# Deliverable D5.1: Documentation on technical concepts and requirements for ACTRIS Observational Platforms

**Authors:** Ulla Wandinger, Arnoud Apituley, Thomas Blumenstock, Nicolas Bukowiecki, Jean-Pierre Cammas, Paul Connolly, Martine De Mazière, Bart Dils, Markus Fiebig, Evelyn Freney, Martin Gallagher, Sophie Godin-Beekmann, Philippe Goloub, Martin Gysel, Martial Haeffelin, Frank Hase, Markus Hermann, Hartmut Herrmann, Tuija Jokinen, Mika Komppula, Dagmar Kubistin, Bavo Langerock, Heikki Lihavainen, Nikos Mihalopoulos, Paolo Laj, Cathrine Lund Myhre, Emmanuel Mahieu, Stephan Mertes, Ottmar Möhler, Lucia Mona, Doina Nicolae, Ewan O'Connor, Mathias Palm, Gelsomina Pappalardo, Andrea Pazmino, Tuukka Petäjä, Sabine Philippin, Christian Plass-Duelmer, Bernhard Pospichal, Jean-Philippe Putaud, Stefan Reimann, Franz Rohrer, Herman Russchenberg, Stéphane Sauvage, Karine Sellegri, Rainer Steinbrecher, Frank Stratmann, Ralf Sussmann, Dominik van Pinxteren, Michel Van Roozendael, Corinne Vigouroux, Chris Walden, Robert Wegener, Alfred Wiedensohler

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# Contents



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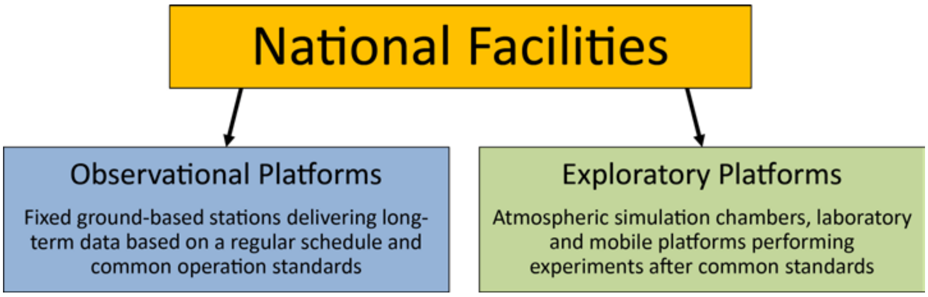
# 1 Introduction

The functionality of ACTRIS is based on a large number of **National Facilities (NFs)** widely distributed over Europe and also located at selected sites outside of Europe. NFs are developed, managed, and operated by the national **Research-Performing Organizations (RPOs)**. Decisions on the implementation and operation of NFs and respective funding solely fall to the member states. The major task of the NFs is the acquisition and delivery of quality-controlled data. NFs can also provide physical access, which will be centrally managed by the **Service and Access Management Unit (SAMU)** within the **ACTRIS Head Office (HO)**.

National Facilities within ACTRIS consist of Observational and Exploratory Platforms. **Observational Platforms** are fixed ground-based stations that deliver long-term data based on a regular measurement schedule and common operation standards. **Exploratory Platforms** are atmospheric simulation chambers, laboratory platforms and mobile platforms that perform dedicated experiments and contribute data on atmospheric constituents, processes, events or regions by following common ACTRIS standards.




This document aims at providing the description of technical concepts and requirements for ACTRIS Observational Platforms. It is complemented by the respective document on Exploratory Platforms (D5.2: *Documentation on technical concepts and requirements for ACTRIS Exploratory Platforms*). The concepts are outlined in sufficient detail to facilitate the substantiated estimation of all efforts and costs for implementation, long-term operation and decommissioning of different kinds of Observational Platforms. The related data can be found in the *ACTRIS Cost Book* (D3.1). With the description of the technical requirements the document also sets the basis for the future labelling of ACTRIS Observational Platforms. The labelling principles are discussed in D5.3 (*Documentation on ACTRIS National Facility labelling principles*).

The document is structured as follows. After this introduction, in Chapter 2 an overview on the ACTRIS observational strategy is given, highlighting the scientific case, user needs and the heritage of established structures and strategies. Chapter 3 outlines the general principles for ACTRIS Observational Platforms. Chapter 4 provides a comprehensive description of the technical concepts and requirements for ACTRIS Observational Platforms in all necessary detail. Chapter 5 describes further organizational and strategic concepts and requirements with view on geographical distribution, co-location, synergies and access capabilities. Annex A summarizes the ACTRIS variables produced by the Observational Platforms and the related instrumentation in tabular form. References and the link to the ACTRIS glossary are provided in Annex B.

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# 2 Overview on ACTRIS Observational Strategy

The goal of ACTRIS is to provide highly reliable information on the four-dimensional distribution of aerosols, clouds and reactive trace gases and on the processes that control their life-cycles, with the grand challenge to reduce uncertainties in future-climate predictions, increase knowledge on climate feedback mechanisms, evaluate air quality and related effects on health and ecosystems and address issues associated with climate–chemistry interaction. The atmospheric constituents investigated by ACTRIS comprise a multitude of species and types that exhibit a large variability in space and time due to the inhomogeneous distribution of natural and anthropogenic sources. The vast variety of complex formation, interaction, transport and removal processes result in relatively short constituent lifetimes of minutes to a few weeks. Therefore, adequate measurement strategies are required to meet the scientific user needs and to provide:

1. Representative long-term, standardized and quality-controlled data for the detection and understanding of trends in the changing atmosphere, the constraining of model predictions of future climate and air quality and the supervision of mitigation measures;
2. Dedicated high-resolved, high-precision and synergistic data for the investigation and understanding of atmospheric processes related to climate and climate feedback mechanisms, air chemistry and climate–chemistry interaction.

For this reason, ACTRIS Observational Platforms perform measurements of aerosols, clouds and reactive trace gases from the Earth surface throughout the troposphere up to the stratosphere by applying state-of-the-art remote-sensing and *in situ* measurement techniques under consideration of harmonized, standardized and quality-controlled instrumentation, operation procedures and data retrieval schemes. Observational sites of ACTRIS cover major geographical areas in Europe and, in addition, important global habitats in order to obtain data representing and contrasting scientifically relevant aspects, e.g., at urban and rural, polluted and clean, mountainous and flat, marine and continental or wet and dry sites or under polar, mid-latitude, sub-tropical, tropical and other climatic conditions. ACTRIS Observational Platforms deliver the data regularly to the ACTRIS DC, where they are accessible and where higher-level products are created and provided to the users. All data have standardized formats, are accompanied with the metadata, contain uncertainty and traceability information and undergo a strict quality control.

The ACTRIS observational strategy has been widely established already over more than two decades. The heritage evolves from European and global observational networks, which have been working on common standards for instrumentation, operation, quality assurance and quality control (QA/QC) and data products over many years. These networks are mainly based on the voluntary association of partners. Their developments have been supported by European infrastructure projects, national agencies, and international activities. ACTRIS incorporates ground-based remote-sensing sites of the European Aerosol Research Lidar Network (EARLINET), the European part of the global Aerosol Robotic Network (AERONET), the European cloud observation network (Cloudnet) and European parts of the global Network for the Detection of Atmospheric Composition Change (NDACC). The ACTRIS network for aerosol *in situ* observations has been established in the framework of the European projects CREATE (Construction, use and delivery of a European aerosol database) and EUSAAR (European Supersites for Atmospheric Aerosol

Research). The heritage builds on the European Monitoring and Evaluation Programme (EMEP) and the Global Atmospheric Watch (GAW) programme of the World Meteorological Organisation (WMO). Interactions with these programmes exist in the form of shared sites and regarding common standards for instrumentation, operation, QA/QC and data curation. ACTRIS standards have been implemented in EMEP and GAW networks on European and global level already in the past and ACTRIS will make a substantial European contribution to these networks in the future. The integration of *in situ* and remote-sensing observations started with the first ACTRIS infrastructure project in 2011. Since then the completion of ACTRIS observation capabilities for short-lived atmospheric species has been steadily pursued, e.g., by establishing standardized European-wide *in situ* observations of reactive trace gases.

One important task of the ACTRIS Implementation Phase is to transform the observational network structures into a consolidated, sustainable, long-term research infrastructure, at the same time maintaining and advancing the long-term efforts of standardization and QA/QC and the capacity to respond to changing scientific requirements. The latter issue is facilitated through the implementation of Topical Centres (TCs), in the form of Central Facilities (CFs), which define the standards, provide operation support and supervise the quality-assurance measures from instrumental setup to data delivery. The present document contributes to the ACTRIS implementation tasks by describing the technical concepts and requirements for the ACTRIS Observational Platforms, considering the heritage of previous developments as well as new aspects needed to improve and substantiate the capabilities of the distributed research infrastructure in the future.

# 3 General Principles for ACTRIS Observational Platforms

ACTRIS Observational Platforms are strategically located in diverse climatic regimes in Europe and outside of Europe. Operated or co-operated by ACTRIS partners, they deliver unique high-quality observational data to the scientific community through the ACTRIS Data Centre (DC) and provide key support to research projects and training activities for the atmospheric and climate science community. ACTRIS Observational Platforms are not necessarily organized at single locations, but can be composed of an ensemble of sub-stations in a regional environment. ACTRIS Observational Platforms follow common general principles listed hereafter. The compliance will be proven through the ACTRIS labelling process (see D5.3).

## General Principles

1. ACTRIS Observational Platforms must support at least one of the **observational components,**
   - aerosol remote sensing,
   - cloud remote sensing,
   - reactive trace gases remote sensing,
   - aerosol *in situ* measurements,
   - cloud *in situ* measurements,
   - reactive trace gases *in situ* measurements,

   by delivering respective high-quality data to the ACTRIS Data Centre, in close cooperation with the associated ACTRIS Topical Centres. The list of ACTRIS variables (to be either directly delivered from the NF or produced within the Data Centre from delivered data) is provided in Annex A of this document, together with the related ACTRIS instrumentation.

2. ACTRIS Observational Platforms are committed to long-term operation for the detection of trends and variability.

3. ACTRIS Observational Platforms are operated by personnel with identified expertise in running the relevant ACTRIS instrumentation. Support for training of personnel will be provided by the Topical Centres.

4. The instrumentation operated at ACTRIS Observational Platforms follows the ACTRIS recommendations (see Chapter 4 and Annex A) and is approved by the Topical Centres. Any deviation from ACTRIS instrumental standards must be documented and approved by the associated Topical Centre.

5. Measurement methodologies and procedures for operating the ACTRIS instruments comply with the standards of calibration, operation and quality assurance defined and recommended by the Topical Centres. Any deviation from ACTRIS standards must be documented and approved by the associated Topical Centre.

6. Data from measurements performed at the ACTRIS Observational Platforms are made available to users through the ACTRIS Data Centre. Data are transferred to the ACTRIS Data Centre following the procedures, formats and timelines described in Chapter 4 and in the Data Management Plan (D4.2). Whenever applicable, data should be transferred in real real-time (RRT, within 3 hours after acquisition) or near real-time (NRT, within 3 days after acquisition).

7. ACTRIS Observational Platforms may provide physical access for users if respective capacity and expertise is proven (see Chapter 5 and D6.3 for specific requirements).

8. ACTRIS Observational Platforms follow the specific technical requirements outlined in Chapter 4. Consequently, ACTRIS Observational Platforms aim at operating an optimum setup of instruments to produce a comprehensive set of ACTRIS variables belonging to one or more of the ACTRIS observational components. In addition, they may deliver individual data belonging to other ACTRIS observational components, in agreement with the related Topical Centres and the Data Centre.

# 4 Technical concepts and requirements for ACTRIS Observational Platforms

In the following, a comprehensive description of the technical concepts and requirements for ACTRIS Observational Platforms, including instrumentation, calibration, operation, data evaluation, data products, data bases, data delivery and the related QA/QC procedures is provided. For each observational component, the respective section describes the entire chain of technical requirements from the instrumentation to data delivery and respective quality control. In the beginning of each section an overview is given, containing recommendations for an optimum setup, minimum technical requirements and suggestions for complementary added-value observations and auxiliary measurements.

The **optimum setup** is considered to be the most suitable configuration of instruments and operation procedures to satisfy the demands of a large user community and to produce a comprehensive set of ACTRIS variables belonging to the respective ACTRIS observational component. **Minimum technical requirements** describe specifications and procedures that are at least necessary to deliver a valuable set of quality-assured variables to the ACTRIS Data Centre. **Complementary added-value observations** may help in the scientific use and interpretation of data from an ACTRIS observational component. Added-value observations are not necessarily part of ACTRIS and thus do not always follow ACTRIS QA/QC procedures. They may however be subject of integration into ACTRIS in the future or follow the standards of other research infrastructures or international bodies. **Auxiliary measurements** cover fundamental parameters (e.g., meteorological data) needed to process or evaluate ACTRIS data and follow established international standards. If adequate, added-value observations and auxiliary measurements are shared among the observational components at the same NF.

In addition to the general principles discussed in Chapter 3, ACTRIS Observational Platforms are expected to fulfil technical concepts and requirements described in the following in order to receive an ACTRIS label. If a different concept than the one described here is used, it has at least to comply with all basic ACTRIS standards and requirements, has to be documented and has to be agreed with the responsible Topical Centre. The technical concepts are subject to innovation and scientific advancement. Thus, the Topical Centres will regularly revise the respective standards and requirements during the lifetime of ACTRIS and help implementing new concepts at the NFs.

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## 4.1 Aerosol remote sensing

### 4.1.1 Introduction

Atmospheric aerosols are highly variable in space and time as well as in their physical and chemical composition, and thus in their optical and radiative properties. The lifetime of particles near the Earth surface ranges from hours to a few days, whereas lofted aerosol layers may be present in the free troposphere over days to weeks and can remain in the stratosphere even over years. Trans-border and inter-continental aerosol transport of, e.g., desert dust, volcanic ash, anthropogenic pollution or biomass-burning smoke, has to be taken into account in the estimation of regional and global direct and indirect radiative effects and climate forcing, but also in the investigation of local and regional air pollution and respective health effects. Therefore, remote-sensing observations in ACTRIS aim at the four-dimensional observation of characteristic aerosol properties at regional, continental and global scales.

This section describes the technical concepts and requirements for ACTRIS aerosol remote-sensing observations. The remote-sensing equipment consists of active and passive instruments, which are operated following principles developed over a long time in the major European and global networks EARLINET (Pappalardo et al. 2006, 2014) and AERONET (Holben et al. 1998, 2001), respectively.

ACTRIS **high-power aerosol lidars** provide quantitative measurements of **aerosol extinction and backscattering profiles,** and thus the **extinction-to-backscatter or lidar ratio,** throughout the troposphere and lower stratosphere with high spatial and temporal resolution. **Spectral and polarization information** (extinction-related and backscatter-related **Ångström exponents** and **particle linear depolarization ratio**) is retrieved in order to classify **aerosol types** and to determine natural and anthropogenic contributions to the aerosol load. ACTRIS variables also include information on **geometrical boundaries of aerosol layers** and **layer-mean optical properties**.

**Automatic sun/sky and moon photometers** measure the **columnar spectral aerosol optical depth and sky radiance**, from which information on **particle microphysical and radiative properties**, e.g., **particle size distribution, absorption, complex refractive index, spherical/non spherical fraction, phase matrix**, is retrieved. The synergistic use of photometer and lidar observations, partly inherited from the AERONET inversion philosophy (Dubovik et al. 2000, 2011, 2014), aims at the retrieval of higher-level variables such as **fine and coarse particle mass concentration** and **spectral extinction, backscatter and absorption profiles**, all consistent with columnar aerosol optical and microphysical properties.

### 4.1.2 Observational capabilities

#### 4.1.2.1 Optimum setup

The optimum setup of an ACTRIS aerosol remote-sensing station consists of a **three-wavelength Raman or high-spectral-resolution (HSR) lidar with polarization discrimination capability** and an **automatic sun/sky and moon photometer** (optionally also polarized) according to ACTRIS/AERONET standards, both operating continuously. Level 0 data of the instruments shall be uploaded automatically to the respective units of the DC (lidar) or TC (photometer) for processing in RRT or NRT, with the aim to provide products for assimilation purposes, fast model evaluation and immediate information of the public about special

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events and hazardous situations. All higher-level ACTRIS variables will be produced and provided by the DC/TC units, including respective QA/QC. A list of variables is provided in Annex A.1 and the products are further described below. Calibration and quality assurance tools for photometer and lidar instruments have to be applied following the guidelines of the Centre for Aerosol Remote Sensing and the requirements outlined below.

#### 4.1.2.2 Minimum requirements

The minimum setup of an ACTRIS aerosol remote-sensing station consists of a **one-wavelength Raman or HSR lidar with polarization discrimination capability** and a **sun/sky photometer**. The photometer has to be set up for automatic operation following the ACTRIS/AERONET standards. Photometer Level 0 data have to be uploaded to the TC in NRT. The lidar must be operated following the measurement schedule for climatological observations and shall in addition contribute to the observation of special events and satellite validation activities. Lidar data have to be uploaded to the DC unit for central processing in NRT in order to provide immediate public Level 1 images (quicklooks). All higher-level lidar and photometer products are centrally produced. Calibration and quality assurance tools for photometer and lidar have to be applied following the guidelines of the Centre for Aerosol Remote Sensing and the requirements described below.

#### 4.1.2.3 Complementary added-value observations

In order to support aerosol process studies, **Raman lidar** measurements of **water vapour** and **temperature** are helpful, e.g., to study hygroscopic growth of particles. For this purpose, the high-power aerosol lidar can be equipped with additional measurement channels. **Microwave radiometer** can be used in synergy to improve the profiling capabilities for water-vapour content and relative humidity.

Complementary observations of the **vertical wind velocity** with **Doppler lidar** and/or **radar wind profilers** are useful to investigate aerosol vertical exchange in the planetary boundary layer and can also contribute to aerosol-cloud-interaction studies.

A continuously operating **low-power lidar** (ceilometer) is useful for stations that do not operate the high-power lidar continuously in order to provide information on atmospheric conditions, e.g., presence of low-level clouds prohibiting useful aerosol observation or indication of special events such as dust or smoke plumes.

**Brewer** and **UVVIS spectrometers** can extend the **aerosol optical depth** measurements towards the UV spectral range and provide a link to observations of **ozone** and **other trace gases**.

Collocated **surface radiation measurements** following the standards of the Baseline Surface Radiation Network (BSRN) help in aerosol-radiation closure studies and trend analysis and facilitate satellite validation activities.

#### 4.1.2.4 Auxiliary measurements

Vertical profiles of **meteorological parameters** (temperature, pressure, relative humidity) are required in the retrievals for calculation of Rayleigh scattering profiles. They can be taken from the output of a high-

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resolution weather forecast model, radiosoundings or standard atmospheric profiles based on surface measurements of **meteorological parameters** (temperature, pressure, relative humidity). The stations should thus be equipped at least with automatic sensors for **standard meteorological measurements** (e.g., **automatic weather station**) to provide useful information on surface conditions. **Radiosondes** measuring vertical profiles of **temperature, pressure, humidity** and **winds** allow calculation of actual Rayleigh scattering profiles independent from model information. Radiosondes should be launched at least twice per day to provide useful information for the processing.

### 4.1.3 Instrumentation and calibration

#### 4.1.3.1 High-power aerosol lidar

ACTRIS Observational Platforms apply sophisticated **high-power aerosol lidars** making use of the **Raman or HSR lidar techniques**, which allow the independent determination of **aerosol extinction and backscattering profiles** based on the separation of pure molecular and particulate atmospheric backscattering. Polarization discrimination is required in order to apply **aerosol typing** algorithms. Measurements of the **particle linear depolarization ratio** permit the identification of large, non-spherical dust particles, which strongly depolarize the backscattered light in contrast to less-depolarizing pollution, smoke or marine aerosols. Measurements of aerosol extinction, backscatter and depolarization-ratio profiles are to be performed at least at one wavelength, either 355 or 532 nm. For an optimized setup, a three-wavelength system is recommended, permitting the measurement of backscatter-coefficient profiles at 355, 532 and 1064 nm and thus the **backscatter-related Ångström exponent** (day and night), extinction-coefficient profiles at 355 and 532 nm and thus the **extinction-related Ångström exponent** (at least at night), and **depolarization-ratio profiles** at 355 and/or 532 nm (day and night). In this way, advanced retrievals of aerosol type and microphysical parameters based on spectral information are possible.

Technical system parameters such as laser power, telescope aperture, receiver bandwidth and data acquisition system must be chosen such that profiles can be acquired throughout the troposphere up to the lower stratosphere with the required accuracy and temporal and spatial resolution. A separate near-range receiving system is recommended for observations in the lower planetary boundary layer, starting at least at 200 m height. Configurations may vary to account for climatic circumstances, e.g., the typical height of the boundary layer for the location of the NF.

Quality assurance measures for aerosol lidars include external intercomparisons and internal check-ups. Intercomparison measurements with one of the reference lidar systems operated by the Centre for Aerosol Remote Sensing shall be performed for new systems and after major upgrades following the methodology described in Wandinger et al. (2015). Internal check-up tools have to be applied regularly based on the recommendations and under the supervision of the Centre for Aerosol Remote Sensing. The checks are outlined by Freudenthaler et al. (2018). Polarization measurements require a detailed system characterization and calibration as described in Freudenthaler (2016).

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#### 4.1.3.2 Automatic sun/sky and moon photometer

For columnar aerosol measurements, the required instrument is a **fully automatic sun/sky photometer**. Only this kind of photometer can provide **aerosol radiative properties** (e.g., size distribution, absorption, complex refractive index, spherical/non spherical fraction, phase matrix) required for aerosol forcing determination. Similarly, for synergetic use of observations (joint photometer/lidar retrievals) **direct-sun** and **diffuse sky radiance** are absolutely mandatory (together with at least two elastic-backscatter lidar signals) to derive, e.g., daytime **aerosol concentration** (fine and coarse modes) and **absorption profiles**. Since moon photometry has recently made significant technical progress, the new sun/sky photometer standard must now include the direct-moon extinction measurement capability, which is again very relevant for aerosol profiling.

Direct-sun and direct-moon-extinction **aerosol optical depth** (AOD) are derived using the Beer-Bouguer-Lambert law. The extra-terrestrial signal has to be determined very accurately to extract AOD with the requested accuracy (0.01 for field instruments and 0.005 for reference instruments). During the operation, optical and electronic components degrade and change the calibration for sun, moon, and sky radiance and polarization observations. Therefore, the regular recalibration of each instrument is mandatory and should be performed every 12 month on average. After the calibration, it is required to set the instrument up again as quickly as possible.

For the standard sun/sky/moon photometer, four major distinct calibrations have to be performed at the Centre for Aerosol Remote Sensing. Day and night AOD calibration must be performed on specific outdoor calibration platforms, whereas radiometric calibrations (sky radiance and polarisation) are performed in the laboratory (for details see the concept paper of the Centre for Aerosol Remote Sensing in D4.1). Since this procedure can last several weeks, spare instruments will be provided by the Topical Centre to cover continuity observation needs at each NF during the calibration phase. The requirement of the annual re-calibration is very strong. A 5% variation in the direct-sun or moon calibration coefficients (caused by filter degradation, deposit of dust on external lenses, etc.) yields to typical 0.05 absolute bias on AOD at noon (Holben et al. 2001, Smirnov et al. 2000). If the period between two calibrations is too long, the assumption of linear variation of the instrument response will be not valid, neither the temporal interpolation performed in the reprocessing phase for getting QA Level 1/Level 2 data products.

### 4.1.4 Operation

#### 4.1.4.1 High-power aerosol lidar

It is recommended to operate ACTRIS high-power aerosol lidars continuously, weather permitting, i.e., in the absence of precipitation or fog. If the instrument is not automated, it must at least provide unbiased long-term regular observations following the pre-defined schedule with 5 observations per week as agreed within the community to avoid a meteorological bias. Furthermore, measurements are to be performed upon alert, e.g., in hazardous situations such as volcanic eruptions, for special events such as dust outbreaks or forest fires, and for dedicated satellite validation purposes. Satellite validation measurements will follow a specific strategy. Alerts and measurement schedules for collocated observations during satellite overpasses will be distributed by the lidar unit of the DC.

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Regular observations shall last for 4 hours, to adequately capture the atmospheric state and to allow for enough observation time to reduce random noise in the measurements and to retrieve a set of aerosol profiles throughout the troposphere. Longer measurement periods are to be considered for special events. In any case, raw data (Level 0) must be recorded with a resolution of at least 60 s in time and 15 m in height in order to permit proper cloud screening and the provision of quicklook images for visual assessment of the atmospheric conditions.

#### 4.1.4.2 Automatic sun/sky and moon photometer

Photometers must be automatic and are operated continuously weather permitting, i.e., in the absence of precipitation. Considering the diversity of photometers operated in regional or global networks, three types of observations can be taken into account: direct sun/moon extinction measurements to retrieve spectral AOD; sky angular radiance measurements; and sky angular polarized radiance measurements. In some cases, cloud radiance observations can also provide Cloud Optical Depth (COD). Spectral AOD and sky angular radiance measurements are mandatory. In addition, sky angular polarization measurements can provide the full picture of the radiation characteristics, but remain optional until a mature data processing chain is implemented.

Direct sun/moon and sky radiance measurements follow a consistent scheduled scenario. Spectral AOD is measured very frequently, whereas simultaneous AOD and sky radiance measurements are performed less frequently, but provide necessary information to retrieve scattering and absorption properties. It must be outlined that new algorithm developments (e.g., Torres et al. 2017) based on the Generalized Retrieval of Aerosol and Surface Properties (GRASP) offer now the possibility to invert spectral AOD to retrieve, both during day and night, the aerosol size distribution. Sky radiance is not measurable at night with the current technology, however, a multi-pixel approach based on GRASP should allow, e.g., the retrieval of absorption at night in the future.

The standard measurement mode of a sun/sky/polarization (and moon) photometer includes two basic measurements, either direct-sun/moon or sky measurements, both within several programmed sequences or protocols at wavelengths of 340, 380, 440, 500, 675, 870, 940, 1020 and 1640 nm. The 940-nm channel is used for column water abundance determination, always relevant when investigating aerosols. AOD is calculated from spectral extinction of direct-beam radiation at each wavelength based on the Beer-Bouguer-Lambert law.

A sequence of three measurements is taken 30 seconds apart creating a triplet observation per wavelength to detect cloud contamination. During the large-air-mass periods, direct-sun measurements are made at 0.25 air mass intervals, while at smaller air masses the interval between measurements is typically 15 minutes. The temporal variation of clouds is usually greater than that of aerosols causing an observable variation in the triplets that can be used to screen clouds in many cases. Additionally, the 15-minute interval allows a longer temporal frequency check for cloud contamination.

In addition to the direct solar irradiance measurements, the instruments must measure the sun aureole and sky radiance (optionally the polarized sky radiance) in at least four spectral bands (440, 675, 870 and

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1020 nm) with different geometries: almucantar, principal plane, hybrid, etc. Sampling must be done typically every hour, or less at large solar zenith angles. This kind of measurements provides spectral sky radiance observations over a large range of scattering angles that are inverted, together with spectral AOD, to retrieve the aerosol size distribution (from 0.04 to 20 µm), absorption and other optical properties.

### 4.1.5 Data production and data products

#### 4.1.5.1 High-power aerosol lidar

Aerosol lidar raw data acquired at NFs are mandatorily processed at the ACTRIS DC using the Single Calculus Chain (SCC). The NFs are responsible for reporting the technical information required for the configuration of the SCC for the specific high-power aerosol lidar system. As support to the NFs, the Centre for Aerosol Remote Sensing provides tools for the NFs for on-site data evaluation procedures and plausibility tests to be performed before starting a measurement or at regular interval for automatized systems. The QA/QC tests performed and/or coordinated by the Centre for Aerosol Remote Sensing are codified and embedded in the SCC for traceability and full documentation of the data quality.

Different levels of products are produced. **Level 0 data** are the **raw lidar data,** which are delivered by the NF to the ACTRIS DC. The processing of Level 0 data allows the provision of higher-level products. **Level 1 data** contain not fully quality controlled data, namely the **pre-processed lidar signals** including all the instrumental correction factors and **profiles of aerosol optical properties** and corresponding **layer products**. In particular, standard products are the **profiles of aerosol extinction coefficient, backscatter coefficient and depolarization ratio**, together with the resulting **profiles of lidar ratio, Ångström exponent and backscatter-related Ångström exponent**. Layer products report statistical values of all these quantities for each identified aerosol layer, together with geometrical features of the layer itself. Additional data products resulting from the **combination** of different observational components, like daytime **aerosol microphysical properties** and **spectral absorption profiles** (Lopatin et al. 2013) retrieved through the combination of aerosol lidar and photometer observations, will also be part of the ACTRIS Level 1 data products.

**Level 2 data** are the same Level 1 products, but fully quality controlled and containing devoted flagging. The full quality control procedure is based on: update of meteorological fields used in the processing; reporting/updating of QA tests performed and traced by the Centre for Aerosol Remote Sensing; and results of ACTRIS DC QC procedures and related feedbacks to the NFs (with potential feedback to the Centre for Aerosol Remote Sensing). **Level 3 data** are climatological, statistical and other products obtained using the Level 2 data. All quantities are reported together with the statistical and systematic errors, according to the state of the art.

#### 4.1.5.2 Automatic sun/sky and moon photometer

Photometer data are automatically transferred to the Centre for Aerosol Remote Sensing where the standard data processing procedures (following AERONET definitions) are performed to convert Level 0 to Level 1 and Level 1 to Level 2 data products. For new products (non-AERONET), Level 0 to Level 1 processing can be performed at the Centre for Aerosol Remote Sensing as well, while the generation of

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specific Level 2 or 3 products, especially those combining column and profile Level 1 data (Dubovik et al. 2011, Lopatin et al. 2013, Dubovik et al. 2014), will be done at the ACTRIS DC (see concept papers of the Centre for Aerosol Remote Sensing and the Data Centre in D4.1). The Level 0 to Level 1 standard automatic processing corrects for various instrumental and atmospheric effects. An automatic cloud screening procedure is also applied to generate either Level 2 aerosol or cloud products.

Standard tools are applied at the TC to evaluate the various data levels and, when necessary, to warn the NFs. Several tools (all centralized and associated to a central relational data base) are recommended to be used by the local site manager of the NF to check the status of the instrument (more details are given in the concept paper of the Centre for Aerosol Remote Sensing in D4.1).

All data levels currently provided by an automatic sun/sky and moon photometer operated in existing operational networks are documented in terms of Standard Operation Procedures (SOPs) and uncertainties. The documentation is publically available. In general, Level 0 data is not made available to the public. QA/QC and calibration procedures are standardized. In principle, average uncertainty on each produced variable is equivalent for each station, since QA/QC and calibration are also standardized. Finally, the uncertainty will be associated to each retrieved aerosol variable (directly or indirectly measured).

### 4.1.6 Data delivery and quality control

#### 4.1.6.1 High-power aerosol lidar

The ACTRIS high-power aerosol lidar products are collected and made available through the ACTRIS Data Centre and the ACTRIS data user interface. The data repository is a version-controlled database in order to accomplish the need for reprocessing the data and for producing new advanced products from the raw data delivered by the NFs.

The NFs are responsible for submitting the Level 0 data to the ACTRIS DC in the agreed and documented format as specified in the Data Management Plan (D4.2). These data are then centrally processed at the ACTRIS DC. Level 1 data products are retrieved and made available in NRT internally and externally, according to the agreed Data Policy (D2.3). Level 1 data are made publicly available as visualizations and on request for specific use (e.g., for assimilation purposes), while the higher-level numerical data products are available for file download by ACTRIS users.

Level 2 data are open and publicly available, when the quality control procedures are completed. Quality control procedures (performed every 3 months) include some formal and automatic procedures, which are completed already on Level 1 data, but also some procedures related to the identification of anomalous behaviour in the aerosol optical properties and the identification of potential instrumental problems. The time between the NRT provision (Level 1 data) and the provision of fully quality controlled data allows the use of more accurate meteorological fields in the processing, the update of instrumental QA flags and signal corrections. Level 3 data are publicly provided based on Level 2 data annually.

The responsibility for the ACTRIS data quality is on the data originator at the NF. The QC performed at ACTRIS DC provides feedback to the data originator, which can be useful for identifying potential problems of the instrument and fixing them at NF level or with the help of the Centre for Aerosol Remote Sensing.

#### 4.1.6.2 Automatic sun/sky and moon photometer

There are three databases for ACTRIS photometer data available. Beside the official (external) AERONET database and processing system operated by NASA, France and Spain have built dedicated databases and processing chains (i.e., Level 0 to Level 1 Data Management and Production) to respond to some specific needs not covered by NASA and to offer an independent production of Level 1 data for ACTRIS and the provision of data through the ACTRIS DC (i.e., production of value-added parameters, Level 2 and higher). Level 0 to Level 1 data processing chains have been developed, e.g., for specific instruments like mobile photometers (Karol et al. 2013, Torres et al. 2017) and for testing of new calibration methodologies (Li et al. 2010, 2013, 2016, 2017, Barreto et al. 2013, 2017) (see concept paper of the Centre for Aerosol Remote Sensing in D4.1).

For standard ACTRIS/AERONET instruments, the Level 0 data are transferred in NRT to one of the three dedicated databases as soon as they have been acquired at the station. All three databases (all levels) are synchronized and are permanently identical. Similarly, the same data management systems (e.g., monitoring, calibration) are in operation in the three units. The data processing system (Level 0 $\rightarrow$ Level 1 $\rightarrow$ Level 2) is centralized and the resulting data products (Level 1, Level 2) are immediately synchronized in the French and Spanish databases.

As mentioned above, the major requirement is to transfer the data NRT to the database, which is mandatory to monitor the instrument and the NRT processing and product delivery. Standardization of the instrument and the data transmission protocol are imposed by the TC. Tools are distributed to each operator to allow NRT transmission through different channels (internet, satellite transmission for very special and remote places). The data are made public immediately.

The Centre for Aerosol Remote Sensing is in charge of most of the quality control activities, as explained previously, by following regularly a list of instrumental parameters, detecting anomalies, informing operators and solving problems. The operators must be continuously involved in the quality control. The visual inspection of the instrument (optics, collimator and cables to solar panel and data transmission system) once a week is required. Furthermore, the operators must react efficiently and immediately on alerts sent by the TC. All operators have access to the monitoring webpage and can see the status of the main instrumental parameters (battery level, tracking system, humidity and temperature sensors, etc.). They also have access to Level 1 data in NRT so that they can potentially detect themselves apparent calibration shifts due to collimator obstruction or similar issues.

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## 4.2 Cloud remote sensing

### 4.2.1 Introduction

Clouds form a major component of the Earth's radiation budget. They vary rapidly in space and time, with associated rapid variation in the radiation and precipitation impinging on the Earth's surface. To obtain quantitative information on how clouds evolve in space and time requires instruments that can capture both the vertical profile and the temporal variation with sufficient resolution.

Within ACTRIS, the primary objective is to obtain the **vertical cloud structure** within an atmospheric column, utilising the temporal dimension to yield the equivalent of a two-dimensional slice through the three-dimensional atmosphere. The resolution required to capture such highly variable entities necessitates the use of active remote sensing in the form of cloud radar and lidar or ceilometer. Both instruments, each sensing a different portion of the electromagnetic spectrum, are required to disentangle ambiguities in the **atmospheric targets** that are detected.

This recommended combination of instruments was instigated in the European FP5 project Cloudnet starting in 2003, where the original objective was the routine automated evaluation of the representation of clouds in numerical models using observations. Evaluating the representation of clouds in climate and numerical weather prediction (NWP) models is not straightforward. For NWP models, this task is compounded by the expectation of a good forecast, as well as the reliable representation of the specific cloud parameters themselves. Cloudnet developed and implemented a comprehensive suite of **objective metrics for the evaluation of model cloud parameters**, in continual joint collaboration with operational modellers. The set of evaluation metrics is designed to investigate both the climatological aspects required of a climate model, and the ability to forecast the correct cloud at the right time, a necessary validation for NWP.

### 4.2.2 Observational capabilities

The objective to provide continuous long-term vertical profiles of **cloud fraction** and **water** and **ice cloud properties** requires the synergistic use of three core instruments—Doppler cloud radar, lidar/ceilometer and microwave radiometer—and an optional Doppler wind lidar. To qualify as an ACTRIS compatible cloud-profiling station, the instrument setup must be capable of continuously providing vertical profiles of clouds at the nominal Cloudnet resolution of 30 seconds and 60 metres. The list of variables is provided in Annex A.2.

#### 4.2.2.1 Optimum setup

With the optimum setup, cloud-profiling stations deliver a comprehensive set of atmospheric quantities such as **cloud and aerosol target classification, cloud fraction**, **liquid water content**, **ice water content**, **drizzle properties (size distribution, water content, water flux), dissipation rate of turbulent kinetic energy, liquid water path, integrated water vapour path, temperature** and **humidity profiles.** To enable these quantities to be derived, the instruments must have the following capabilities:

**Doppler cloud radar** providing the full Doppler spectrum, together with the first 3 moments of the Doppler spectrum (reflectivity, Doppler velocity, and spectral width) and linear depolarisation ratio is the basic instrument. The minimum sensitivity should be at least −60 dBZ at 1 km for 10 second integration time enabling the detection of almost all radiatively significant **ice clouds** in non-precipitating conditions. This sensitivity can be achieved with both pulsed and frequency-modulated continuous-wave (FMCW) Doppler radars operating at 35 or 94 GHz (and potentially at higher frequencies). At these frequencies, correction for attenuation by atmospheric gases and, more importantly, liquid water clouds is necessary; attenuation is less at 35 GHz, so this frequency is preferable to 94 GHz. In addition, radome wetting during periods of rainfall leads to large signal losses and unreliable data.

Lower-frequency radar (e.g., 10 GHz more typical of weather radar) can also achieve the desired sensitivity in vertically-pointing mode and be able to provide reliable data during periods of rainfall. However, lower frequencies pose additional constraints such as enhanced sensitivity to insects and clutter issues at near range (larger sidelobes due to antenna size constraints limiting how focused the transmit beam is), and a minimum range that may preclude measurements of liquid layers in the boundary layer.

Higher temporal resolution (especially 1 second integration time) permits the generation of products based on the velocity variation (e.g., **turbulence**, **drizzle products** based on skewness) in addition to the standard products. The full Doppler spectrum permits the analysis of situations where more than one distinct hydrometeor population is occupying the same volume (e.g., **mixed-phase clouds** with both supercooled liquid and ice particles, stratocumulus containing liquid droplets and drizzle drops). The velocity resolution, usually determined from the Nyquist velocity and the number of points in the FFT (Fast Fourier Transform) used to obtain the Doppler spectrum, should be 10 cm $s^{-1}$ or better to make maximum use of these capabilities.

Inclusion of additional radar frequencies also expands the range and accuracy of products that can be derived. Dual-frequency (e.g., 35 and 94 GHz) permits the vertical **profile of liquid water content** to be derived without restrictive assumptions, and triple-frequency (e.g., 10, 35, 94 GHz) permits **ice microphysical properties** to be deduced without certain density and habit assumptions through accounting for Mie scattering at higher frequencies. Multiple frequencies also assist in accounting for atmospheric attenuation, especially if one of the selected frequencies is around 10 GHz or less.

**High-power aerosol lidar** capable of detecting **thin ice clouds**, **elevated aerosol layers** and the molecular backscatter signal provides additional retrieval capabilities and improves high-altitude cloud statistics. A depolarization channel is desirable for unambiguous **particle phase discrimination**. The ability to retrieve extinction directly through high-spectral-resolution or Raman methods also greatly improves retrieval uncertainties and provides a consistency check. Aerosol properties at high resolution permit synergy between aerosol (see Sec. 4.1) and cloud remote sensing retrievals allowing investigation of **aerosol-cloud interactions** in the same profile.

**Multi-channel scanning microwave radiometer** permits the retrieval of **temperature** and **humidity profiles**, in addition to the standard column-integrated measurements. The addition of an extra-high frequency channel (such as 89 or 180 GHz) provides extra sensitivity to thin clouds with very low liquid water path (LWP) that are still radiatively important (such as supercooled layers found in the Arctic).

**Doppler wind lidar** provides the **dynamical features** of the atmospheric boundary layer, including winds, turbulent properties, shear, mixing-level-height, low-level jets, and classification of the turbulent sources.

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In combination with aerosol and cloud retrievals, such properties permit the identification of aerosol layers and clouds that are directly coupled to the surface, extend the *in situ* measurements at the surface vertically through the atmospheric column and provide the **timescales for turbulent transport**.

#### 4.2.2.2 Minimum requirements

The minimum setup of a cloud-profiling station consists of less powerful core instruments that may operate on just one channel. The measurements are used to derive the minimum set of atmospheric quantities: **cloud fraction**, **liquid water content**, **ice water content** and **drizzle properties.** To enable these quantities to be derived, the three core instruments must have the following capabilities:

**Cloud radar** with Doppler capability providing profiles of radar reflectivity factor and Doppler velocity: Minimum sensitivity should be about −50 dBZ at 1 km in the absence of attenuation.

**Ceilometer** (low-power lidar) capable of detecting liquid water layers, including supercooled liquid layers, up to 7.5 km in altitude: In this mode, the primary function of the ceilometer is purely the detection of liquid water in the lower troposphere.

**Dual-frequency microwave radiometers**, where the liquid water path and water vapour path are derived from two brightness temperatures ideally measured at frequencies close to 23.8 and 36.5 GHz. The approach by Gaussiat et al. (2007) is then used to derive an accurate liquid water path by correcting for instrumental drifts in calibration and unknown absorption coefficients by adding a calibration offset to the derived optical depths. The offset is determined in clear-sky periods as indicated by the ceilometer, when it is expected that the liquid water path be zero.

#### 4.2.2.3 Complementary added-value observations

**Water vapour** and **temperature** profiles measured with **Raman lidar** can provide useful information on the atmospheric conditions under which clouds develop. The profiling capabilities for water vapour content and relative humidity can be further improved when Raman lidar and **microwave radiometer** measurements are combined in synergistic retrievals. For this purpose, the high-power lidar used in the optimum setup can be equipped with additional measurement channels.

**Radar wind profilers** provide the vertical profile of **horizontal and vertical winds**. The horizontal wind profile can be used to determine appropriate advection-based averaging for cloud variables, provide suitable length scales for deriving turbulent parameters and statistical-based algorithms and determine the beam-broadening component for radar vertical velocity uncertainties. The profile of the vertical wind (determined from clear-air returns) can be used to provide the 'true' vertical wind. The cloud radar measures the hydrometeor velocity, which is the sum of the hydrometeor fall velocity and vertical air motion. The hydrometeor fall velocity provides excellent information on the hydrometeor size, density and shape; after correction for the vertical air motion, algorithms can use the cloud radar Doppler velocity as an additional component to constrain microphysical properties. Winds throughout the full tropospheric profile are of interest.

Combination of a **sonic anemometer** and a **Licor gas analyser** permits the calculation of the **sensible and latent heat flux** (and $CO_2$ flux) at the surface. Together with radiation measurements, the full surface energy balance can be obtained using micrometeorological methods by including a **soil heat plate** to determine the **heat flux into the ground**.

The **atmospheric emitted radiance interferometer** (AERI) is a ground-based instrument that measures the **downwelling infrared radiance** with sufficient spectral resolution to discriminate among gaseous emitters (e.g., carbon dioxide and water vapour) and suspended matter (e.g., aerosols, water droplets and ice crystals). These upward-looking surface observations can be used to obtain vertical profiles of tropospheric **temperature and water vapour**, as well as measurements of **trace gases** (e.g., ozone, carbon monoxide and methane) and **downwelling infrared spectral signatures** of clouds and aerosols.

The **micro rain radar** (MRR) is a very low-power vertically-pointing FMCW Doppler radar operating at 24 GHz providing the full Doppler spectrum, from which vertical profiles of the **drop size distribution of precipitation** are derived. This instrument complements the cloud radar in the nearest 2 km by providing the precipitation profile to the surface, enabling correction for any saturation in the cloud radar near field, and aiding calibration activities.

**Drop-counting raingauges** and **snowgauges** provide closure methods for microphysical profiles of precipitation derived from the active remote sensing vertical profiles. Various types of **disdrometers** and **cameras** can provide information on the **hydrometeor size distribution, phase, shape and density**.

**Broad-band shortwave** and **longwave radiation** measurements at the surface (e.g., BSRN station) are an obvious complement to cloud profiling, and also provide an opportunity to implement closure studies on the vertical profile of microphysical properties derived from the cloud-profiling measurements. For full closure, it is recommended that all radiation components are measured (shortwave down, net, direct and diffuse, and longwave down and net).

#### 4.2.2.4 Auxiliary measurements

Vertical profiles of **meteorological parameters** (temperature, pressure, specific humidity and winds) are required for quantifying instrument, atmospheric attenuation and retrieval uncertainties. They may be taken from the output of a high-resolution weather forecast model or radiosoundings. **Radiosondes** measure high-resolution vertical profiles of **temperature, humidity and winds**, thus providing the parameters necessary for specific instrument corrections within the cloud profile processing scheme, independent from any model that might be evaluated. However, only radiosonde launches at sites where the frequency is twice per day or higher are suitable for inclusion within the processing.

**Standard meteorological measurements** (e.g., **automatic weather station**) provide useful information on surface conditions, especially those that may impact the core measurements, such as precipitation, strong winds, extreme heat or cold, and can be used within the QA system. The measurement system should include a precipitation detection system with fast response times (i.e., optical rain gauge or present weather detector).

### 4.2.3 Instrumentation and calibration

#### 4.2.3.1 Cloud radar

**Cloud radars** are active systems similar to weather radar, but operating at higher frequencies, typically 35 and 94 GHz. These higher frequencies permit much smaller antennae and power consumption than weather radar frequencies but suffer more from gaseous and liquid attenuation, which must be corrected for. Higher frequencies also have an advantage with clutter suppression, due to the more focused radar beam, and a reduction in the amount of scattering by insects ubiquitous in the lower atmosphere; insect sizes relative to the radar wavelength mean they are scattering in the Mie regime. The radar must be Dopplerized, as **Doppler velocity** measurements are required for hydrometeor diagnosis (e.g., liquid cloud droplets versus drizzle drops, identification of the melting layer as slowly falling snowflakes melt to become rain drops with significant terminal fall speeds), and for discriminating between insects and other hydrometeors. The second moment of the Doppler spectrum, **Doppler spectral width**, is a useful but not strictly necessary additional parameter. Both pulsed and frequency-modulated continuous-wave (FMCW) Doppler radars are suitable, provided there is no saturation. Cloud radars capable of measuring **Linear Depolarisation Ratio** (LDR) provide significant advantages in insect discrimination, melting layer determination and ice crystal classification.

The preferred measurement mode is vertical pointing, since this permits the direct use of Doppler velocities (after correction for the motion of the air) in microphysical retrieval and reduces the severity of attenuation due to gases and liquid. Scanning is permitted but is not directly applicable for ACTRIS measurements. Note that without measurements of liquid water path, it is not possible to determine how strongly the profile of radar reflectivity is attenuated by an intervening liquid layer. Sensitivity to ice clouds above a liquid layer is then reduced by an unknown amount, potentially causing issues in determining cloud fraction, and there is an unknown bias in the reflectivity profile harming measurements in ice above the liquid layer.

The amount of radar reflectivity attenuation due to liquid is frequency dependent. The two-way attenuation due to a cloud with a liquid water path of 500 g $m^{-2}$ is around 4.5 dB at 94 GHz, but only 1.2 dB at 35 GHz, and less at lower frequencies. Hence, it is possible to sidestep the issue of liquid attenuation in particular locations under certain conditions through the use of a lower-frequency radar – such as the Arctic in winter when there are no warm liquid layers present, only thin supercooled liquid layers with very low liquid water path.

The cloud radar must be capable of detecting the vast majority of optically relevant clouds, which can be directly expressed in terms of radar reflectivity. Comparing radar returns with the optical depth derived from lidar, for ice clouds up to a height of 9 km, Protat et al. (2006) show that a radar with a sensitivity of –55 dBZ at 1 km should detect 80% of the ice clouds with an optical depth above 0.05 and 97% of clouds with an optical depth greater than 0.1. For a radar with –60 dBZ sensitivity at 1 km the percentages are 98% and 100%, respectively. Hence, a minimum requirement is −50 dBZ at 1 km with a temporal resolution of 30 seconds and 60 m resolution in the vertical. Calibration of the reflectivity is vital for removing bias in both calculating cloud fraction amounts and in deriving ice water contents; a systematic 1 dB radar calibration error results in a 15% error in mean ice water content when using the radar reflectivity–

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temperature method of Hogan et al. (2006). Hence, radar reflectivity calibration should take place at least twice a year (see calibration methods described in the concept paper of the Centre for Cloud Remote Sensing in D4.1). Doppler velocity calibration is usually not necessary but can be checked by pointing at a hard target. Ensuring that the instrument is indeed pointing at vertical is very important; off-vertical Doppler velocity measurements will contain a component from the horizontal wind which may be significant at altitudes close to the tropopause where horizontal wind speeds can easily exceed 50 m $s^{-1}$.

Precipitation can cause wetting of the radome or antenna, causing significant attenuation which is difficult to ascertain. Reflectivity data is not reliable in these conditions and should be flagged. Atmospheric attenuation, including gaseous, liquid rain, and the melting layer, is diagnosed and corrected for, if appropriate, in the data processing stage.

#### 4.2.3.2 Ceilometer/Lidar

**Ceilometers** are single-wavelength, low-power, automatic lidars typically operating at wavelengths ranging from 850 to 1064 nm, originally designed to provide the cloud base altitude. Since clouds are very strong scatterers at near-infrared wavelengths, these systems do not require the high power expected for aerosol lidar systems. However, the sensitivity of current ceilometers is sufficient to detect aerosol within the boundary layer, and thicker ice clouds. High-power aerosol lidar systems can also be used (see Sec. 4.1).

The key parameter for the ceilometer or lidar is detection of **liquid layers**, including supercooled liquid layers. To improve sensitivity, averaging of data to 15–30 m in the vertical and 15–30 seconds in time is therefore appropriate. The minimum range should be 200 m or less to enable detection of fog layers, which might be missed by the cloud radar causing unaccounted-for attenuation. Maximum range should exceed 7.5 km to enable detection of supercooled liquid layers down to almost −40 °C. Note that ceilometers with extended maximum range are required in regions where supercooled layers may be expected above 7.5 km, such as the tropics. Instrument design may mean that full overlap between receiver and transmitter is not reached until 1 km or so, with correction of the signal possible in part of the overlap region; this is permissible as long as detection of liquid layers at 200 m is still possible. Possible saturation of the lidar signal in clouds at low altitudes must be flagged and mitigation procedures adopted to prevent this occurring.

Instrument sensitivity is dependent on the signal-to-noise ratio (SNR), which is a function of the emitted power, telescope design, averaging time, background light and the strength of the backscattered return from atmospheric targets. Thus, stray background light (solar radiation) entering the detector chain leads to a drop in sensitivity during the day.

The required sensitivity for liquid-layer detection can be expressed in terms of extinction, with typical values exceeding 10 $km^{-1}$. Since the lidar ratio for cloud droplets is about 20 sr at almost all lidar wavelengths, this translates to a backscatter coefficient of about 0.5 $km^{-1}$ $sr^{-1}$ which is achieved by all current ceilometer systems up to 7 km even during daytime as long as the instrument is operating at designed performance levels. Note that this sensitivity is not sufficient to detect high ice clouds, which can have lower extinction than 0.05 $km^{-1}$.

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Ceilometer instruments are calibrated by the manufacturer, and the calibration is regarded as stable over time. However, the calibration should be checked on installation, and then periodically over time using a standard naturally occurring atmospheric target with a known backscatter, such as molecular backscatter or liquid clouds that fully extinguish the signal (see calibration methods described in the concept paper of the Centre for Cloud Remote Sensing in D4.1). These calibration methods yield a calibration accurate to about 10% (O'Connor et al. 2004, Wiegner and Geiß 2012), suitable for cloud detection and target categorization.

High-power aerosol lidar systems can also be used instead of ceilometers. These should utilise a near-range channel to avoid overlap issues, and include neutral-density filters to mitigate saturation in liquid layers. Full calibration should follow the specifications given in the concept paper of the Centre for Aerosol Remote Sensing in D4.1.

Further use of the lidar signal in specific algorithms may require much more stringent tests on calibration, stability, and the calculation of the influence of multiple scattering.

#### 4.2.3.3 Microwave radiometer

**Microwave radiometers** are passive receivers calibrated to measure the down-welling thermal emission from the atmosphere; from which some atmospheric thermodynamic properties can be deduced. The quantity measured is atmospheric radiance (W $m^{-2}$ $sr^{-1}$ $Hz^{-1}$), typically converted into brightness temperature (Tb, in Kelvin). Thermal emission is usually measured in the 20–60 GHz range. The 22–35 GHz band provides information on water vapour and cloud liquid water, with at least two channels (usually 23.8 and 30–31 GHz) required to retrieve the **column-integrated water vapour path and liquid water path**. Additional channels in this region can provide information on the vertical distribution of water vapour content. Some instruments make observations at 50–60 GHz to derive **temperature** information, with a vertical profile usually obtained through scanning at multiple elevation angles. Current systems have a temporal resolution better than 1 minute.

Microwave radiometers are continuously calibrated internally using a black-body target at ambient temperature and noise power injected by diode sources. In addition, external calibration should be performed using a tipping curve method (for scanning systems) and by an external target (liquid nitrogen). Calibrated microwave radiometers are then expected to be capable of providing brightness temperatures with an absolute accuracy of 0.3–0.5 K. This results in measurements of LWP with an accuracy of about 20 g $m^{-2}$. External calibration with a liquid nitrogen target is recommended at least twice a year (see calibration methods described in the concept paper of the Centre for Cloud Remote Sensing in D4.1).

Precipitation causes wetting of the radome, with similar attenuation issues as experience by the cloud radars. The data is not reliable in these conditions and must be flagged.

#### 4.2.3.4 Doppler wind lidar

**Doppler wind lidars** are single-wavelength lidar systems that provide profiles of SNR and **radial Doppler velocity**. These instruments are typically low-power, eye-safe, automatic lidar systems operating at wavelengths close to 1500 nm, and Doppler velocity is usually obtained using the heterodyne technique.

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The scattering targets are aerosol particles and cloud droplets, which act as tracers from which winds and turbulent properties can be derived, and larger hydrometeors such as ice and rain drops. Vertical profiles of the horizontal wind are obtained by pointing off-zenith, whether by combining three or four orthogonal beams (Doppler Beam Swinging – DBS) or by conical scanning (Velocity Azimuth Display – VAD), hence one key requirement is that the Doppler lidar instrument is configured with multi-beam or scanning capability.

The other key requirement for the Doppler lidar is that it must have sufficient sensitivity to obtain velocity information throughout the extent of the boundary layer. The majority of the scattering targets in the boundary layer are aerosol particles and the required sensitivity is therefore similar to ceilometer systems. The minimum measurement height should be 100 m or less, but this can be mitigated through the use of scanning at low elevation angles (minimum range may exceed 100 m), and the maximum range should extend beyond the boundary layer (i.e., maximum range should be at least 2 km in most cases).

Quantitative measurements of winds and turbulent mixing in the atmosphere require accurate characterization of the uncertainties in the radial SNR and Doppler velocities. Since radial Doppler velocity uncertainty estimates are derived from SNR, full characterization of the background noise behaviour of the instrument, and possible subsequent post-processing, is necessary (Manninen et al. 2016). This improvement in the radial Doppler velocity uncertainty estimate propagates directly through to wind retrievals and is **vital for deriving reliable higher order velocity statistics** such as variance, skewness and dissipation rates; for example, the observed variance contains contributions from both the true variance and the error variance (e.g., O'Connor 2010).

Doppler velocity calibration is performed by the manufacturer and the calibration is regarded as stable over time. However, the velocity calibration should be checked periodically using stationary targets in the far field of the instrument, such as towers, masts, buildings, or hills. Such targets, especially towers, masts and buildings, also enable the azimuthal and elevation pointing accuracy to be assessed.

If the telescope function is known accurately, the attenuated backscatter profile can be obtained from the SNR profile (Hirsikko et al. 2014), and the Doppler lidar can act as a surrogate ceilometer. Calibration should be checked periodically over time using a standard naturally occurring atmospheric target with a known backscatter, such as liquid clouds that fully extinguish the signal (see calibration methods described in the concept paper of the Centre for Cloud Remote Sensing in D4.1). This method yields a calibration accurate to about 15% (O'Connor et al. 2004, Westbrook et al. 2012), suitable for cloud detection and target categorization. Note that the molecular backscatter return is too low to detect at typical Doppler lidar operating wavelengths.

Further use of the Doppler lidar signal in specific algorithms may require much more stringent tests on calibration, stability and the post-processing corrections applied.

#### 4.2.3.5 Auxiliary data sources: temperature and humidity profiles

The target categorization includes profiles of temperature, humidity and horizontal winds for assisting in quantifying uncertainties in particular retrievals, initialising a background state, estimating temporal or spatial scales, and for determining constants or variables that are temperature or humidity dependent where appropriate. Certain instrument uncertainties also require these parameters as an input. The

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**profiles of temperature, humidity and horizontal winds** are normally taken from the output of a **high-resolution weather forecast model**. **Radiosoundings** can also be used if available, and the ingest code will provide them in a format that emulates the weather forecast model input file. In addition, horizontal winds from a wind profiler can also be incorporated if preferred.

#### 4.2.3.6 Auxiliary sources: raingauge

Precipitation has several potential sources of impact, arising from radome wetting (both cloud radar and radiometer), scattering assumptions no longer applicable (microwave radiometer), and attenuation in the atmospheric column (cloud radar). Periods when the measurements are potentially affected by precipitation can usually be determined from the measurements themselves. However, the addition of a **raingauge** provides the **surface rainrate** which will aid identifying those periods where only radome wetting is an issue (weak precipitation), and periods where the precipitation is strong enough to cause serious attenuation of the radar reflectivity profile. For identifying radome wetting conditions, a fast response instrument sensitive to weak precipitation must be employed, such as optical sensors and disdrometers; a standard tipping bucket raingauge has very slow response times to weak precipitation (has to wait for the internal bucket to fill before tipping) and is not suited for this application. A tipping bucket raingauge may be more accurate in strong precipitation conditions and when calculating accumulations.

### 4.2.4 Operation

Cloud profiling operates on a continuous basis, rather than targeted or routine dedicated measurement periods. The goal is to operate at or above the nominal temporal resolution of 30 s continuously, i.e., 24 hours a day/7 days a week. The preferred measurement mode is continuous vertically-pointing, although occasional scanning is also permitted as long as it does not dominate the measurement schedule. Usually, only extended continuous measurement periods (greater than 1 month) are considered suitable.

The required temporal resolution for mandatory instrumentation is nominally 30 seconds, although this can be relaxed to 1 minute for the multi-channel microwave radiometer. The minimum required vertical resolution is 60 m for the active instruments: cloud radar and ceilometer/lidar. The required temporal and spatial resolution is necessarily high, since cloud parameters also vary rapidly at these measurement scales. The temporal and spatial requirements are not necessary for any complementary instrumentation, since most other atmospheric parameters vary much less rapidly than do clouds.

Standard operation procedures relating to the mandatory instrumentation are described in the concept paper of the Centre for Cloud Remote Sensing in D4.1.

### 4.2.5 Data production and data products

Raw data acquired from the cloud profiling instruments at NFs are processed at the ACTRIS DC using the Cloudnet processing suite, which provides the necessary tools for data processing, automated quality control and product generation, together with a standard template for generating new products and tools within the community. In addition, the processing suite provides an extensive set of procedures for both model evaluation and for data evaluation.

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NFs are responsible for providing the instrument technical information necessary for performing QA/QC tests coordinated by the Centre for Cloud Remote Sensing, which then embeds this within the metadata to ensure full traceability of the data within the processing chain. This includes updates to instrument calibration, performance and parameter information.

Instrument synergy is necessary to create cloud products. Level 1 data deals with the processing of Level 0 instrument data provided by the NF to the DC, and their subsequent combination to provide a single synergistic product on a well-defined time-height grid. All individual observations are pre-processed and quality-checked. The target categorization dataset (Hogan and O`Connor 2004) is the basis from which all ACTRIS cloud products are created, and provides the harmonized dataset that contains all instrument uncertainties and quality control flags for propagation through the various retrieval algorithms, as well as providing the underlying target identification for these retrievals to operate on (Illingworth et al. 2007).

High-resolution products, at the native instrument resolution if possible, are created in Level 2a, and are used for all scientific studies. Specific products for model evaluation are created in Level 2b, where the high-resolution products are averaged onto the grid of each individual model, and in Level 3 and beyond, amassed into monthly and yearly files containing a wide range of statistical measures. These include: means, distributions, and joint-pdfs for creating the contingency tables used for deriving the skill score of choice. From these files, a wide range of metrics are then routinely plotted and analysed. The full list of products and accompanying metadata is detailed in the Data Management Plan (D4.2).

### 4.2.6 Data delivery and quality control

The ACTRIS cloud profiling products are collected and made available through the ACTRIS DC and the ACTRIS data user interface. The data repository is a version-controlled database enabling an iterative process concerning calibration updates and manual quality control.

NFs are responsible for providing Level 0 or Level 1 data in RRT to the ACTRIS DC in the agreed and documented format specified in the Data Management Plan (D4.2). Processing through Levels 1–3 is then performed centrally at the ACTRIS DC and made available according to the agreed Data Policy (see D2.3).

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## 4.3 Reactive trace gases remote sensing

### 4.3.1 Introduction

Trace gases play an important role in the atmosphere, e.g., in environmental issues like air quality and climate change, and it is not only the concentration of the trace gas at the surface that is relevant but also the abundance of the trace gas in the troposphere and above, as well as the vertical distribution of the trace gas throughout the atmosphere. For example, ozone in the troposphere plays a very different role in air quality and climate change than ozone in the stratosphere.

While the *in situ* observation techniques focus on local concentrations at the surface and at specific heights in the troposphere, the remote-sensing techniques provide access to column abundances and vertical profiles of the trace gases. Both techniques are therefore complementary to each other. Moreover, the ground-based remote-sensing techniques provide column and vertical profile data that are better comparable to satellite measurements than the local *in situ* observations. The remote-sensing observations together with the local *in situ* observations can be used to get information about the transport in the atmosphere.

The trace-gas products that can be obtained by ground-based remote-sensing techniques and that ACTRIS will be focusing on at start include the **ozone ($O_3$) column, partial column and vertical profile**, **nitrogen dioxide ($NO_2$) column, partial columns and lower tropospheric profile**, as well as the **formaldehyde (HCHO) column and lower tropospheric profile** and **ethane ($C_2H_6$) column.** The latter two are important components in the family of volatile organic compounds (VOC) that play an important role in the abundance of ozone and the self-cleansing capacity of the atmosphere. The **ammonia column ($NH_3$)** will be provided in special conditions**.** The characteristics of the different products (columns, partial columns, profiles) are further described in Sec. 4.3.1.

In ACTRIS the following trace-gas remote-sensing techniques are considered: **Fourier Transform Infrared spectrometry (FTIR)**, **Ultra-Violet and Visible spectrometry (UVVIS)** and **Differential Absorption Lidar (DIAL)**. These techniques have been developed and demonstrated in the Network for the Detection of Atmospheric Composition Change (NDACC). Also protocols for observations and data QA/QC have been developed within that network (http://www.ndsc.ncep.noaa.gov/organize/protocols/). They will be adopted and further developed in ACTRIS. For the history, structure and observational capacities of NDACC, we refer to the AMT/ACP/ESSD Inter-journal Special issue 'Twenty-five years of operations of the Network for the Detection of Atmospheric Composition Change (NDACC)' – in particular the overview paper by De Mazière et al. (2018).

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## 4.3.2 Observational capabilities

### 4.3.2.1 Optimum setup

The optimum setup of an ACTRIS Observational Platform dedicated to remote sensing of reactive trace gases consists of a configuration of instruments that enables the measurement of **total columns of HCHO, $C_2H_6$ and $O_3$**, as well as **partial columns or profiles of HCHO, $O_3$ and $NO_2$**. This can be achieved in the following configurations:

(1) The Observational Platform hosts together (co-located) an FTIR instrument and a UVVIS instrument, both satisfying the optimum technical specifications, as described in Sec. 4.3.3; these are the so-called **double FTIR and UVVIS MAXDOAS instruments,** or
(2) The Observational Platform hosts together (co-located) an FTIR instrument satisfying the minimum technical specifications (so-called **single FTIR,** see Sec. 4.3.3) **plus an $O_3$ DIAL and a UVVIS MAXDOAS instrument** (satisfying the optimum requirements for the UVVIS instrument).

Each FTIR and UVVIS instrument must satisfy the layout, observation procedures, data production and data delivery requirements established by the Centre for Reactive Trace Gases Remote Sensing, as described in the respective concept document (see D4.1) and in the following sections. The $O_3$ DIAL must provide $O_3$ vertical profiles according to the standard operation procedures established in NDACC. The list of produced variables is provided in Annex A.3, and the products are further described below.

### 4.3.2.2 Minimum requirements

To satisfy the minimum requirements for an ACTRIS Observational Platform dedicated to remote sensing of reactive trace gases, it is required to have a configuration of instruments that enables the measurement of **total columns of HCHO and $C_2H_6$** and **total/partial columns of $O_3$ and $NO_2$**. This can be achieved in two configurations:

(1) The Observational Platform hosts an FTIR instrument satisfying the optimum technical specifications (so-called **double FTIR**, see Sec. 4.3.3), or
(2) The Observational Platform hosts together (co-located) an FTIR and a UVVIS instrument, both satisfying the minimum technical specifications (i.e., the so-called **single FTIR and UVVIS-zenith-sky** spectrometers, see Sec. 4.3.3).

In all configurations, the FTIR and UVVIS instruments must comply with the technical specifications as described below (see Sec. 4.3.3) and with all the observation procedures, data processing and data delivery requirements established by the Centre for Reactive Trace Gases Remote Sensing, as described in the respective concept document (see D4.1) and in the following sections.

### 4.3.2.3 Complementary added-value observations

For any reactive-trace-gases remote-sensing facility, co-location with instrument(s) for ***in situ* trace-gas monitoring** provides an added value.

For the sites equipped with a UVVIS-type instrument, co-location with an **aerosol lidar** instrument and/or a **sun photometer** provides an additional added value. MAXDOAS UVVIS systems can provide **aerosol**

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**extinction profiles in the lower troposphere** as well as the total **AOD**. If the platform hosts an $O_3$ DIAL, this also provides **aerosol backscatter coefficient** and information of **cloud height** using the lidar signal less absorbed by ozone.

Complementary co-located **water-vapour lidar profiles** or **water-vapour sonde measurements** are useful but not mandatory for the retrieval of the FTIR data (water vapour is often an interfering species).

Since cloud occurrences and the types of clouds can be useful for the quality assessment of both UVVIS and FTIR observations, the availability of **cloud information** at the site is of interest.

The availability of regular nearby **$O_3$ sonde profiles,** or complementary **Dobson/Brewer total ozone column** measurements, is helpful for the quality control of the ACTRIS $O_3$ products.

#### 4.3.2.4 Auxiliary measurements

For any of the three techniques for remote sensing of reactive trace gases, it is useful for the geophysical exploitation of the data to also have **wind** (direction and strength) information at the observation site. Also local soundings of **pressure**, **temperature** and **relative humidity profiles** are useful but not mandatory. For the automated FTIR observations that require cloud-free conditions, meteorological information is needed, but in general, a small **meteorological station** is part of the FTIR experimental setup. The mandatory parameters are **wind speed and direction**, **precipitation**, **surface pressure and temperature** and **direct solar irradiance**. If the FTIR system is not automated and such small meteorological station is not included, then the availability of complementary meteorological information should be assured to interpret the quality of the recorded interferogrammes.

### 4.3.3 Instrumentation and calibration

#### 4.3.3.1 FTIR

The potential of modern ground-based, fast, wide-bandpass FTIR spectrometers using the sun as source of radiation is their ability to regularly record solar spectra over the entire middle and thermal-infrared spectral domain (from 2 to 15 µm) under daytime clear-sky conditions, with very high spectral resolution and large signal-to-noise ratios. Today, they are the standard instruments in the NDACC for making solar-absorption remote-sensing measurements of total and partial columns of a large variety of trace gases in the atmosphere.

The FTIR instruments at ACTRIS Observational Platforms must satisfy the minimum criteria outlined in the NDACC Measurements and Validation Protocols (http://www.ndsc.ncep.noaa.gov/organize/protocols/) and in particular the criteria spelled out in the Appendix II 'Infrared Instruments' of the Validation Protocol.

The main technical specifications are:

1. Optical path difference (OPD): a minimum of 120 cm is acceptable; however, 250 cm is recommended for high-resolution instruments for optimal profile retrieval;
2. Spectral range: <u>minimum</u> 1900–4100 $cm^{-1}$ ($CaF_2$ beamsplitter), <u>optimum</u> 700–5000 $cm^{-1}$ (KBr beamsplitter);

3. Continuous spectral coverage (except for the 6–7 µm $H_2O$ region) in a small number (less than 8) of spectral (filter) bands;
4. Ability to record full-resolution spectrum (in one filter band) in approximately one minute;
5. Ability to make regular timely (sub-diurnal) measurements on an ongoing basis (decadal).

The FTIR spectrometers that satisfy the minimum requirements for specification (2) are indicated as ***'single FTIR'*** instruments in this document: their measurement spectral range is smaller because they include only one detector of the InSb (Indium-Antimonide) type. In terms of ACTRIS products, it implies that they cannot measure the ozone products (neither total nor partial columns) and the $NH_3$ product.

The FTIR spectrometers that satisfy the optimum requirements for specification (2) are indicated as ***'double FTIR'*** instruments hereinafter: their measurement spectral range is larger because they include two detectors, one detector of the InSb type and the other one of the MCT (Mercury-Cadmium-Telluride) type. In terms of ACTRIS products, it implies that they do measure the ozone products (total and partial columns) and they can measure the $NH_3$ product, if the concentration surpasses the detection threshold (Dammers et al. 2016).

In addition, the ACTRIS FTIR instruments will have to comply with specific quality criteria established by the Centre for Reactive Trace Gases Remote Sensing. Moreover, the operations will have to comply with the Standard Operating Procedures that will be developed and maintained by the Topical Centre.

The FTIR instruments are operated in the solar absorption mode. The Level 1 data are solar absorption spectra in spectral bands in the mid-infrared spectral range, in which the target gases have well-identified absorption lines. Since the zero absorption background is also observed, the spectrum is self-calibrating. Nevertheless, to derive from the spectrum accurate quantitative and traceable information about the target gas' column abundance and/or vertical distribution, a retrieval or spectral inversion procedure must be applied for which it is important to characterize the Instrument Line Shape (ILS) function. The Centre for Reactive Traces Gases Remote Sensing will be the housekeeper of the standard retrieval and ILS characterization procedures and software and associated retrieval strategies to be used by the ACTRIS FTIR NFs.

With the optimum specifications (double FTIR), the target species that can be observed – with the required accuracy and precision – are $O_3$, $NO_2$, HCHO, $C_2H_6$ and $NH_3$ (if the concentration is above the detection limit). For most species, the retrieved product is the total column. The characteristics of the product and the vertical sensitivities are discussed by Hendrick et al. (2012) for $NO_2$, by Vigouroux et al. (2018) for HCHO, by Dammers et al. (2016) for $NH_3$ and by Franco et al. (2015a) for $C_2H_6$. For $O_3$, approximately four partial columns (troposphere, lower, middle and upper stratosphere) can be retrieved (Vigouroux et al. 2015). It must be highlighted that the FTIR $O_3$ partial column product provides information about the $O_3$ vertical distribution with a vertical resolution not better than 5 to 8 km. This is much lower than the vertical resolution of the order of 0.1 to a few km that the $O_3$ DIAL can provide.

Mandatory target species are **$C_2H_6$** and **HCHO**, while **$O_3$** will be provided in the optimized double FTIR setup. **$NH_3$** is considered to be a specialised variable because it can be provided only by the double FTIR and only at some sites where its concentration is high enough to be above the detection limit. Since the vertical sensitivity for FTIR $NO_2$ measurements lies essentially in the stratosphere, the **$NO_2$ total column** is essentially a partial stratospheric column. More technical details are provided in the ACTRIS concept document of the Centre for Reactive Trace Gases Remote Sensing (see D4.1).

#### 4.3.3.2 UVVIS

Passive UVVIS spectrometry using direct or scattered sunlight as a light source provides one of the most effective methods for routine remote sensing of atmospheric trace gases from the ground. While zenith-sky observations have been used for several decades to monitor stratospheric gases (e.g., Pommereau and Goutail 1988), measurements scanning the sky vertically at elevation angles close to the horizon have been established only more recently. Owing to its multi-angular observation geometry, the MAXDOAS (Multi-Axis Differential Optical Absorption Spectroscopy) technique allows the derivation of vertically resolved information on tropospheric species and aerosols (e.g., Hönninger et al. 2004, Wagner et al. 2004, Frieß et al. 2006) as well as the total tropospheric column of the observed trace gases. When combined with the direct-sun geometry, these systems also provide accurate trace-gas column measurements integrated over the full atmosphere (e.g., Herman et al. 2009).

The trace gases that the UVVIS instruments will provide in ACTRIS are **$O_3$**, **$NO_2$** and **HCHO**. The UVVIS $O_3$ product is described in Hendrick et al. (2011) and Herman et al. (2015), the $NO_2$ products are discussed in Hendrick et al. (2012, 2014) and Vlemmix et al. (2015) and the HCHO products in Franco et al. (2015b) and Vlemmix et al. (2015). As an added value, MAXDOAS UVVIS systems can provide aerosol extinction profiles in the lower troposphere as well as the total AOD (Clémer et al. 2010, Vlemmix et al. 2015).

The UVVIS instruments at ACTRIS National Facilities must at minimum comply with the following requirements:

- Zenith-sky viewing mode with one channel covering the visible range (400–550 nm);
- Fully automated acquisition, including data transfer to central processing system;
- Spectral resolution better than 2.0 nm (full width at half maximum);
- Minimum signal-to-noise ratio of 1500 at the wavelengths where the target gases feature absorption signatures that are used for the retrievals;
- No significant spectral features due to polarization sensitivity (it is recommended to use optical fibre bundle to depolarize the incoming scattered sunlight);
- Instrument Spectral Response Function (ISRF) characterised using emission lines (HgCd) at minimum one wavelength per channel;
- Spectral stray-light < 2% at wavelengths relevant for trace gas retrievals.

The UVVIS instruments satisfying the above minimum requirements are referred to as UVVIS-zenith-sky or **UVVIS-ZS** instruments.

The optimum setup should feature the additional technical specifications:

- MAXDOAS elevation scanner covering the range from 0 to 90° elevation in at least one azimuthal direction, with accuracy and repeatability better than 0.2° and field of view better than 1.5°;
- Sun-tracking system allowing for measurements in direct-sun mode;
- One or more spectral channels covering the UV (300–400 nm) at a resolution of 0.8 nm or better and/or the visible (400–550 nm) at a resolution of 1.5 nm or better.

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The UVVIS instruments satisfying these optimum requirements are referred to as **UVVIS-MAXDOAS** instruments.

Moreover, the ACTRIS UVVIS instruments have to comply with specific quality criteria defined by the Centre for Reactive Trace Gases Remote Sensing as well as with certification criteria established as part of regular intercalibration campaigns, organised by the Centre for Reactive Trace Gases Remote Sensing. ACTRIS quality and certification criteria will be compliant with NDACC criteria, but may be more strict. The operations also have to comply with the Standard Operating Procedures to be developed and maintained by the Topical Centre.

Instrument intercalibration campaigns are considered necessary every 5 to10 years. Such exercises need to be organised in a location that allows optimal observing conditions with respect to the required viewing geometry. Auxiliary observations of the atmospheric column, aerosol profile and cloud properties, as well as *in situ* trace gas observations should be available during such campaigns. The Centre for Reactive Trace Gases Remote Sensing should identify an ACTRIS site for this purpose. More technical details are provided in the concept document of the Centre for Reactive Trace Gases Remote Sensing (see D4.1).

#### 4.3.3.3 $O_3$ DIAL

The **DIAL technique** is used for the measurement of the **ozone vertical distribution**. This technique requires the simultaneous emission of two laser beams with different wavelengths characterised by different ozone absorption cross-sections. The laser wavelengths are chosen in the ultraviolet where ozone absorption is most efficient. Tropospheric and stratospheric measurements require different wavelength pairs and laser sources. Since the ozone profile is derived from the derivatives of the lidar signals, the technique does not require any calibration, but correction terms in the DIAL equation require the use of auxiliary total number density and temperature profile data.

ACTRIS $O_3$ DIAL instruments that are included in the optimum setup of an ACTRIS Observational Platform for remote sensing of reactive trace gases have to comply with the specific procedures defined by the Centre for Reactive Trace Gases Remote Sensing. Such procedures include periodic intercomparison campaigns with a reference mobile lidar instrument, regular comparisons with nearby satellite measurements or ozonesonde profiles and evaluation of the retrieval algorithm using synthetic data.

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### 4.3.4 Operation

#### 4.3.4.1 FTIR

The measurement mode is the solar absorption mode. The Centre for Reactive Trace Gases Remote Sensing will prescribe the specific operation procedures for the ACTRIS target gases, i.e., spectral resolution and optical band of the solar spectrum to be recorded for each target species.

For the regular monitoring, measurements are recorded during daytime under clear-sky conditions – preferably from sunrise to sunset, and alternating between the different target gases. For the ACTRIS targeted short-lived climate pollutants, it is important to have several measurements per day, in order to cover the diurnal cycle. The automation of the observations, with remote-control access, is highly recommended, in order to have a good temporal coverage (diurnal, seasonal, interannual) of the observations at an affordable cost.

#### 4.3.4.2 UVVIS

The standard measurement mode of UVVIS instruments consists in scanning the sky from the zenith down to the horizon. The simplest instruments (zenith-sky systems) measure the sky light scattered at the zenith only and are only sensitive to total integrated columns. Best sensitivity to the near-surface trace-gas concentrations is obtained when observing at multiple elevation angles close to the horizon. This geometry is known as the MAXDOAS geometry. In addition, some systems also include a solar absorption mode (or direct-sun mode).

For the regular monitoring at ACTRIS Observational Platforms, measurements are recorded during daytime under all weather conditions from sunrise to sunset, and alternating between sky-light scanning and direct-sun modes, if the latter one is available. For the MAXDOAS type instruments, the standard operation mode typically consists of 3 scans hourly at solar zenith angles smaller than 85°.

All MAXDOAS systems must be fully automated, preferable with remote-control access, and setup to deliver spectral data to the centralised data base at least once in a day. The Centre for Reactive Trace Gases Remote Sensing will prescribe the specific operation procedures for the ACTRIS target gases, i.e., spectral intervals to be recorded for each target species, elevation angles to be scanned, repetition frequency of the elevation scans, reference spectra acquisition, etc.

For the instruments of the MAXDOAS type for which profile inversion is feasible, the selection of data suitable for profile inversion is performed as part of the retrieval process using cloud detection methods making use of intensity ratios (colour index) and $O_4$ measurements. In case of direct-sun observations, the presence of the sun is determined using measured intensities.

#### 4.3.4.3 $O_3$ DIAL

Stratospheric ozone lidar measurements are performed during night time and require clear-sky meteorological conditions – laser radiation is rapidly attenuated by clouds and only cirrus can be tolerated for accurate lidar measurements. Tropospheric lidar measurements are also performed at night to be used with the stratospheric data. Requirements for clear sky are less stringent for tropospheric profiling which can be less than 30 min and be obtained below the strongly attenuating cloud layers. Both stratospheric and tropospheric lidar profiles are necessary for the measurement of ozone in the upper troposphere/lower stratosphere.

Lidar sites measuring composition are chosen for their quality for atmospheric transparency and allow quasi-daily operation capabilities. Generally, one measurement per day is provided with a duration ranging from one to several hours depending on the altitude range of the target profile.

### 4.3.5 Data production and data products

#### 4.3.5.1 FTIR

The Level 0 data acquired at the NF that operate FTIR instruments are interferogrammes and corresponding housekeeping data. The conversion of Level 0 to Level 1 data is done at the NFs and consists of (1) the rejection of bad interferogrammes, taking into account the housekeeping data and the meteorological conditions (for example, interferogrammes contaminated by clouds are rejected) and (2) conversion of the interferogrammes to solar absorption spectra accompanied by relevant metadata. The quality of the Level 1 data will be verified regularly by the Centre for Reactive Trace Gases Remote Sensing; if issues with the Level 1 data are detected, the Topical Centre may request access to the Level 0 and/or Level 1 data for verifying the quality. It is the responsibility of the NF to care for the long-term archiving of the Level 1 data, including the housekeeping data and metadata. Long-term archiving of the Level 0 data at the NFs is also recommended.

Data processing from Level 1 to the Level 2 data, i.e., the retrieval of the target gases' concentrations, is done generally at the NF, but the data processing software is standardised. The comparison between the two existing standard retrieval software packages (SFIT4 and PROFFIT) will be done in the Centre for Reactive Trace Gases Remote Sensing to ensure that both software codes deliver consistent retrieval products and associated uncertainties (Level 2 data). In recent years, a lot of effort has been spent on improving and harmonising the procedures for the evaluation of the uncertainties (see, e.g., the documents 'NORS uncertainty budgets' and 'Spatial representativeness of NORS observations' on http://nors.aeronomie.be/index.php/documents). More recent additional efforts have been made in the EU H2020 projects QA4ECV and GAIA-CLIM and a publication is in preparation (Langerock et al., in preparation). The progress made in these recent projects will be implemented at the Centre for Reactive Trace Gases Remote Sensing in the retrieval procedures and software that will be distributed to the ACTRIS NFs.

The required auxiliary data are the vertical profiles of pressure and temperature that can be taken from NCEP or ECMWF, if local observations are not available. Also some *a priori* climatological information is required in the algorithms using the Optimal Estimation Method, which is taken from global models or historical data.

In ACTRIS, the NFs will have to comply with strict harmonised processing requirements including retrieval strategies, *a priori* information, processing parameters and auxiliary data, established by the Centre for Reactive Trace Gases Remote Sensing, and the Topical Centre will quality-control the retrieval products. The NFs will also have to respond to requests for re-processing of the time series from the Centre for

Reactive Trace Gases Remote Sensing, whenever the latter will distribute a significant update of the processing software, spectroscopic linelist and/or retrieval strategies.

The Level 2 data will be submitted in the GEOMS HDF format (https://avdc.gsfc.nasa.gov/index.php?site=1178067684) to the TC, where the QA/QC is done, and the TC will then submit them to the ACTRIS Data Centre.

NFs can request that their data are processed at the TC, however, this option is no general obligation of the TC. It is highly recommended to automate to a large extent the data processing procedures, to enable the timely delivery of the data.

No standardized L3 data are foreseen.

#### 4.3.5.2 UVVIS

The Level 0 data acquired at NFs operating UVVIS instruments are uncalibrated radiance spectra and corresponding housekeeping data. Like for FTIR instruments, the conversion of Level 0 to Level 1 data is done at the NF and consists of various calibration steps (wavelength registration, dark-current, non-linearity and stray-light correction) as well as filtering for possible anomalies during the spectral acquisition process (e.g., saturation). The quality of the Level 1 data submitted to the Centre for Reactive Trace Gases Remote Sensing will be further checked as part of the QA/QC procedure of the central processing unit, leading to possible additional screening of the Level 1 data.

Data processing from Level 1 to the Level 2 data, i.e., the retrieval of the target atmospheric species concentrations, is performed using standardised algorithms implemented in the central processing units operated by the Centre for Reactive Trace Gases Remote Sensing. Centralised processing units are based on systems developed for the different UVVIS instrument types as part of NDACC and within the ESA-funded Pandonia and $FRM_4DOAS$ projects. Common retrieval methods selected after round-robin intercomparison and peer-reviewed publication are being implemented allowing for a high level of traceability and standardisation in the data processing and delivery. The central processing units also execute systematic QA/QC procedures at each step of the data processing, resulting in the generation of various quality flags attached to the data products.

In ACTRIS, the NFs will have to comply with the requirements defined to join in the centralised processing units. Such requirements concern the operation, calibration and quality control of the instruments providing spectral data to central processors. In turn, the central processing units will provide feedback to the data providers including alerts in case of instrument failure identified as part of the QA/QC procedures. All UVVIS Level 2 data products will be generated using a common data format following the internationally recognised GEOMS metadata standard. They will be made available via the ACTRIS Data Centre.

#### 4.3.5.3 $O_3$ DIAL

The Level 0 data acquired at the NFs that operate lidar instruments are individual raw signal data files corresponding to signal averages of a few thousands lidar pulses. The conversion of Level 0 to Level 1 data is done at the NFs and consists of (1) the rejection of spikes in lidar signals and rejection of files with insufficient signal to noise ratio due to meteorological conditions (arrival of clouds during the measurement period) and (2) summation of these individual files. The quality of the Level 1 data will be verified regularly by the Centre for Reactive Trace Gases Remote Sensing; if issues with the Level 1 data are detected, the Topical Centre may request NFs for verifying the quality of the Level 0 data. It is the responsibility of the NF to care for the long-term archiving of the Level 0 and Level 1 data, including the housekeeping data and metadata.

The Level 2 data processing, e.g., retrieval of the ozone number density profile from the average lidar signal data (Level 1 data) is done at the NF with proven and standardised processing software tested at the Centre for Reactive Trace Gases Remote Sensing. Efforts have been made for improving and harmonising the procedures for the evaluation of the uncertainties and vertical resolution, as discussed in Leblanc et al. (2016a, b, and c).

### 4.3.6 Data delivery and quality control

ACTRIS FTIR, UVVIS and $O_3$ DIAL data handling must deliver the data products to the associated unit of the ACTRIS Data Centre within three months after data acquisition. More rapid data delivery is recommended; in particular NRT delivery is recommended whenever feasible (e.g., the UVVIS data will probably be delivered by the Centre for Reactive Trace Gases Remote Sensing in NRT).

The data format will be the NDACC GEOMS HDF format (https://avdc.gsfc.nasa.gov/index.php?site=1178067684). For each instrument type, specific GEOMS templates have been defined and the submitted data files must be formatted according to these templates (https://avdc.gsfc.nasa.gov/index.php?site=1989220925 for FTIR; https://avdc.gsfc.nasa.gov/index.php?site=1876901039 for UVVIS and https://avdc.gsfc.nasa.gov/index.php?site=455555165 for $O_3$ DIAL). For data collected at ACTRIS NFs, the entry 'ACTRIS' will be added in the global file attribute 'FILE_ASSOCIATION' in the file's metadata.

The quality of the submitted data files will be controlled by the Centre for Reactive Trace Gases Remote Sensing, not only as to format but also as to file content – in order to avoid that files in the ACTRIS Data Centre provide erroneous information to the data users. Experience from the past has demonstrated that this quality control is a very useful step in the data archiving process. This means that data will transit through the Centre for Reactive Trace Gases Remote Sensing on their way from the data provider to the ACTRIS Data Centre, while it guarantees that all the data in the Data Centre satisfy the quality requirements.

## 4.4 Aerosol *in situ* measurements

### 4.4.1 Introduction

Aerosol particles are highly important actors 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.

### 4.4.2 Observational capabilities

#### 4.4.2.1 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 Tab. 1.

#### 4.4.2.2 Mandatory and specializing variables

The **minimum requirement** for ACTRIS aerosol *in situ* measurement stations includes measurements of three mandatory variables (**particle number size distribution**, **particle light scattering & backscattering coefficients** and **particle light absorption coefficient & equivalent black carbon concentration**) and at least two free-choice specializing variables (see Tab. 1 for the two complete list). The reasons that these three variables are mandatory are i) their importance 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 SOPs developed by the ACTRIS community and endorsed by the Centre for Aerosol In Situ Measurements. Among the two free-choice variables, at least one must be a chemical variable. Chemical composition is not as well characterized as physical parameters of aerosol particles, yet it is as important.

#### 4.4.2.3 Added-value variables

Complementary added-value variables permit the full characterization of aerosol particle properties and providing insight to many processes linked to emission, transformation or ageing of particles. Measurements of **trace gases** – $O_3$, CO, $NO_x$ ($NO+NO_2$) and $SO_2$ – should be performed which are useful

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tracers for anthropogenic pollution events and therefore parallel measurements of these gases are a clear asset.

#### 4.4.2.4 Auxiliary variables

Aerosol *in situ* observations should be accompanied by measurements of **meteorological parameters** (wind speed, wind direction, temperature, and relative humidity) and **radiation** (UV, IR, total radiation) in order to interpret the measured data in an appropriate manner. At least the meteorological auxiliary variables must be measured at an Observational Platform connected to the Centre for Aerosol In Situ Measurements.

### 4.4.3 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. As in most cases there is a need to move the instruments during the calibration against the reference at the TC, an extra one to cover up the data while calibrating or in cases of failure would be useful.

#### 4.4.3.1 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. It needs regular checks on-site to quality-assure the measurements. Into the MPSS, a **Condensation Particle Counter** (CPC) is included, which also has to undergo frequent on-site checks. Additionally, MPSS systems must be calibrated every one to two years against a reference instruments at the TC.

#### 4.4.3.2 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. 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 instruments at the TC.

#### 4.4.3.3 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 and yearly or every two years calibrations against a reference instruments at the TC are required.

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Tab. 1: 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 on-line 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) |

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| | | | |
|---|---|---|---|
| | Mass concentration of non-refractory particulate organics and inorganics | Aerosol Mass Spectrometer | in preparation |
| | | | |
| | Nanoparticle number concentration | nCNC | 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 / On-line equivalent technique | CEN |
| | | | |
| | Mass of major ions in $PM_{10}$ or $PM_{2.5}$ | Filter-based Ion chromatography | WMO/EMEP |
| | | | |
| | Atmospheric concentrations of $O_3$, NO Atmospheric concentrations of $NO_2$ | Chemiluminescence Multiple techniques | 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 |

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#### 4.4.3.4 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.

#### 4.4.3.5 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 an **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 instruments at the TC are required.

#### 4.4.3.6 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. They need regular checks on-site to quality-assure the measurement. Additionally, yearly or every two years calibrations against a reference instruments at the TC are required.

#### 4.4.3.7 Mass concentration of particulate elements

Mineral dust particles consist of crustal material originating mostly from suspension of exposed soil by wind 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.

#### 4.4.3.8 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.

#### 4.4.3.9 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. CCNC need regular calibrations and checks on-site to quality-assure the measurement. Additionally, yearly or every two years calibrations against a reference instruments at the TC are required.

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##### 4.4.3.10 Mass concentration of non-refractory organic and inorganic aerosols

**Aerosol Mass Spectrometers** (AMS) measure **concentrations of particulate sulphate, nitrate, ammonium, chloride, and organic mass** at the same time. Upon contact with the heater, the non-refractory 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. They need regular calibrations and checks on-site to quality-assure the measurement. Additionally, yearly or every two years calibrations against a reference instruments at the TC are required.

##### 4.4.3.11 Nanoparticle number concentration (< 0.01 µm)

**Nano-CNCs** (nCNC) are used for **counting particles in the range of 1–10 nm**. The working principle of a Nano-CNC 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 instruments at the TC are required.

##### 4.4.3.12 Nanoparticle number size distribution (0.001 – 0.02 µm)

The **size distribution below 20 nm** can be measured with **N-MPSS** systems, where the sampling and instrumental losses are minimized and a suitable CPC is used for a detector. Furthermore, **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 instruments at the TC are required.

### 4.4.4 Operation

Operations at ACTRIS Observational Platforms are expected to follow guidelines recommended in the reports and papers listed in Tab. 1 and any additional material provided by the Centre for Aerosol In Situ Measurements.

It is expected that data coverage should allow robust documenting of variability at different scales: diurnal, monthly, seasonal and annual. This implies that instruments should be operated at least 70% of the time under normal operating conditions. Participation to the calibration exercise organized by the TC is mandatory.

Within ACTRIS aerosol *in situ* data production for on-line data, by default and whenever possible a RRT schedule submission should be set up, according to the agreed principles.

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### 4.4.5 Data production and data products

The final data product (ACTRIS data Level 1 and Level 2) consists of various ACTRIS aerosol particle properties with the respective precision and accuracy, metadata and time dependent flags as specified by the Data Centre and in the standard operating procedures. All operational and planned aerosol *in situ* variables are listed in Annex A.4.

Raw measurement data (Level 0) at temperature and pressure conditions as provided by the on-line instruments (*in situ* measurement) has to be stored together with the relevant standard and calibration measurements and all information and metadata, which is needed to calculate the higher-level data products. Off-line measurements (*in situ* sampling) do not deliver Level 0 data. Details for the data production are given in the ACTRIS Data Management Plan (D4.2) and the associated data production descriptions and documents provided by the Data Centre and the Centre for Aerosol In Situ Measurements. All data products, pre-products and software tools are version controlled and identified by the associated DC unit.

ACTRIS aerosol *in situ* data production follows one of two main workflows, on-line or off-line. For the **on-line workflow**, data production is based on Level 0 data, i.e., all raw data and signals provided by an instrument in its native time resolution and native conditions of temperature and pressure, brought to a harmonized format, and annotated with all discovery and metadata needed in the further data production process. Level 0 data are to be submitted and archived at the Data Centre unless the ACTRIS Data Management Plan (D4.2), with the associated data production descriptions, defines an exception caused by, e.g., large raw data volumes. In this case, an alternative storage procedure has to be agreed between the Centre for Aerosol In Situ Measurements and the Data Centre, which meets long-term archive criteria. The Level 0 data submission includes relevant calibration measurements and measurements of traceable standards needed for data quality control, which are flagged as such. From Level 0 data, Level 1 and Level 2 data are produced. Level 1 data are quality-controlled, calibrations are applied, final variable calculated, native time resolution, invalid and quality control measurements removed, and transferred to standard conditions of temperature and pressure where applicable. Level 2 data is averaged Level 1 data to typically hourly averages, with measure of atmospheric variability included. The Level 1 and Level 2 data can be produced either by the NF or the associated Data Centre unit, depending on variable. The distribution of work is included in the associated data production descriptions available from the Data Centre, and indicated in Annex A.4. The quality control step between Levels 0 and 1 can be automatic (RRT data production) or manual, performed by the NF. Data level identifiers distinguish between data having received automatic or manual QC. The details of the steps producing Level 1 from Level 0, and Level 2 from Level 1, are specified in the associated data production descriptions and the standard operating procedures.

For the **off-line workflow**, the steps of sample medium pre-exposure treatment, exposure, preparation, sampling, and analysis are documented with standard operating procedures and protocols including discovery and use metadata in machine-readable form. Items to be included are specified in the associated data production descriptions and the standard operating procedures. The archive for the protocols is located at the NF, its operating protocols coordinated with and approved by the DC and the TC. From these protocols, the Level 2 data products are produced in the temporal resolution determined by the

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sampling schedule, and transferred to the DC using the tools provided for data submission to ensure required documentation, flagging and metadata. The details of the procedure are specified in the associated data production descriptions.

### 4.4.6 Data delivery and quality control

It is compulsory for the NF to produce at least the Level 1 and Level 2 data for archiving at the associated Data Centre unit. Archiving of Level 0 data will depend on the specific variable. For the submission of aerosol *in situ* data, required procedures are described in the ACTRIS Data Management Plan (D4.2) and the associated data production descriptions. Manually quality controlled data has to be submitted on a regular, scheduled frequency, at least yearly to the ACTRIS DC following the scheme in the ACTRIS Data Management Plan (D4.2), and associated documents. Submission to the DC has to be done before 31 May, using the submission tools and automatic quality control software available within the DC. Data originators at the NF are responsible for checking the data using the procedures in the associated data production descriptions. Data is then reviewed by the Centre for Aerosol In Situ Measurements and will be discussed at the annual data quality meeting or teleconference, in collaboration with the DC. An issue tracker is operated in the process of data evaluation to ensure full documentation and traceability of the data production and quality control process. This comes into place yearly following the initial data submission by stations to the ACTRIS DC. Upon errors, the data has to be re-submitted and will be reviewed again for compliance with suggested changes.

Whenever possible by measurement principle and connectivity to the station, Level 0 data must be transmitted to the Data Centre in RRT, i.e., latest within 3 hours of measurement, for delivery of an RRT data product for operational services.

## 4.5 Cloud *in situ* measurements

### 4.5.1 Introduction

Clouds are an important component of the atmosphere, influencing a large number of physical and chemical properties of the Earth's atmosphere and thereby strongly impacting climate, air quality, ecosystems and associated interactions. Cloud observations in ACTRIS and preceding networks have so far focussed on remote-sensing techniques, delivering information on temporal and vertical variation of cloud properties and structures. *In situ* observations of clouds and cloud-related parameters provide additional, very detailed insights into important processes related to the formation, the structure, and the chemical composition of clouds, which feedback to associated aerosol properties and thus impact the atmosphere as a whole.

Cloud i*n situ* measurements will therefore be an important new observational component within ACTRIS. They will be performed at ground-based field stations, typically on mountains, which are frequently covered in clouds. Being a multiphase system consisting of gas, particle, liquid-water and ice phases with complex interactions, clouds represent a challenging system to study. ACTRIS cloud *in situ* observations will focus on a set of easily accessible variables and extend to technically more demanding parameters in the future. In contrast to other observational components, ground-based cloud *in situ* measurements still lack a long record of standardisation efforts. These will, however, be enforced within the ACTRIS implementation phase, such that this gap will be closed and high-quality data will be ensured until the start of the operational phase of the RI in 2025.

### 4.5.2 Observational capabilities

#### 4.5.2.1 Optimum setup

The optimum setup of cloud *in situ* observations consists of a number of **microphysical and chemical measurements**, which provide crucial parameters to study cloud processes, see also Annex A.5: **Liquid water content (LWC)**, **effective droplet diameter ($D_{eff}$)**, **cloud droplet number concentration and size distribution**, **ice particle number concentration and size distribution** (in mixed-phase clouds), **ice nucleating particles (INP) number concentration and temperature spectra** (outside cloud periods), **cloud condensation nuclei (CCN) number concentration**, **interstitial particle number concentration and size distribution**, **cloud residuals particle number concentration and composition**, **total particle number concentration and size distribution**, **bulk cloud water chemical composition**.

As the microphysical parameters can be measured in an automated fashion by the instrumentation given below, they should be provided for all clouds occurring at the site. In contrast, the chemical measurements need manual interaction and are more labour intensive, which is why they should be provided at least for a 6-weeks campaign each year with sampling of all occurring clouds and a maximum collection time per sample of 24 hours or – alternatively – over a period of 4 months per year with more infrequent sampling of occurring clouds, but at least one cloud water sample per cloud event.

#### 4.5.2.2 Minimum requirements

The minimum requirements to qualify as an ACTRIS cloud *in situ* observational site are (i) the **occurrence of clouds** at the site, defined by periodical **LWC** > 0.05 g $m^{-3}$ at least during two seasons of a year, (ii) the measurements of **LWC** and **$D_{eff}$,** and (iii) the measurements of at least two other specializing cloud variables, which are listed in Annex A.5 and for which the Centre for Cloud In Situ Measurements is providing operation support.

#### 4.5.2.3 Complementary added-value observations

Measurements of **visibility**, **precipitation intensity**, **diffuse radiation** and **vertical wind speeds** can provide additional value to the observation of cloud *in situ* parameters and are therefore recommended, as well as the measurement of **total condensed water content** in mixed-phase clouds.

#### 4.5.2.4 Auxiliary measurements

Measurements of **meteorological parameters** (temperature, pressure, relative humidity, wind speed, wind direction, global radiation) can supplement cloud *in situ* data and support dedicated process studies. Stations should therefore be equipped with automatic weather stations, ideally including sensors for precipitation.

### 4.5.3 Instrumentation and calibration

#### 4.5.3.1 *In situ* observations of cloud liquid water content

A number of instruments are available to measure the **LWC**, commonly expressed in gram of liquid water per cubic meter of air. Instruments can be divided into two types: (i) **integrating probes** like the Particle Volume Monitor (PVM) and the Present Weather Detector (PWD) that integrate the scattering of cloud droplets over a given open path, and (ii) **size distribution probes** like the Forward Scattering Spectrometer Probe (FSSP), Fog Monitors (FM) and Cloud Droplet Probes (CDP) that actively operate with a controlled flow entering the probe. The most commonly used of these instruments at ground-based stations is the PVM probe, which was shown to give a stable and reliable measurement most adapted for monitoring purposes and does not suffer from bias due to the orientation of the probe into the wind direction (Guyot et al. 2015). There are approximately 5 of these instruments operating on a regular basis at ACTRIS facilities throughout Europe. These probes have been the subject of intercomparison campaigns during ACTRIS-2 (deliverable D3.12).

The ground-based PVM probes are usually installed on a fixed platform on the roof of the sampling site. The PVM measures the laser light (at $\lambda$ = 0.780 µm) scattered in the forward direction by an ensemble of cloud droplets which crosses the probe's sampling volume of 3 $cm^3$. The light scattered is collected by a system of lenses and directed through two spatial filters. The first filter converts scattered light to a signal proportional to the particle volume density (or LWC).

Recommended SOPs for the liquid water content measurements have been supplied in ACTRIS-2 (deliverable D3.12).

#### 4.5.3.2 *In situ* observation of cloud droplet effective diameter

**$D_{eff}$** is a single variable that gives an indication on the average size of a given cloud droplet population. It is commonly expressed in µm, and it is derived from **integrated measurements** performed by PVM-type instrumentation. In the PVM, the first filter converts scattered light into LWC, while the second filter converts scattered light to a signal proportional to the particle surface area density (PSA, Gerber et al. 1994). From the ratio of these two quantities, $D_{eff}$ is derived. These two filters guarantee a linear relationship between scattering intensity and LWC or PSA for droplet diameters from 3 to 50 µm (Gerber et al. 1994). Calibration for instrument droplet diameter is the same as that above for LWC.

Recommended SOPs for cloud droplet distributions measurements ($D_{eff}$) have been supplied in ACTRIS-2 (deliverable D3.12).

#### 4.5.3.3 *In situ* observation of cloud droplet number concentration and size distribution

The **number size distribution of cloud droplets** varies and depends on many things like CCN concentration, CCN chemical composition and water supersaturation. The mean cloud droplet diameters are typically 5–15 µm, the size distribution varies between 1 and 100 µm. Clouds typically contain few hundred droplets in one cubic centimetre, varying from few tens to few thousands in a cubic centimetre (e.g., Henning et al. 2002, Miles et al. 2000). Number size distributions of cloud droplets are measured usually optically taking advance of forward scattering of light from liquid droplets (e.g., Spiegel et al. 2012). There are several **cloud droplet probes** available, most of them are designed to be installed into aircraft (e.g., Lance et al. 2010). Such cloud probes need special inlet arrangements to get droplets through the measurement area when applied in *in situ* cloud measurements. The alignment of the inlet of the probes should also be facing directly towards the wind. The probes typically measure the number size distribution between about 3 and 50 µm. Probes are usually calibrated with known sized glass beads and spinning pinholes.

Recommended SOPs will be developed within the implementation and pre-operational phases by the Centre for Cloud In Situ Measurements.

#### 4.5.3.4 *In situ* observation of ice particle number concentration and size distribution

The **ice particle number concentration** is important for those platforms where mixed-phase or ice clouds occur naturally. It is usually measured with the following cloud-ice probes:

- **Photodiode imaging spectrometers**, e.g., 2D-Stereoscopic spectrometers (2DS, 2DS-GS) and Cloud/Precipitation Imaging Probes (CIP-15, CIP-15, PIP), Cloud Aerosol Precipitation Spectrometers (CAPS), High Volume Precipitation Spectrometer (HVPS);
- **CCD Imaging Probes**, e.g., Cloud Particle Imager (µCPI, µCOPP);
- **2D spatial scattering imaging probes**, e.g., Small Ice Detectors and Phase Particle Discriminators (SID, PPD-2);
- **Holographic Spectrometers**, e.g., HaloHolo, Holimo;

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- **Depolarisation Particle Spectrometers**, e.g., Cloud Aerosol Spectrometer with Polarisation (CAS-POL), backscatter Cloud Probe with Depolarisation (BCP-D).

Cloud-ice particle phase monitoring is problematic due to the large range of particle sizes and shapes, from 1 µm to 2 cm or more, and the definition of ice particle size. No one instrument can fully define the necessary ice cloud parameters, and field experiments use a combination of the above instruments. Ice cloud parameters include ice crystal number size distribution, $N_{ice}(D)$, and ice crystal shape/habit. At present, although some information on the response of the bulk cloud instrument, PVM, to ice particles is available, more work is required to deliver quantitative information, e.g., total ice particle concentration, $N_{ice}$, Ice Water Content (IWC) and ice particle size distribution, $N_{ice}(D)$. Most of the above instruments have been developed for airborne applications, but have been used successfully in laboratory, chamber and ground-based field applications using appropriate aspirated inlets. These have been well characterised, documented and intercompared at ground-based field sites (Lloyd et al. 2015) and recommendations for specific instrument operation is available based on feedback from extensive cloud instrument workshops.

Field operation and protocols follow those for the cloud liquid water spectrometers for calibration particles and particle generator gun, with the addition of spinning disk rigs for simulated large ice particle size, absolute ice number concentrations and ice particle shape calibration. Annual to biennial calibration and maintenance with operator training at a chamber facility is recommended using repeatable, simulated ice cloud conditions.

#### 4.5.3.5 *In situ* observation of ice nucleating particle number concentration and temperature spectra

INP can currently only episodically be measured with **aerosol sampling** based methods and **off-line analysis** of the temperature spectra of ambient concentrations. These methods have a poor time resolution of only a few hours to a few days, but can deliver accurate INP concentrations in the temperature range from about −5°C to −25°C. These techniques, though relatively labour intensive, should be used for both exploratory and observational ACTRIS activities, but require a thorough assessment and calibration of the aerosol sampling methods (e.g., filters or impingers) and the INP analysis systems. Furthermore, the storage of the samples as well as their shipment to the laboratory should be standardized to assure comparability between different sampling locations and systems. It is anticipated that in the near future new INP instruments with higher time resolution and more automated operation may be available. The Centre for Cloud In Situ Measurements has to provide guidance for such new developments and develop calibration protocols and procedures.

#### 4.5.3.6 *In situ* observation of total and interstitial particle number concentration and size distribution

The simultaneous measurement of the **total and interstitial aerosol particle size distribution** provides the opportunity to derive the activation diameter ($D_{50}$) and (with assumption/knowledge of the particle hygroscopicity) the maximum supersaturation ($SS_{max}$) of the cloud (e.g., Krüger et al. 2014). Both parameters are important for cloud microphysical modelling purposes (Reutter et al. 2009). The needed size distribution of the activated particles (CCN) is then inferred by the difference of the total and interstitial particle size distribution. Both direct *in situ* observations require the combination of a dedicated inlet and an aerosol sizing instrument, which is able to measure down to at least 20 nm.

This approach was already successfully applied in numerous *in situ* cloud studies (Anttila et al. 2009, Anttila et al. 2012, Asmi et al. 2012, Ditas et al. 2012, Hammer et al. 2014, Henning et al. 2002) at different research field stations (Jungfraujoch, Pallas, Puy de Dôme). The **dedicated total and interstitial inlets** used at these field sites were individual versions and thus their sampling specifications might be different. For future cloud studies the total inlet should follow the design of Weingartner et al. (1999) to sample particles up to a size of 40 µm for wind speeds up to 20 m $s^{-1}$. The interstitial inlet should have a sharp cut-off at 2.5 µm either as a cyclone (Verheggen et al. 2007) or an impactor (Schwarzenböck et al. 2000). Further standards and SOPs regarding the inlets will be developed within the implementation and pre-operational phases by the Centre for Cloud In Situ Measurements.

The second component is the aerosol particle size distribution measurement device. In order to derive the $D_{50}$ at high supersaturation and the presence of highly soluble aerosol particles, the **scanning mobility particle sizer** (SMPS) would be the best choice for this purpose. This kind of size distribution instrument has been frequently intercompared, calibrated and technically standardized (Wiedensohler et al. 2012) and the respective standards and SOPs are defined by Centre for Aerosol In Situ Measurements and will need to be followed. Both inlets and SMPS systems can be operated in an autonomous way, so that their deployment is proposed as a minimum requirement at each future cloud station.

#### 4.5.3.7 *In situ* observation of cloud residuals number concentration and composition

Special inlets with inertial separation of large hydrometeors form smaller, interstitial aerosol particles, so-called **counterflow virtual impactors** (CVI), have been developed and designed in order to selectively sample droplets and ice particles into dry, particle-free air, evaporate the condensed water and analyse the **residual particles** with various techniques (Ogren et al. 1985, Noone et al. 1988, Twohy et al. 1997, Mertes et al. 2001). Based on the CVI principle, Boulter et al. (2006) have developed a pumped CVI (PCVI) with for stationary operation at both laboratory and observational platforms. This device has cut-off diameters of only a few µm for separating small cloud droplets and ice crystals from interstitial aerosols. It was further improved and modified towards the larger ice-selective PCVI (IS-PCVI) with cut-off diameters larger than 10 µm for separating ice crystals from droplets in mixed-phase clouds (Hiranuma et al. 2016). The residuals can either be sampled for off-line physical and chemical analysis, e.g., with electron microscopy (Worringen et al. 2015), or directly be analysed with proper instruments like CPC, SMPS or single particle mass spectrometers continuously sampling from the PCVI (Cziczo et al. 2009). PCVI residual sampling and analysis provides valuable insight into the formation mechanisms of droplets and ice crystals, but require proper control and maintenance for setup, sampling connection and operation procedures in order to achieve high quality data.

#### 4.5.3.8 *In situ* observation of cloud water chemical composition

The **chemical composition of cloud water** is most often determined from **bulk cloud water collectors** that rely on the principle of droplet inertial impaction and the collection of impacted droplets of all sizes into one collection vessel. For passive samplers (e.g., Reynolds et al. 1996), droplet impaction typically takes place on strings or meshes and is driven by the ambient wind only. So-called rotating arm collectors force droplet impaction by rotating a rod around its centre point at high speed (e.g., Krämer und Schütz 1994). In other active samplers, droplet-laden air is drawn through the device to ensure sufficient droplet velocities for impaction even under calm conditions. Impaction then takes place on a set of vertically clamped strings (e.g., Demoz et al. 1996) or on flat surfaces (e.g., Berner 1988). As active samplers show less dependency of collection efficiencies on wind speeds, they are the preferred instruments for ground-based cloud water sampling. After sampling, the integral cloud water sample is typically analysed off-line, i.e., in a laboratory away from the sampling device, for its chemical composition. For inorganic ions, ion chromatography is most often applied, while for the organic composition a range of analytical separation techniques are available, including gas and liquid chromatography and capillary electrophoresis, coupled either to optical or mass spectrometry detectors. Such combinations have been frequently applied in cloud chemistry campaigns (e.g., Collett et al. 1990, Lihavainen et al. 2008, Marinoni et al. 2004, van Pinxteren et al. 2005) and efforts to harmonize and standardize both the collection and the chemical analysis will be reinforced within the ACTRIS implementation and pre-operational phases to define standards and SOPs for the determination of cloud water chemical composition.

### 4.5.4 Operation

Measurement strategies given in the following will serve as a starting point to further refine standard operation procedures within the implementation and pre-operational phases of the RI (until 2024).

The LWC as well as $D_{eff}$ should be measured continuously for all clouds. A PVM is capable of generating data at a 1-second time resolution. For ground-based observations, data averaging over 1 minute provides sufficient temporal resolution, however. The droplet size distribution should also be measured for all clouds with a time resolution of 1 min, covering a size range of at least 5–50 µm diameter. Interstitial, residual and total particle size distributions need to be obtained during all clouds occurring at a site as well, with a cycle time of 20 min. It is suggested to run the particle spectrometers continuously, i.e., also outside cloud periods, to support data interpretation of INP and CCN measurements, taking place outside clouds as well. The chemical composition of cloud water is more difficult to obtain in an automated fashion. It should be provided at least for a 6-week campaign each year with sampling of all occurring clouds and a maximum collection time per sample of 24 hours, but preferably much shorter (1 h). Alternatively, it can be determined over a period of 4 months per year with more infrequent sampling of occurring clouds, but at least one cloud water sample per cloud event. Regarding the inorganic composition, the minimum set of constituents to be analysed comprises the ions sulphate, nitrate, chloride, ammonium, potassium, calcium and sodium. Regarding the organic cloud water composition, marker compounds that will be defined by the Centre for Cloud In Situ Measurements should be provided as a minimum set of constituents.

### 4.5.5 Data production and data products

All data processing from raw data to the different data levels will be done at the NFs according to the standards developed and defined by the Centre for Cloud In Situ Measurements.

### 4.5.6 Data delivery and quality control

Data delivery and quality control given in the following will serve as a starting point to further refine standard operation procedures within the implementation and pre-operational phases of the RI (until 2024).

Quality controlled data has to be submitted on a regular, scheduled frequency, at least yearly to the ACTRIS *in situ* data repository following the scheme in the ACTRIS Data Management Plan (D4.2) and associated documents. Data originators at the NF are responsible for checking the data using the procedures in the associated data production descriptions and the QA/QC tools provided by the Centre for Cloud In Situ Measurements.

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## 4.6 Reactive trace gases *in situ* measurements

### 4.6.1 Introduction

Reactive gas species in the Earth's lower atmosphere are a large group of compounds with lifetimes between minutes and a few months. These gases are the primary source of the highly reactive free radical species that drive the gas-phase chemistry of the atmosphere. This radical chemistry is essential for cleansing the atmosphere of a range of pollutants and greenhouse gases by initiating their oxidation. Key reactive gases, which are also readily observable, are tropospheric ozone, carbon monoxide, volatile organic compounds (VOCs), nitrogen oxides ($NO_x$), and reactive sulfur species. Assessing the role and impacts of reactive gases in the atmosphere requires knowledge of the global distribution and long-term changes in their abundance.

This section describes the technical concepts and requirements for the ACTRIS Observational Platforms that perform *in situ* **$NO_x$** and **VOC** measurements. $NO_x$ and VOCs are key components in the formation of tropospheric ozone and secondary aerosols, which affect human health, food security and climate change. Accurate and precise measurements of $NO_x$ and VOCs are crucial for improving air-quality models and emission inventories and to monitor long-term trends as an independent measure for air quality and anthropogenic emission mitigation strategies. Additionally, climate change alters the temperature driven biospheric emission patterns (especially of VOCs) and its impact is still difficult to predict due to missing long-term observations.

**Nitrogen oxides, $NO_x$**, are the combination of NO and $NO_2$. NO is mainly emitted from anthropogenic sources such as combustion processes. It is rapidly oxidized in the atmosphere to $NO_2$ by ozone and peroxyradicals, originating from the degradation of VOCs. NO and $NO_2$ are the key substances for ozone formation in the presence of sunlight leading to photochemical smog formation. $NO_x$ is removed from the atmosphere by dry and wet deposition or by formation of organic nitrates. Having a longer lifetime than $NO_x$ itself, these organic nitrates can be subject to long-range transport in the atmosphere and can act as $NO_x$ sources in remote regions when ultimately decomposed. The atmospheric lifetime of $NO_x$ ranges from a few hours to one or two days. Since both NO and $NO_2$ are involved in essential reactions in the troposphere they have to be measured individually.

**VOCs** summarizes species of short-chain, non-methane hydrocarbons (NMHCs; alkanes, alkenes, alkynes and aromatics, terpenes) and oxygenated hydrocarbons (OVOCs; e.g., alcohols, ketones, aldehydes) with a high enough vapour pressure to be gaseous under tropospheric conditions. They are emitted from anthropogenic and biogenic sources and are subsequently oxidised mostly by OH radicals, resulting in formation of ozone and secondary organic aerosols. VOC oxidation products include also highly oxygenated molecules (HOM) that partition to the aerosol phase and contribute to gas-to-particle conversion in concert with e.g., sulfuric acid.

The atmospheric lifetimes of VOCs are linked to their reactivity and range from minutes (alkenes) to a few months (light alkanes). Together with long-term measurement of anthropogenic and biogenic VOCs as well as their degradation products, this information can be used to assess the reactivity of the atmosphere and to study atmospheric processes.

### 4.6.2 Observational capabilities

#### 4.6.2.1 Optimum setup

**$NO_x$ specific setup:**

In addition to NO and $NO_2$, ozone and relative humidity have to be measured to enable the correction of interferences. Additional $J(NO_2)$ data are needed for further data analysis. Ideally and in addition to final data (Level 2), RRT or at least NRT data should be submitted, i.e., within 3 hours or 3 days of measurement, respectively. Automated quality control has to be used, based on tools specified in SOP-NOx (SOP-NOx, 2014; Deliverable D4.10 of ACTRIS-I3 project: Standardized Operating Procedures (SOPs) for $NO_{xy}$ Measurements).

**VOC specific setup:**

Measurement of all relevant non-methane hydrocarbons (NMHCs; alkanes, alkenes, alkynes, aromatic compounds) in the $C_2$–$C_9$ range (around 30 compounds) should be performed.

Measurement of all relevant oxygenated VOCs (OVOCs; alcohols, ketones, aldehydes, ethers, esters) in the $C_1$–$C_5$ range (around 10 compounds) should be performed.

Measurements of biogenic VOCs (BVOCs; monoterpenes) should be performed.

Measurements of direct aerosol precursors like HOM and sulfuric acid should be performed (e.g., by online techniques, such as CI-APi-TOF) when the station also performs aerosol and gas-to-particle conversion studies.

Ideally and in addition to final data (Level 2), RRT or NRT data should be submitted whenever possible at reasonable quality, i.e., within 3 hours or 3 days of measurement, respectively. Automated quality control has to be used, based on tools specified in SOP-VOC (SOP-VOC, 2014; Deliverable D4.9 of ACTRIS-I3 project: Standardized Operating Procedures (SOPs) for VOC Measurements).

#### 4.6.2.2 Minimum requirements

Observational Platforms for *in situ* measurements of reactive trace gases must have collocated measurements of VOCs and $NO_x$ as specified below and in Annex A.6.

For calibration, a standard has to be used which is traceable to the Centre for Reactive Trace Gases In Situ Measurements, which provides the link to the Central Calibration Laboratories (CCLs) of the World Meteorological Organisations' Global Atmosphere Watch program (WMO-GAW) holding the SI traceable scales for VOCs and $NO_x$.

The performance of the measurement instrument has to be checked against a target gas in regular intervals (e.g., monthly). The target gas consists either of an ambient air standard with known compound concentrations or of an artificial standard within the ambient concentration range of the target compounds.

Reported measurement data have to include the measured mixing ratios, their associated precisions and uncertainties as specified in SOP-VOC (2014) and SOP-NOx (2014), and flags as commonly accepted by the

ACTRIS reactive trace gases measurement community and specified by the Centre for Reactive Trace Gases In Situ Measurements.

During the course of the years, data have to be regularly (e.g., monthly) reviewed for consistency with existing data from the same measurement site and against similar European measurement sites. Tools for these checks are provided by the ACTRIS Data Centre and the Centre for Reactive Trace Gases In Situ Measurements. Data are submitted following strictly the data submission procedures as outlined in Section 4.6.5 together with metadata and data flagging.

The data providers of the Observational Platforms have to participate in round-robin exercises when organized by the Centre for Reactive Trace Gases In Situ Measurements. In case of on-going non-compliance with the Key Performance Indicators (KPI) set by Centre for Reactive Trace Gases In Situ Measurements they have to accept and organize performance audits by the Centre for Reactive Trace Gases In Situ Measurements.

**$NO_x$ specific requirements:**

For $NO_x$ both NO and $NO_2$ measurements have to be reported separately. $NO_2$ has to be measured mandatorily, either with chemiluminescence detection (CLD) and photolytic converter (PLC), Blue Light converter (BLC), with Cavity Attenuated Phase Shift instrumentation (CAPS) or with any other $NO_2$-specific measurement technique approved by the Topical Centre. Explicitly not considered as ACTRIS compatible are $NO_2$ measurements using a molybdenum-based converter. NO and $NO_2$ values have to be corrected for conversion caused by the reaction with ozone inside of the inlet line. If this is not done by the instrument directly, also $O_3$ and relative humidity have to be measured and submitted to allow for data correction, as specified by SOP-NOx (2014).

**VOC specific requirements:**

At least 6 different VOCs have to be measured at an Observational Platform for *in situ* measurements of reactive trace gases.

Atmospheric VOCs have to be preconcentrated, subsequently separated by gas chromatography and finally analysed by mass spectrometry (GC-MS) or flame ionization detection (GC-FID). Alternatively, VOCs can also be measured without preconcentration, using specific detection such as proton transfer reaction–mass spectrometry (e.g., PTR-MS). Analysis can be performed on-line (at the site) or off-line (i.e., sampling at the site and analysis remotely in the lab).

Off-line sampling intervals have to be at least twice a week and sampling has to follow a station-specific protocol, where station-characteristic air masses are sampled with little contamination due to local sources. This will allow obtaining a consistent climatology of VOCs and assessing the influence of emission mitigation measures or changes of climate and transport regimes (e.g., El Niño-Southern Oscillation – ENSO, North Atlantic Oscillation – NAO) in the atmosphere.

On-line sampling has to be performed continuously, with an interval of at least two times daily but preferably in hourly intervals. With respect to off-line sampling, this setup allows obtaining high-resolution information on the impact of specific processes/events and provides time series useful for source quantification by inverse modelling.

#### 4.6.2.3 Complementary added-value observations

**CO, $CO_2$, $CH_4$, $SO_2$** and **$NO_y$** are useful tracers for anthropogenic pollution events and therefore parallel measurements of these gases are highly recommended. The analysis of the $NO_x$ and VOCs also benefits from co-located measurements of **ozone** for photochemical studies and of **aerosol components** for studies on formation of secondary aerosols.

In addition to the *in situ* data, **remote-sensing measurements of trace gases and aerosol parameters** can be used to further enhance the potential of the observational platform.

#### 4.6.2.4 Auxiliary measurements

**Ozone** and **water vapour** must be measured according to the rules of WMO-GAW at Observational Platforms for reactive trace gases.

Furthermore, measurements of reactive trace gases have to be accompanied by measurements of **meteorological parameters** in high time resolution near the place of the air intake port for the analysers. The minimum set of parameters includes wind speed, wind direction, air temperature, and air pressure. These auxiliary data are essential for checking the quality of the data and for advanced data products (e.g., emission estimation, long-term trend analysis). In addition, so-called footprints from meteorological transport models should be available in order to connect measured data with potential source regions.

### 4.6.3 Instrumentation and calibration

#### 4.6.3.1 *In situ* observations of $NO_x$

The **chemiluminescence detection** (CLD) is the state-of-the-art technique for **NO** observations. No other technique for direct detection of NO is recommended so far (SOP-NOx, 2014). **$NO_2$** can either be detected indirectly by converting $NO_2$ to NO or by newly evolving measurement techniques, e.g., **Cavity Enhanced Phase Shift** (CAPS) or **Quantum Cascade Laser systems** (QCLAS).

The instrument performance should target to fulfil the ACTRIS Data Quality Objectives (SOP-NOx, 2014) for NO and $NO_2$ dependent on the atmospheric regimes (e.g., urban, rural, remote). Sensitivity drifts of the instrument response have to be corrected by regular calibrations, which need to be adapted to the specific instrument. The detection limit has to be at least <50 ppt and <100 ppt for NO and $NO_2$, respectively.

For the NO observations, low-maintenance CLDs instruments are commercially available from different manufacturers. In principle, no supply gases are needed during operation. However, the precision is greatly enhanced by suppling pure oxygen for the in-built ozone generator. Though reaching the ACTRIS quality goals, the ACTRIS quality assurance and quality control procedures have to be strictly followed (SOP-NOx, 2014).

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For **$NO_2$** observations the photolytic conversion of $NO_2$ to NO using **Blue Light** (BLC) or **photolytic converters** (PLC) and subsequent detection by CLD is the recommended measurement technique. Molybdenum converters are not recommended due to their insufficient selectiveness to $NO_2$. Direct $NO_2$ detection methods (CAPS, QCLAS) are able to reach the same performance as BLC/PLC-CLD instruments and are also recommended.

Calibration for NO has to be performed by dynamic dilution of a reference standard (low mixture of NO in $N_2$, in the order of 5 ppm). The reference standard has to be traceable to standards provided by the Centre for Reactive Trace Gases In Situ Measurements. Regular calibrations are necessary to correct for drifting instruments. Two calibration points (zero and one concentration) are recommended to be performed on a weekly basis at least.

Calibration for $NO_2$ has to be performed by using a gas phase titration system. As for the NO calibration, a dynamic dilution of an NO in $N_2$ reference standard is produced. Ozone, produced by UV-lamps is added to the mixture, quantitatively converting NO in $NO_2$. Depending on the concentrations, different $NO_2$ concentrations are achieved. The converter efficiency of the BLC/PLC is checked with one $NO_2$ concentration after the regular NO-calibration on a weekly basis. Since dilution is a key component of the calibration process, a specific device for zero air generation and a systematic check of the mass flow controller calibration must be conducted in agreement with SOP-NOx (2014).

#### 4.6.3.2 *In situ* observations of VOC species

The equipment for analysing **VOCs** in ambient air varies in specification and performance depending on the measured species. A sample of atmospheric VOCs can be introduced to the analytical system directly from ambient air (on-line), or via a canister or an adsorptive sampling tube (off-line).

**On-line sampling** avoids storage issues and minimizes leak issues, however, requires an analytical system at the sampling site. The air sample is directly transferred via a sampling line into the instrument. Use of on-line systems is encouraged for ACTRIS stations if the required well-trained personal, the appropriate equipment and the resources necessary for QA/QC including regular zero, calibration and target gas measurements are available. Otherwise, it is recommended to use **off-line sampling** and conduct the sample analyses in an experienced laboratory. For precursor gases measured with the CI-APi-TOF or similar instrumentation, such as HOM and sulfuric acid, on-line sampling is mandatory in order avoid condensation to the walls and thus loss of analysed compounds. Filter inlets such as FIGAERO may be used for simultaneous measurements of gas and condense phase HOM.

For on-line and off-line analyses of VOCs from ambient air gas chromatography (GC) systems equipped with flame ionization detection (GC-FID) and/or mass spectrometry (GC-MS) are key instruments. For light OVOCs (aldehydes and ketones) a possible off-line method combines sampling through a silica gel adsorbent coated with 2,4-Dinitrophenylhydrazine (DNPH) and analysis with the High Performance Liquid Chromatography and UV detection (HPLC-UV). For measuring formaldehyde in air an on-line analyser with fluorimetric detection of the product formed by the Hantzsch-Reaction may be used.

An alternative are the PTR-MS systems with high-time-resolution measurements. PTR-MS systems are capable of measuring only compounds with higher proton affinity than water molecules, thus selected

OVOC, unsaturated NMHCs (aromatics and few alkenes) can be measured. Furthermore, they cannot separate compounds with identical molecular masses, though recent developments in high resolving time-of-flight (TOF) MS have overcome this problem for isobaric but not for isomeric compounds. The main purpose of PTR-MS is the measurement of OVOCs and BVOCs.

A list of prior species has been defined regarding their interest in atmospheric science (WMO, 2017). The Observational Platform has to define its measurement strategy considering this list. $C_2$–$C_9$ VOC species have to be measured with a detection limit of at least 15 ppt for individual VOC species.

For details of GC-FID and GC-MS systems consult SOP-VOC (2014), the new measurement guidelines for VOCs of WMO (to be published in 2018) and the Section 3 of the concept document for the Centre for Reactive Trace Gases In Situ Measurements. Furthermore, an overview of available systems for the analysis of VOCs from ambient air and their performance is available from Hoerger et al. (2015). For the PTR-MS system a guideline is under progress within ACTRIS-2. Precursor gases system (CI-APi-TOF) and calibration procedures and schedules and measurement guidelines are under progress.

For VOCs, calibration has to be performed using a multicomponent mixture, containing all analysed species in the lower ppb-range. The target concentrations must be traceable to the WMO-GAW scale for VOC, with the Centre for Reactive Trace Gases In Situ Measurements as anchor point. For NMHC and BVOCs, scales are available by the Central Calibration Laboratories (CCLs) for NMHC (NPL, UK) and Monoterpenes (NIST, USA), whereas for OVOC and ELVOCs no CCL has been approved yet. Thus, in case of OVOCs, the Centre for Reactive Trace Gases In Situ Measurements will host a preliminary scale for these compounds in close cooperation with the CCQM (Consultative Committee for Amount of Substance: Metrology in Chemistry and Biology) Working Group on Gas Analysis (GAWG) of the International Office for Weight and Measures (BIPM). Calibration has to be performed in regular periods. For the observations with a GC-FID a monthly calibration cycle is recommended, if no manual interference or system break occurs. For the GC-MS systems a daily calibration is a minimum requirement. In addition, a target sample has to be measured at least monthly. This standard sample consists of a pressurized air cylinder which is again traceable to the WMO-GAW scale. The Centre for Reactive Trace Gases In Situ Measurements provides both calibration gas and target gas samples for regular checks. Recalibration is performed after the approved lifetime of the gas cylinder or when the pressure of the gas/air in the cylinder becomes less than 5 bar.

### 4.6.4 Operation

For $NO_x$, measurements are performed continuously (i.e., native raw data aggregated on 1-minute time resolution). For VOCs, a minimum of two measurements per week is required. Hourly measurements are however preferred. Standard operation procedures are outlined in the SOP-NOx (2014) and the SOP-VOC (2014), as well as their updates in ACTRIS-2 deliverable D3.17. Updated Measurement Guidelines for $NO_x$ and VOCs are in progress and will be available at least by end of 2018. Measurement Guidelines for aerosol precursor gases are being prepared and will be available by the end of 2020.

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### 4.6.5 Data production and data products

The final data product (ACTRIS Level 1 and Level 2 data) consists of measured concentrations of the reactive trace gases listed in Annex A.6 connected with the respective measurement uncertainty and precision, metadata and time dependent flags as specified by the DC, and in the standard operating procedures. Raw ambient measurement data has to be stored together with the relevant standard measurements and all information and metadata, which is needed to recalculate the higher-level data products. Details for the data production will be given in the ACTRIS Data Management Plan (D4.2) and the associated data production descriptions and documents provided by ACTRIS Data Centre and the Centre for Reactive Trace Gases In Situ Measurements. All data products, per-products and software tools are version controlled and identified by the DC.

ACTRIS *in situ* data production follows one of two main workflows, on-line or off-line. For the **on-line workflow**, data production is based on Level 0 data, i.e., all raw data and signals provided by an instrument in its native time resolution, brought to a harmonised format, and annotated with all discovery and metadata needed in the further data production process. Level 0 data are to be submitted and archived at the Data Centre, unless the ACTRIS Data Management Plan and the associated data production descriptions define an exception caused by large raw data volumes. In this case, an archive procedure has to be agreed between the Centre for Reactive Trace Gases In Situ Measurements and the Data Centre. The Level 0 data submission includes relevant calibration measurements and measurements of traceable standards needed for data quality control which are flagged as such. From Level 0 data, data Level 1 and Level 2 are produced. Level 1 data are quality controlled and calibrations are applied, final concentrations calculated, native time resolution, invalid and quality control measurements removed, and transferred to standard conditions of temperature and pressure where applicable. Level 2 data is averaged Level 1 data to typically hourly averages, measure of atmospheric variability included. The Level 1 and Level 2 data can be produced either by NF or the respective unit of the Data Centre, depending on variable, the distribution of work is included in the associated data production descriptions available from the Data Centre, and indicated in Annex A.6. The quality control step between Levels 0 and 1 can be automatic (RRT data production) or manual, performed by the Observational Platform. Data level identifiers distinguish between data with automatic or manual QC. The details of the steps producing Level 1 data from Level 0, and Level 2 from Level 1, are specified in the associated data production descriptions and the standard operating procedures.

For the **off-line workflow**, the steps of sample medium pre-exposure treatment, exposure, sampling time, preparation, and analysis are documented following standard operating procedures and protocols including metadata in machine-readable form. Items to be included are specified in the associated data production descriptions and the standard operating procedures. The archive for these protocols is located at the Observational Platform, its operating protocols coordinated with and approved by the Data Centre and the Centre for Reactive Trace Gases In Situ Measurements. From these protocols, the NF produces the Level 2 data product in the temporal resolution determined by the sampling schedule, and submits it to the Data Centre using the tools provided for data submission to ensure required documentation, flagging and metadata. The details of the procedure are specified in the associated data production descriptions.

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### 4.6.6 Data delivery and quality control

It is compulsory for the Observational Platform to produce the Level 1 and Level 2 data for archiving at the Data Centre. Archiving of Level 0 data will depend on specific variables. For the submission of trace-gas *in situ* data required procedures are described in ACTRIS Data Management Plan (D4.2) and the associated data production descriptions. Manually quality controlled data has to be submitted on a regular, scheduled frequency, at least yearly to the ACTRIS *in situ* data repository following the scheme in the ACTRIS Data Management Plan, and associated documents. Preliminary, manually quality controlled data has to be submitted by the end of March in the following year, the latest. Data originators at the NF are responsible for checking the data using the procedures in the associated data production descriptions.

Data is then reviewed by the Centre for Reactive Trace Gases In Situ Measurements and will be discussed at the annual data quality meeting in May, in collaboration with the respective unit of the Data Centre. An issue tracker is operated in the process of data evaluation to ensure full documentation and traceability of the data production and quality control process. This comes into place yearly following the initial data submission by stations to the DC. After review of the data according to the suggestions of the Centre for Reactive Trace Gases In Situ Measurements and the measurement community attending the meeting, data has to be resubmitted and will be reviewed again for compliance with suggested changes. Final submission to the DC has to be done before 31 May, using the submission tools and automatic quality control software available within the DC. Figure 1 shows the cooperation between the Observational Platforms, the Topical Centre and the Data Centre.

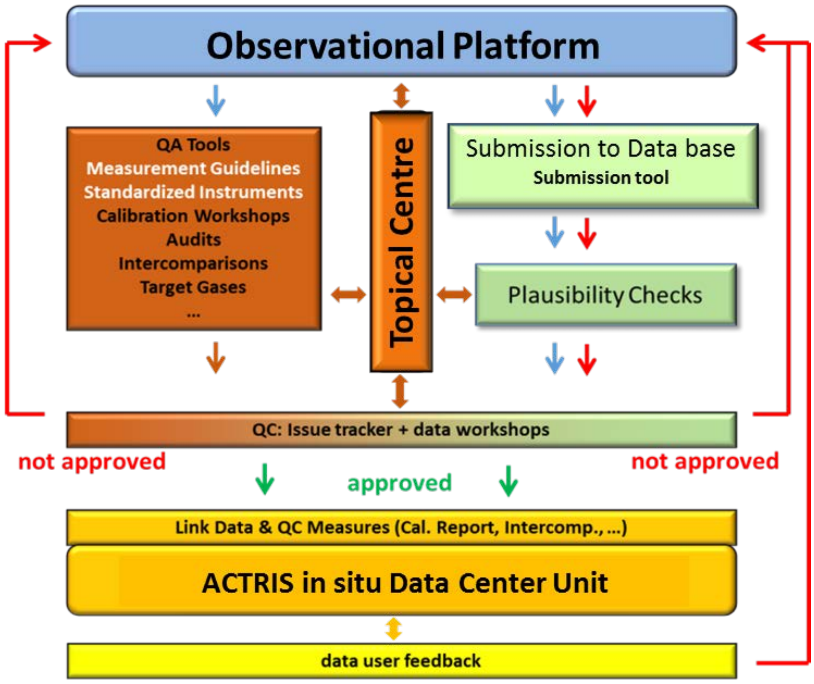


*Figure 1: Scheme of the QA-system envisioned for the Operational Platforms together with the Centre for Reactive Trace Gases In Situ Measurements and the Data Centre.*

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# 5 Organizational and strategic concepts for ACTRIS Observational Platforms

Experience from ACTRIS heritage shows that typically two kinds of Observational Platforms evolve in the research infrastructure: a) advanced, well-equipped Observational Platforms, which contribute to the observational strategy with optimized and combined observations leading to substantial synergistic effects (described in Sec. 5.1), and b) specialized Observational Platforms, which deliver a limited number of variables with focus on regional coverage and specific topics (described in Sec. 5.2). In the following, a brief description of respective requirements for these two types of Observational Platforms is given. Details of requirements and procedures that will be used in the respective labelling of ACTRIS Observational Platforms are discussed in D5.3 (*Documentation on ACTRIS National Facility labelling principles*).

## 5.1 ACTRIS Observational Platforms focussing on synergy

### 5.1.1 Observational requirements

Advanced ACTRIS Observational Platforms apply sophisticated and optimized instrumentation in a synergistic manner in order to deliver a comprehensive set of aerosol, cloud and/or reactive-trace-gas data, together with auxiliary parameters. It is expected that several of the observational components described in Sec. 4.1–4.6 are joined at such stations or that ACTRIS observational components are deployed together with an extensive set of non-ACTRIS instrumentation, e.g., at existing national observatories or at sites shared with another RI. Instruments at these advanced ACTRIS Observational Platforms should run continuously (24 hours/7 days a week if applicable; otherwise whenever measurement conditions are suitable) and data should be delivered in RRT or NRT in order to allow for data assimilation, on-line validation of model or satellite products and immediate information of the public.

### 5.1.2 Geographical requirements

Advanced ACTRIS Observational Platforms require substantial implementation and operation efforts, i.e., it is expected that only a limited number of such stations can be realized. Most probably, they will be set up at already existing national observatories, often also called “supersites” (a term that is however not adopted by ACTRIS). Thus, the geographical location of these sites, in many cases, has been already chosen in the past. It may be supposed that major general requirements have been considered in the selection, e.g., representativeness for a larger area or homogeneity of the surrounding in terms of orography, vegetation, cultivation, population density, etc. The sites should usually not be located in an isolated micro-environment with very specific conditions, except if the performed research is specifically dedicated to such an environment, which could be the case, e.g., for high-mountain sites. When new synergistic Observational Platforms are planned the locations should be chosen accordingly.

Moreover, synergistic Observational Platforms should be well distributed across Europe, covering the major climatic conditions and all typical air masses present over the continent. Due to the limited number of the sites, typical distances between them will be of the order of several hundred to thousand kilometres. Consequently, each advanced Observation Platform will be of major importance as key location and anchor point for observations in a larger region.

## 5.2 ACTRIS Observational Platforms focussing on regional coverage

### 5.2.1 Observational requirements

Specialized ACTRIS Observational Platforms contribute to at least one observational component described in Sec. 4.1–4.6 following at least the minimum ACTRIS requirements discussed above. Specific operation procedures may be applied at such stations, if they are in line with the ACTRIS standards.

### 5.2.2 Geographical requirements

Specialized ACTRIS Observational Platforms require less implementation and operation efforts. Therefore, a larger number of sites, involving also a larger number of national institutions, are expected. These Observational Platforms may be dedicated to the observation of distinct short-lived species under certain conditions. For instance, aerosols and short-lived trace gases relevant for human health need to be observed in and around industrialized urban regions, whereas for cloud observations rural mountainous sites are of much higher interest. Specialized ACTRIS Observational Platforms are important for geographical coverage and the investigation of the variability of different ACTRIS species in between the bigger observatories.

## 5.3 Access requirements

The major task of Observational Platforms is the collection and delivery of quality-controlled data for provision to users via the ACTRIS Data Centre. In addition, selected ACTRIS Observational Platforms, in particular large observatories, may offer physical access to users. Adequate personnel, equipment, logistics and resources at the respective sites are required, i.e.:

- Capabilities to run large scientific experiments;
- Possibilities to run instruments on user request for specific investigations, in specific modes, etc.;
- Possibilities to set up and run instruments of the user, including supply of power, water, technical gases, internet connection, etc.;
- Logistics to perform specific campaigns, e.g., with mobile ground-based or airborne platforms;
- Resources to host users, including working (office) and storage space and all necessary auxiliary facilities and supplies;
- Capabilities to train and support users by experienced staff;
- Resources to support users in administrative and logistic issues, e.g., customs, shipping, travel, transport, accommodation, etc.;
- Capabilities to ensure the ACTRIS observational requirements during physical access provision.

Physical access to Observational Platforms will be managed by the SAMU. The selection of Observational Platforms that will provide physical access will be part of the labelling process. Details are specified in D5.3, D2.6 and D6.3.

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## 5.4 Recommendations for national strategies

Setting up ACTRIS Observational Platforms following the concepts described above requires coordination and funding efforts at the national level. Thus, cost-effective solutions for maximum scientific value are demanded. The more instrumental and data synergy is achieved the more valuable information on atmospheric processes can be extracted from the observations. Thus, bundling efforts at national level or even collaboration of member states in order to set up high-sophisticated, synergistic Observational Platforms is strongly recommended. Such strategies may also consider co-location of sites with other environmental RIs, if added value can be achieved in this way.

ACTRIS focusses on highly variable short-lived species originating from various sources and undergoing vast atmospheric processes. Therefore, as discussed above, observational sites should be located such that, on the one hand, data representative for a larger area can be collected, and, on the other hand, sufficient information on the variability of atmospheric parameters in different environments is gathered. Therefore, the coverage of scientifically relevant geographical areas and ecosystems should be considered in national strategies and Observational Platforms distributed accordingly. Decisions on locations of observational sites, in particular when new sites are planned, should be reconciled within ACTRIS to allow for a coordination of efforts to enclose the scientific areas of interest. Furthermore, national and common initiatives for setting up observational sites at global hot spots are highly appreciated. Collaboration with local partners at such locations outside of Europe and respective outreach strategies will be strongly supported by ACTRIS.

# Annex A: ACTRIS Variables and Related Instruments

***Version 23 April 2018***

This section comprises a catalogue with ACTRIS Level 1 (L1) and Level 2 (L2) data from Observational Platforms associated to recommended instrument techniques.

## Abbreviations and symbols

| **Colour codes** | |
|---|---|
| Variable produced from a single measurement technique | (dark teal) |
| Variable produced from synergy of measurement techniques | (medium teal) |
| Variable produced from synergy of measurement techniques where combinations are possible | (light blue) |

| **Abbreviations used in the tables** | |
|---|---|
| **NF** | National Facility |
| **DC** | Data Centre |
| **TC** | Topical Centre |
| | |
| **CARS** | Centre for Aerosol Remote Sensing |
| **CAIS** | Centre for Aerosol In Situ Measurements |
| **CGas-SiM** | Centre for Reactive Trace Gases In Situ Measurements |
| **CIS** | Centre for Cloud In Situ Measurements |
| **CCRES** | Centre for Cloud Remote Sensing |
| **CREGARS** | Centre for Reactive Trace Gases Remote Sensing |
| | |
| **RRT-O** | Real real time (RRT) data stream implemented and operational. Most cases less than 3 h (real real time) but can be near real time (less than 3 days) |
| **RRT-S** | Real real time (RRT) possible and scheduled |
| | |
| **M** | Mandatory variables required for ACTRIS site |
| **S** | Specializing variable provision of at least 1 specializing variable are mandatory for ACTRIS sites connected to Aerosol in-situ TC - |
| **O** | Optimum - recommended |

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## A.1 Aerosol remote sensing

| *ACTRIS variable* | NF requirements Mandatory - M Specializing - S Optimum - O | Associated Topical Centre | Data producer L1, L2 | RRT-O= operational in RRT now RRT-S = scheduled from 2020 | Approx. height resolution | High-power aerosol lidar | Automatic sun/sky/lunar photometer |
|---|---|---|---|---|---|---|---|
| Attenuated backscatter profile | M | CARS | DC | NRT-S | 60 m | | |
| Volume depolarization profile | M | CARS | DC | NRT-S | 60 m | | |
| Particle backscatter coefficient profile | M | CARS | DC | NRT-S | 60 m | | |
| Particle extinction coefficient profile | M | CARS | DC | NRT-S | 60 m | | |
| Lidar ratio profile | M | CARS | DC | NRT-S | 60 m | | |
| Ångström exponent profile | O | CARS | DC | NRT-S | 60 m | | |
| Backscatter-related Ångström exponent profile | O | CARS | DC | NRT-S | 60 m | | |
| Particle depolarization ratio profile | M | CARS | DC | NRT-S | 60 m | | |
| Particle layer geometrical properties (height and thickness) | M | CARS | DC | NRT-S | 60 m | | |

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| *ACTRIS variable* | **NF requirements Mandatory - M Specializing - S Optimum - O** | **Associated Topical Centre** | **Data producer L1, L2** | **RRT-O= operational in RRT now RRT-S = scheduled from 2020** | **Approx. height resolution** | High-power aerosol lidar | Automatic sun/sky/lunar photometer |
|---|---|---|---|---|---|---|---|
| Particle layer optical properties (extinction, backscatter, lidar ratio, Ångström exponent, depolarization ratio, optical depth) | M | CARS | DC | NRT-S | 60 m | | |
| Column integrated extinction | M | CARS | DC | NRT-S | 60 m | | |
| Planetary boundary layer height | O | CARS | DC | NRT-S | 60 m | | |
| Spectral Downward Sky Radiances | M | CARS | TC | NRT-O | NA | | |
| Direct Sun/Moon Extinction Aerosol Optical Depth (column) | M | CARS | TC | NRT-O | NA | | |

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## A.2 Cloud remote sensing

| *ACTRIS variable* | NF requirements Mandatory - M Specializing - S Optimum - O | Associated Topical Centre | Data producer L1, L2 | RRT-O= operational in RRT now RRT-S = scheduled from 2020 | Approx. height resolution | High-power aerosol lidar | Automatic low-power lidar and ceilometer | Doppler cloud radar | Radiosonde | Microwave radiometer | Doppler lidar | Drop-counting raingauge | Disdrometer | NWP model input required |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Radar reflectivity factor | M | CCRES | DC | RRT-O | 60 m | | | | | | | | | |
| Radar Doppler velocity | M | CCRES | DC | RRT-O | 60 m | | | | | | | | | |
| Radar Doppler spectral width | M | CCRES | DC | RRT-O | 60 m | | | | | | | | | |
| Radar linear depolarisation ratio | O | CCRES | DC | RRT-O | 60 m | | | | | | | | | |
| Attenuated backscatter profile | M | CARS | DC | RRT-O | 60 m | | | | | | | | | |
| Cloud/aerosol target classification | M | CCRES | DC | NRT-O | 60 m | | | | | | | | | |
| Drizzle drop size distribution | M | CCRES | DC | NRT-O | 60 m | | | | | | | | | |
| Drizzle water content | M | CCRES | DC | NRT-O | 60 m | | | | | | | | | |

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| *ACTRIS variable* | NF requirements Mandatory - M Specializing - S Optimum - O | Associated Topical Centre | Data producer L1, L2 | RRT-O= operational in RRT now RRT-S = scheduled from 2020 | Approx. height resolution | High-power aerosol lidar | Automatic low-power lidar and ceilometer | Doppler cloud radar | Radiosonde | Microwave radiometer | Doppler lidar | Drop-counting raingauge | Disdrometer | NWP model input required |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Drizzle water flux | M | CCRES | DC | NRT-O | 60 m | | | | | | | | | |
| Ice water content | M | CCRES | DC | NRT-O | 60 m | | | | | | | | | |
| Liquid water content | M | CCRES | DC | NRT-O | 60 m | | | | | | | | | |
| Dissipation rate of TKE (turbulent kinetic energy) | O | CCRES | DC | NRT-S | 60 m | | | | | | | | | |
| Atmospheric boundary layer classification | O | CCRES | DC | RRT-S | 60 m | | | | | | | | | |
| Liquid water path | M | CCRES | DC | NRT-O | - | | | | | | | | | |
| Temperature profile | O | CCRES | DC | NRT-O | variable | | | | | | | | | |
| Relative humidity profile | O | CCRES | DC | NRT-O | variable | | | | | | | | | |
| Integrated water vapor path | O | CCRES | DC | NRT-O | - | | | | | | | | | |

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## A.3 Reactive trace gases remote sensing

| *ACTRIS variable* | **NF requirements Mandatory - M Specializing - S Optimum - O** | **Associated Topical Centre** | **Data producer L1, L2** | **RRT-O= operational in RRT now RRT-S = scheduled from 2020** | **Approx. height resolution** | Single FTIR | Double FTIR | UVVIS-Zenith Sky | UVVIS MAXDOAS | O3 DIAL |
|---|---|---|---|---|---|---|---|---|---|---|
| Ozone profile | O | CREGARS | NF | - | few hundred meters to few km | | | | | ■ |
| Ozone partial columns | O | CREGARS | NF | - | 5 to 8 km | | ■ | | | |
| Ozone column | M | CREGARS | FTIR: NF; UVVIS: TC | UVVIS: NRT-S | NA | | ■ | ■ | ■ | |
| Formaldehyde column | M | CREGARS | FTIR: NF; UVVIS-MAXDOAS: TC | UVVIS MAXDOAS: NRT-S | NA | ■ | ■ | | ■ | |
| Formaldehyde lower tropospheric profile | O | CREGARS | TC | NRT-S | few hundred meters to few km | | | | ■ | |
| NO2 column | M | CREGARS | FTIR: NF; UVVIS: TC | FTIR: after 3 months; UVVIS: NRT-S | NA | ■ | ■ | ■ | ■ | |
| NO2 partial columns | S | CREGARS | FTIR: NF; UVVIS: TC | FTIR: after 3 months; UVVIS: NRT-S | stratospheric column | ■ | ■ | ■ | ■ | |
| NO2 lower tropospheric profile | O | CREGARS | TC | NRT-O | - | | | | ■ | |
| NH3 column | S | CREGARS | NF | NRT-O | NA | | ■ | | | |
| C2H6 column | M | CREGARS | NF | NRT-O | - | ■ | ■ | | | |

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## A.4 Aerosol *in situ* measurements

| ***ACTRIS variable*** | **NF requirements Mandatory - M Specializing - S Optimum - O** | **Associated Topical Centre** | **Data producer L1, L2** | **RRT-O= operational in RRT now RRT-S = scheduled from 2020** | Integrating Nephelometer | Mobility Particle Size Spectrometer | Aerodynamic & Optical Particle Size Spectrometer | Absorption Photometer | Condensation Particle Counter | Scanning PSM, (N)AIS, N-MPSS | Particle Size Magnifier (PSM) | Cloud Condensation Nuclei Counter | Filter sampling | Thermal-optical analyser | Offline filter-based IC, GC-MS, HPLC-MS, LC/MS | Aerosol Mass Spectrometer | X-Ray Fluorescence, Particle Induced X-ray Emission |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Particle light scattering and backscattering coefficients | M | CAIS | NF | NRT-O | | | | | | | | | | | | | |
| Particle number size distribution - mobility diameter | M | CAIS | NF | NRT-O | | | | | | | | | | | | | |
| Particle number size distribution - optical and aerodynamic diameter | S | CAIS | NF | NRT-S | | | | | | | | | | | | | |
| Particle light absorption coefficient and equivalent black carbon concentration | M | CAIS | NF | NRT-O | | | | | | | | | | | | | |
| Particle number concentration | S | CAIS | NF | NRT-S | | | | | | | | | | | | | |
| Nanoparticle number size distribution | S | CAIS | NF | NRT-S | | | | | | | | | | | | | |

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| *ACTRIS variable* | **NF requirements Mandatory - M Specializing - S Optimum - O** | **Associated Topical Centre** | **Data producer L1, L2** | **RRT-O= operational in RRT now RRT-S = scheduled from 2020** | Integrating Nephelometer | Mobility Particle Size Spectrometer | Aerodynamic & Optical Particle Size Spectrometer | Absorption Photometer | Condensation Particle Counter | Scanning PSM, (N)AIS, N-MPSS | Particle Size Magnifier (PSM) | Cloud Condensation Nuclei Counter | Filter sampling | Thermal-optical analyser | Offline filter-based IC, GC-MS, HPLC-MS, LC/MS | Aerosol Mass Spectrometer | X-Ray Fluorescence, Particle Induced X-ray Emission |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Nanoparticle number concentration | S | CAIS | NF | NRT-S | | | | | | | | | | | | | |
| Cloud condensation nuclei number concentration | S | CAIS | NF | NRT-S | | | | | | | | | | | | | |
| Mass concentration of particulate organic and elemental carbon | S | CAIS | NF | - | | | | | | | | | | | | | |
| Mass concentration of particulate organic tracers | S | CAIS | NF | - | | | | | | | | | | | | | |
| Mass concentration of non-refractory particulate organics and inorganics | S | CAIS | NF/TC | NRT-S | | | | | | | | | | | | | |
| Mass concentration of particulate elements | S | CAIS | NF | - | | | | | | | | | | | | | |

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| ACTRIS variable | Comment |
|---|---|
| Particle light scattering and backscattering coefficients | multi-wavelength |
| Particle number size distribution - mobility diameter | 0.01 - 0.8 µm |
| Particle number size distribution - optical and aerodynamic diameter | 0.7 - 10 µm |
| Particle light absorption coefficient and equivalent black carbon concentration | |
| Particle number concentration | > 0.01 µm |
| Nanoparticle number size distribution | 0.001 - 0.02 µm |
| Nanoparticle number concentration | < 0.01 µm |
| Cloud condensation nuclei number concentration | at various supersaturations |
| Mass concentration of particulate organic and elemental carbon | |
| Mass concentration of particulate organic tracers | |
| Mass concentration of non-refractory particulate organics and inorganics | |
| Mass concentration of particulate elements | |

## A.5 Cloud *in situ* measurements

| *ACTRIS variable* | NF requirements<br>Mandatory - M<br>Specializing - S<br>Optimum - O | Associated Topical Centre | Data producer L1, L2 | RRT-O= operational in RRT now<br>RRT-S = scheduled from 2020 | Mobility Particle Size Spectrometer | Condensation Particle Counter | Integrating Cloud Probe | Cloud Droplet Probe | Cloud Ice Probe | Aerosol Particle Sampler | Bulk collectors | INP instrument |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Liquid Water Content | M | CIS | NF | NRT-S | | | ■ | | | | | |
| Droplet effective diameter | M | CIS | NF | NRT-S | | | ■ | | | | | |
| Droplet number concentration | S | CIS | NF | NRT-S | | | | ■ | | | | |
| Droplet size distribution | S | CIS | NF | NRT-S | | | | ■ | | | | |
| Interstitial aerosol number concentration | S | CIS | NF | NRT-S | | ■ | | | | | | |
| Interstitial aerosol size distribution | S | CIS | NF | NRT-S | ■ | | | | | | | |
| Total aerosol number concentration | S | CIS | NF | NRT-S | | ■ | | | | | | |
| Total aerosol size distribution | S | CIS | NF | NRT-S | ■ | | | | | | | |
| Cloud residuals number concentration | O | CIS | NF | NRT-S | | ■ | | | | | | |
| Cloud residuals composition | O | CIS | NF | NRT-S | | | | | | ■ | | |
| Ice particle number concentration | S | CIS | NF | NRT-S | | | | | ■ | | | |
| Ice particle size distribution | S | CIS | NF | NRT-S | | | | | ■ | | | |
| Ice nucleating particle number concentration | S | CIS | NF | NRT-S | | | | | | | | ■ |
| Ice nucleating particle temperature spectrum | S | CIS | NF | NRT-S | | | | | | ■ | | |
| Bulk cloud water chemical composition | S | CIS | NF | NRT-S | | | | | | | ■ | |

## A.6 Reactive trace gases *in situ* measurements

| *ACTRIS variable* | **NF requirements Mandatory - M Specializing - S Optimum - O** | **Associated Topical Centre** | **Data producer L1, L2** | **RRT-O= operational in RRT now RRT-S = scheduled from 2020** | On-line GC-FID | On-line GC-MS | On-line GC-FID/MS | On-line GC-Medusa | On-line PTR-MS | On-line Hantzsch | Off-line traps: ads-tubes | Off-line traps: DNPH-cartridge-HPLC | Off-line steel canister | Off-line glass flask | NO-$O_3$ chemiluminescence | Potentially other measurement technique supported by the TC | Cavity Attenuated Phase Shift Spectroscopy (CAPS) | CI-APi-TOF |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| NMHCs | M*, O | CGas-SiM | NF | NRT-S | | | | | | | | | | | | | | |
| OVOCs | M*, O | CGas-SiM | NF | NRT-S | | | | | | | | | | | | | | |
| Terpenes | M*, O | CGas-SiM | NF | - | | | | | | | | | | | | | | |
| NO | M | CGas-SiM | NF/TC | NRT-S | | | | | | | | | | | | | | |
| $NO_2$ | M | CGas-SiM | NF/TC | NRT-S | | | | | | | | | | | | | | |
| Condensable vapours | O*, S | CGas-SiM | NF/TC | NRT-S | | | | | | | | | | | | | | |

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| ACTRIS variable | Comments |
|---|---|
| NMHCs | NMHCs ($C_2$-$C_9$, detailed list available). Time resolution depends on sampling frequency, typical maximum 1/hour. M*: At least 6 different VOCs (NMHCs, OVOCs, terpenes) have to be measured at an NF, can be partly NMHCs. |
| OVOCs | Oxidised volatile organic compounds (detailed list available). Time resolution depends on sampling frequency, typical maximum 1/hour, less for PTR-MS. M*: At least 6 different VOCs (NMHCs, OVOCs, terpenes) have to be measured at an NF, can be partly OVOCs. |
| Terpenes | Monoterpenes (detailed list available). Time resolution depends on sampling frequency, typical maximum 1/hour, M*: At least 6 different VOCs (NMHCs, OVOCs, terpenes) have to be measured at an NF, can be partly terpenes. |
| NO | Needs to be accomplished by water vapour and ozone measurements, ideally also global radiation or J(NO2) |
| $NO_2$ | Needs to be accomplished by water vapour and ozone measurements, ideally also global radiation or J(NO2) |
| Condensable vapours | Sulfuric acid, highly oxygenated molecules (HOM) |

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# Annex B: References

## B.1 Applicable ACTRIS-PPP Documents

ACTRIS Glossary: https://www.actris.eu/About/ACTRIS/ACTRISglossary.aspx

D2.3: ACTRIS Data Policy

D2.6: ACTRIS Access and Service Policy

D3.1: ACTRIS Cost Book

D4.1: Concept document on ACTRIS Central Facilities structure and services

D4.2: ACTRIS Data Management Plan

D5.2: Documentation on technical concepts and requirements for ACTRIS Exploratory Platforms

D5.3: Documentation on ACTRIS National Facility labelling principles

D6.3: Report on access rules and modalities and recommendations for ACTRIS access policy

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