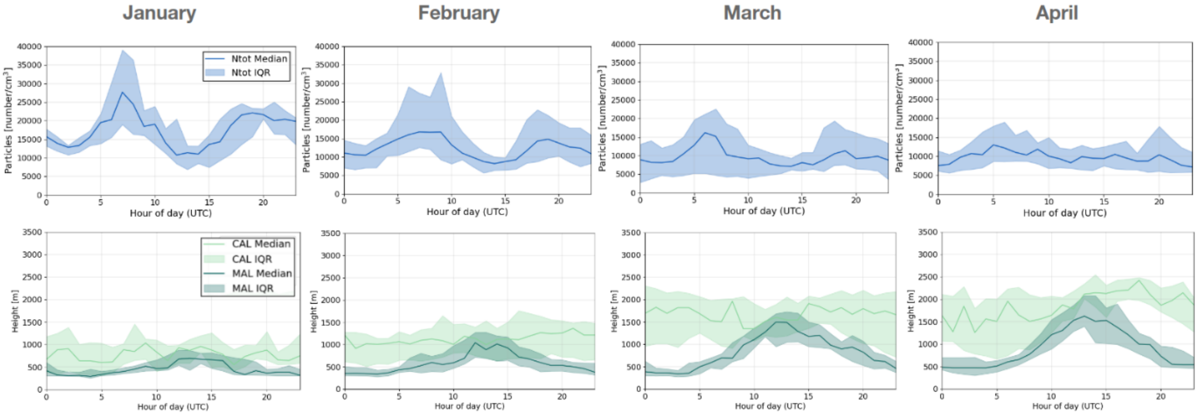


Figure 3: Monthly diurnal variation of the total number of fine particles for year 2023 compared with mixed aerosol layer (MAL) and continuous aerosol layer (CAL).

REFERENCES

1. Crotwell, A., Lee, H., Steinbacher, M.: 20th WMO/IAEA Meeting on Carbon Dioxide, Other Greenhouse

Gases and Related Measurement Techniques (GGMT-2019). Glob. Atmos. Watch Rep. 1–141 (2020).

2. ICOS RI: ICOS Atmosphere Station Specifications V2.0. 0, (2020)
3. Sandradewi, J., Prév?t, A.S., Szidat, S., et al. (2008) Using Aerosol Light Absorption Measurements for the Quantitative Determination of Wood Burning and Traffic Emission Contributions to Particulate Matter. Environmental Science & Technology, 42, 3316-3323. http://dx.doi.org/10.1021/es702253m
4. Schultz, M.G., Akimoto, H., Bottenheim, J., Buchmann, B., Galbally, I.E., Gilge, S., Helmig, D., Koide, H., Lewis, A.C., Novelli, P.C., Plass-Dölmer, C., Ryerson, T.B., Steinbacher, M., Steinbrecher, R., Tarasova, O., Tørseth, K., Thouret, V., Zellweger, C.: The global atmosphere watch reactive gases measurement network. Elementa. 3, 1–23 (2015). https://doi.org/10.12952/journal.elementa.000067
5. WMO: World Meteorological Organization Global Atmosphere Watch Global Atmosphere Watch Measurements Guide. WMO Publ. (2001)