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

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Structure of the deliverable

This deliverable contains concepts documents for all eight Central Facilities in ACTRIS. The document is divided into eight sections, each consisting of the concept document of one ACTRIS Central Facility. Each section has its own cover page, heading, and page numbering.

Section 1

Concept of ACTRIS Head Office

ACTRIS PPP WP 4 Task 4.1

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1 Purpose of the document

This document describes the requirements, functions and relations of the ACTRIS Head Office. The document includes description and the role of the Head Office within the ACTRIS, and its role to the user communities of the ACTRIS, the foreseen organisational structure and the governance of the Head Office. This document describes the responsibilities of the Head Office, required capabilities, human resources, and facilities.

2 Description and role of the ACTRIS Head Office

2.1 Framework

Vision statement of ACTRIS

ACTRIS is the fundamental European research infrastructure for short-lived atmospheric constituents increasing the excellence in Earth system research and developing sustainable solutions to environmental challenges.

Mission statement of ACTRIS

ACTRIS shall establish, operate, and develop a pan-European distributed research infrastructure for short-lived atmospheric constituents. ACTRIS shall provide effective access for a wide user community to its resources and services in order to facilitate high-quality Earth system research.

ACTRIS is the European Research Infrastructure (RI) for fostering the use of research data and data analysis tools, and world-class research facilities in the field of atmospheric aerosols, clouds, and reactive trace gases. The ACTRIS Central Facilities (CFs) represent the key operative entities of this RI and have a fundamental role as they provide services to the users according to the ACTRIS service and access policy as well as operation support to the National Facilities (NFs). CFs are operated at the European level and are part of the governance and decision-making structure of the RI. Each CF may have several operational Units that can be located in different locations, and are operated by research performing organizations (RPOs) or by ACTRIS ERIC. The CFs link the NFs, i.e. the observational and exploratory platforms, which are operated at the national level and produce the majority of the ACTRIS measurement data.

The ACTRIS Head Office (HO) is one of the ACTRIS Central Facilities besides ACTRIS Data Centre and six Topical Centres, which are organized around the main scientific themes of ACTRIS: aerosols, clouds, and reactive trace gases, each with a particular focus on either remote sensing or in situ measurement techniques. Users access the services of ACTRIS through the Service and Access Management Unit (SAMU), administered by the HO.

2.2 Organisational relevance

ACTRIS is a large and complex Pan-European distributed research infrastructure worth of several Million euros, with high scientific ambition and with operations in more than 20 European countries. ACTRIS

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engages a large community of stakeholders, commits the RPOs in the operations, oversees the high standards of the services for the users and ensures the sustainability of its operations. All of these call for well-coordinated and managed operations, organisational framework and governance, which are the tasks of the Head Office to arrange and manage. The Head Office is responsible for establishing and improving the Quality Management System for ACTRIS.

The ACTRIS HO manages the governance bodies of the RI by acting as facilitator and secretariat for many of the bodies. It manages stakeholder liaisons, formal interactions with national and European members, observers and other partners. It manages any agreements with the NFs, CFs and collaborators approved by the General Assembly of the ACTRIS ERIC (European Research Infrastructure Consortium).

The HO administers the Service and Access Management Unit (SAMU) as a single access point to ACTRIS services. The SAMU optimizes physical access and scientific and technical services provided by ACTRIS Topical Centres and NFs. The HO promotes ACTRIS data and services to the wide user communities.

The HO coordinates and promotes the ACTRIS at the European and international levels. It manages liaison and outreach activities and works for building the general ACTRIS identity and raising awareness of its services. HO supports and coordinates the strategic and scientific development and innovation activities by cooperating with other RIs, organisations and private sector at EU and global level.

2.3 Scientific relevance

ACTRIS focuses on producing high-quality observations of short-lived climate forcers (SLCFs) and knowledge about processes driving their atmospheric lifetime. Short-lived atmospheric components have a residence time in the atmosphere from hours to few weeks and their level of concentration and physical, chemical and optical properties affect:

- The Earth's radiation balance through direct albedo effect or indirect cloud-related processes, one of the major sources of uncertainty in future-climate predictions.
- Public health as aerosol particles and gases, at concentrations typically found across Europe, give rise to severe and unacceptable health effects in the European population
- Extreme phenomena whether man-induced or not, by contributing to changing energy balance at the ground and in the atmospheric column.

An additional level of complexity is linked to the issue of man-induced climate–chemistry interaction. Emissions of pollutants change the atmospheric composition contributing to climate change through the aforementioned climate components, and, vice-versa, climate change influences atmospheric composition through a series of feedback process including changes in temperature, dynamics, hydrological cycle, atmospheric stability, emission intensity of biogenic compounds, temperature-dependent transformation processes in the troposphere, etc. The level of scientific understanding of the climate drivers, interactions and impacts is very low. ACTRIS provides user-oriented access to high-quality data and physical access to large facilities and laboratories, including simulation chambers, to conduct excellence research in the atmospheric domain. *The task of ACTRIS HO is to serve the users by providing the access to ACTRIS facilities and coordinate the ACTRIS data production. HO is in charge of the strategic development and planning of the ACTRIS services for users to solve important scientific questions.*

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ACTRIS is an important RI in the atmospheric research infrastructure landscape as it provides high-quality data and information that are very relevant for atmospheric science and are not covered by any other European RIs. ACTRIS integrates five atmospheric science communities (aerosol, cloud, LIDAR, trace gases, and simulation chamber communities) in Europe into one coherent research infrastructure, making ACTRIS the biggest in size, covering most of the atmospheric observations and experiments, and providing the broadest set of atmospheric variables in the atmospheric research infrastructure domain.

Through collaboration with other RIs, with international organisations and programmes, ACTRIS can address scientific and societal challenges through synergies and complementarities. The Head Office manages the ACTRIS scientific and technological development project portfolio and ensures that these collaborations lead to benefits for the ACTRIS users (development in services and operations) and is according to the ACTRIS strategy.

ACTRIS HO also manages and oversees the future cooperation with RIs from other domains and in particular joint development of data interoperability, data provision, technologies and provision of common services and tools for users. In addition to collaboration with other RIs, the ACTRIS HO shall conclude mutual agreements with a number of organizations, either to facilitate the production of services, or to ensure that a specific service is provided or to ensure that the role of the ACTRIS is clearly established. These organisations and programmes are for example:

- WMO (World Meteorological Organisation)
- ECMWF (European Centre for Medium range Weather Forecasting)
- COPERNICUS
- NWS (National Weather Services)
- EMEP (European Monitoring and Evaluations Programme)
- ESA (European Space Agency)
- EUMETSAT (European Organisation for the Exploitation of Meteorological Satellites)
- EEA (European Environment Agency)
- European Commission (under a legal entity status the ACTRIS ERIC will be able to participate as unique and sole beneficiary in any projects funded by the European Commission)
- Private partnerships

2.4 ACTRIS HO mission

The ACTRIS Head Office (HO) mission is to serve as central hub for the research infrastructure providing organizational resource and support to the ACTRIS community, making strategic plans and coordinating, overseeing and integrating the operations into a Pan-European research infrastructure. The HO coordinates and promotes the ACTRIS services, operates the legal entity, and ensures the strategic development and sustainability of the ACTRIS.

The HO operates from a user oriented and service based perspective, which is delivered consistently with quality, excellence, professionalism, and integrity.

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3 Internal organisational support and significance of the HO

The HO is responsible for planning, improving and securing all aspects related to the sustainability of the whole RI: scientific excellence, successful user strategy, efficient governance and management (incl. human resources), financial sustainability, technological development and upgrading of the RI, innovation, measuring the socio-economic impacts, and accounting for risks.

The HO ensures overall quality assurance and control of the research infrastructure including organising the KPI process, regular impact analysis, user satisfaction surveys, and regular RI level evaluation by external evaluators. Based on the evaluations and analysis of the performance, the HO develops RI level strategies and plans, such as user strategy, access policy and management plans to be decided by the General Assembly (GA) of ACTRIAS ERIC in order to improve the scientific excellence and societal relevance of the RI. The requirements for the HO functions are divided in four categories: 1) management of ACTRIS ERIC and coordination of the ACTRIS; 2) ACTRIS service and access management; 3) Coordination of the ACTRIS operations and technological development; and 4) ACTRIS scientific and operations strategy development, and establishment and management of external relations.

HO has to establish and maintain an efficient management methodology consisting of documentation of processes, methods, rules and standards that are used to accomplish the HO specific responsibilities but also to manage the decision-making, adopting a new technology or service, managing risks and performance evaluation etc. All processes, procedures, rules and practices deployed by ACTRIS and described in this chapter should be covered in this HO management methodology. The established HO methodology should be predictable, repeatable, based on standards and best practices. The established methodology promotes high quality results and efficient use of resources. The HO is also a keeper and archive of the RI standards and processes related to the operations at the other CFs.

3.1 Management of the ACTRIS ERIC and coordination of the ACTRIS

This requirement relates especially to the sustainability aspects: a) efficient governance and management (incl. human resources), b) financial sustainability, c) measuring the socio-economic impacts, and d) accounting for risks. The ACTRIS Head Office needs to manage the day-to-day legal entity operations, such as financial planning and budget allocation, annual accounting, work plans, reporting, HR management, and all the other activities required to efficiently run an organisation. At the RI level, the HO supervises the preparation of all necessary administrative documents such as the annual activity report approved by the GA, it handles the overall management and administration issues in the RI and formulates and further develops the RI management plan. The Head Office shall work closely with the other CFs and, thus, it shall support and oversee the management of the CFs.

3.1.1 Efficient governance and management (incl. human resources)

HO is in charge of the whole administrative tasks of ACTRIS ERIC. The administrative responsibilities of the HO includes preparing and coordinating the procurement of administrative services required by Head Office (such as pay-roll administration, working time management, travel and expense recording, contract management and archiving) ensuring that the process is run in accordance with the organizations' policies

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and procedures. Contract management of the ACTRIS ERIC is one of the major administrative duties of the HO. It includes management of any agreements with the ACTRIS Central Facilities and collaborators approved by the General Assembly of the ACTRIS ERIC.

The HO should prepare and facilitate the GA meetings, the work of external advisory bodies, and the RI Committee work. This task includes the meeting material preparations and document management and archiving.

ACTRIS will be regularly subjected to external evaluations and assessments at both the European and national level. HO has the responsibility to respond to these evaluations and assessments. In addition, internal self-assessments of the ACTRIS service provision and European level operation performance (Key Performance Indicators) should be organised and managed by the HO. The HO should create, manage and develop an internal reporting system and establish relevant KPIs in order to gather relevant data and information from ACTRIS operators. This includes organising the quality assurance system of ACTRIS ERIC operations and governance. This task of managing the quality assurance processes feeds to the task of scientific and operations strategy development. Based on the data, the HO shall identify if and where processes are not working as they should and advising on changes to be made and ensuring the implementation of the changes.

The HO is responsible for the human resources policy and strategy of the ACTRIS ERIC. The HO manages issues related to employment contracts and leave of absences. HO is obliged to provide and manage the staff rules and exercise employer´s duties according to the agreed legal framework (national and ERIC). The HO can give recommendations to the CFs and NFs that are not part of the ERIC. The HO should organise the training for managers in the HO and training of the CF managers, heads and directors in ACTRIS that support the success and improvement of the quality of the RI management. The HO task is to promote mobility of the ACTRIS managers and operators to “gain brain”, improve performance, to benchmark and to learn best practices used in other organisations.

3.1.2 Financial sustainability

HO ensures proper financial management according to the ACTRIS financial and work plans at the RI level. Financial management covers for example preparing of the budgets and work plans of the RI, management of the approved budget and processing of the transactions, managing the funds collected within the legal entity for common operations of the RI as well as establishment and tracking of the internal financial rules, fiscal reporting and the annual financial reports. The HO also prepares the balanced budget estimates and gathers work plans of the RI which are approved by the GA and the financial committee.

The Head Office has a central resource management role in planning, coordinating, and allocating the share of annual budget of ACTRIS ERIC for the services provided by the Central Facilities and the HO. The HO prepares runs and supervises all compulsory duties concerning ACTRIS ERIC finances incl. budgetary planning and tracking of costs and revenues throughout the year, invoicing, cash flow management, calculation of salaries and tax administration. The HO has to ensure proper accounting, auditing and preparation of the financial statements.

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3.1.3 Measuring the socio-economic impacts

The relevance of the ACTRIS services and operations for the society and science need to be demonstrated regularly. This also implies for the cost-benefit analysis of the ACTRIS service provision. The services needs to meet the user needs with the most cost-efficient manner. For the overall sustainability it is important to demonstrate in consistent manner and articulate well the socio-economic impact of ACTRIS. The HO is responsible for organising the analyses of the impacts of ACTRIS and communicating results to the stakeholders. This task feeds also to the task of scientific and operations strategy development.

3.1.4 Accounting for risks

The process of risk management should be described as part of the HO management methodology. The HO is responsible for collecting annual risk reports, updating the risk management plan, and organising and managing the risk register. The risk register managed by HO is the basis for the European level risk management and a tool to monitor the risk management plan. Risk register keeps track of identified risks, current assessment of their likelihood and impact and the exposure that the project is subject to, who is currently responsible for taking action to minimisation that exposure, and a note of the actions or strategy adopted. The risk register will be held in the form of a spreadsheet accessible for interested parties on request.

3.2 ACTRIS service and access management

This task of HO is especially related to the establishment and maintenance of the successful user strategy and implementing the ACTRIS access and service provision.

The management of services and access is a core function of the ACTRIS Head Office as it enables excellence in research to the European and international scientific and private sector communities by using ACTRIS services. This function is entrusted to a specific organizational Unit within the HO structure – the Service and Access Management Unit (SAMU) – responsible for steering and coordinating all activities involved in the provision of ACTRIS services, studying and implementing open access best practice.

The Unit is the single entry point for the user access to ACTRIS, being in charge of the management of the physical and remote access to all Topical Centres' services, the access on demand to specific digital services provided by the Data Centre, and the physical access to selected National Facilities. Therefore SAMU shall organize and coordinate on the behalf of the entire ACTRIS the access and service management. In addition, SAMU need to be a place where the ACTRIS policies and strategies on access, data and users are implemented and where feedback and recommendations arising from the interaction with users can be collected.

SAMU shall maintain the service portfolio of ACTRIS. This includes access to calibration services, use of high-class instruments and equipment, knowledge transfer, training and educational services.

Based on the ACTRIS access policy and strategies, SAMU shall be responsible at least for the following activities:

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3.2.1 Establishment and management of the *peer review* access process

The Unit shall **establish and manage the competitive access process during all the relevant phases** from the application, feasibility check, evaluation, selection and approval phases as well as feedback collection.

SAMU need to take care of developing and maintaining the centralized requests submission process as well as the review, and of guaranteeing the transparency and impartiality of the evaluation of the submitted proposals, in line with relevant rules and procedures.

The peer review panel organised by HO/SAMU shall include internationally recognised scientific experts for both scientific and technical review and assessment. It shall be called upon by SAMU when necessary for the review. During the process SAMU shall ensure that applicants have the opportunity to reply to possible questions or concerns that may be raised by experts, establishing a right to reply period before the final assessment.

The Unit shall receive the access requests and cooperates with the relevant Central or National Facility for the feasibility of the access based on the available capacity (laboratories, equipment, services, facility staff providing the support needed, schedule, user needs, etc.).

At the end of the peer review process SAMU need to communicate to applicants the results of the evaluation.

3.2.2 Interface between users and ACTRIS Facilities

SAMU will be at the centre of the relationship ensuring the smoothness and fairness of all interactions between users and ACTRIS CFs/NFs, and supports both so that each takes advantages of the interaction.

The Unit shall promote access opportunities to potential user communities with relevant communication on how to apply for ACTRIS services, eligibility and terms of access, details and timeline of the peer review process, evaluation criteria, etc.

SAMU shall receive and transmit users' requests to Central and National Facilities assisting the exchanges and the identification of possible solutions to accommodate their needs. The Unit need to operate also as **User Service Helpdesk** for any user enquires, providing **day-to-day support** and information to users willing or admitted to access to ACTRIS whenever they have any issues with or questions about ACTRIS services.

3.2.3 Monitoring access and services provided

SAMU need to play a crucial role in monitoring the service provision and its results.

Following the **user-driven approach** of ACTRIS, the monitoring activities of SAMU will provide ACTRIS Facilities and governing bodies with helpful information to consent an evaluation of ACTRIS activities and services from the perspective of those who make effectively use of them. Comments, opinions and

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suggestions coming from users' experience need to be routed back to TCs/DC/NFs as *input* into the services development and ongoing management process.

SAMU shall produce, keep and make accessible appropriate information, documentation, and statistics on user, services, and access:

- on the users (e.g., number of users, names, origin, affiliation) and user needs;
- on the quantity of access provided (e.g. number of units of access provided), type of services requested, selection procedures and results (including information on the impact of scientific outcomes acknowledging the use of the ACTRIS Facilities (publications, patents, etc.).
- on the quality of services, based on the analysis and elaboration of the **feedback** collected from users with specific surveys or arisen during the access.

The need for monitoring is to evidence the quantity and quality of ACTRIS service provision and, in case, to identify areas of enhancement so to consent the ACTRIS Facilities and governance bodies to consider/plan actions to improve service provision, develop further services and advance the user strategy.

This activity is considered crucial also to provide needed input for the overall continuous socio-economic impact analysis of ACTRIS.

Information on access, access impact and the continuous effort to accommodate the user needs improving their ACTRIS experience is needed to be disseminated at conferences, on websites and in publications.

3.2.4 Management of the Science and User Forum

On the behalf of ACTRIS SAMU shall also be responsible for the coordination and development of the **ACTRIS User Forum**, the virtual place where researchers interested in ACTRIS services and resources for their research can gather together to discuss their needs and expectations regarding the services.

Open to scientific and private sector user communities, the Forum is foreseen to be the main communication channel between users and ACTRIS Facilities. The Forum shall provide an organized framework for discussion and exchange, and can also serve as platform for fostering collaboration between different user communities to stimulate synergies that will increase the scientific and economic impact of ACTRIS.

SAMU shall:

- put in place forum features to help gaining valuable insights on the users' requirements (type, size, origin) and their research interests
- steer the discussion and analysis of present and future scientific and technical challenges regarding usage of CF/NF resources
- distil recommendations from the discussions in the Forum mediating bottom up initiatives/requests to the ACTRIS governance bodies.

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3.2.5 Training of users

SAMU shall contribute to the organization of **training** for RI users, including industry users, to better take advantage of the opportunities connected to the access. Ad-hoc training on how to use the ACTRIS facilities or research data to solve specific research problems is offered in cooperation with the Central/National Facilities. Seasonal schools, workshops and scientific and industrial seminars shall be designed on the basis of the educational needs of users, upon a preliminary thorough understanding of their existing skills and competencies.

3.2.6 Interlinkages with other HO units

Due to foreseen activities, SAMU shall have a crucial role in fostering the RI's knowledge of the user communities and related needs in terms of services. Interlinkages and relations with the other HO organizational units responsible for legalities, RI operations, strategic development & external relations are decisive to ensure that the knowledge of the user communities will guide and inform the RI decision-making and will influence future strategies and roadmap.

SAMU shall maintain close relations with:

- the Legal Entity Management Unit, to properly deal with all access aspects related to the Intellectual Property (IP) protection and requirements, confidentiality issues, privacy protection, applicable regulations, etc. as well as for informing the self-assessment/evaluations activities with results and impact of the access
- the RI Operations, to support the development of joint strategies for use and upgrade of the TCs and the entire infrastructure, based on the needs and feedback of users.
- the Development and relations Unit, to cooperate to the design of tailored communication strategies for different user communities and to maintain the Science and User Forum.

3.3 Coordination of the ACTRIS operations and technological development

This task relates especially to the sustainability aspects of technological development, upgrading of the RI, innovation, and data management.

3.3.1 Management of well-integrated RI operations

The HO shall maintain and develop the scientific focus of ACTRIS according to the vision and mission statements and the strategies agreed in the General Assembly. The HO should **coordinate and integrate the research infrastructure operations**, the core mission of the RI, by communicating effectively the ACTRIS strategy, sharing timely information and making recommendations. The HO shall facilitate development and implementation of ACTRIS strategy by organizing necessary consultations in the community and collecting information and giving advice on streamlining the activities.

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3.3.2 Technological development of RI operations

The HO should promote **technological development and knowledge transfer** within RI and the users. It should arrange workshops for the RI managers (CF and NF) and the private sector users with this aim, and contribute to technology development and innovation. The HO need to facilitate novel public-private collaborations to develop the CF and NF operations and should support in developing new services to users based on user needs. The HO need to be tasked to seek private and public partnerships (public-private-partnership (PPP)) for innovation and to provide information on the availability of test beds, downstream activities, and to promote development of new instruments, technology transfer (including IPR, legal issues etc.), and pre-commercial procurements.

3.3.3 Optimizing the RI operational work flows

The HO shall be responsible for overseeing and developing the **internal operational process flow** of the CFs and NFs and to solve bottlenecks. The work flow management need to take place in close cooperation with the ACTRIS Data Centre and other CFs and NFs. The HO shall monitor and analyse the performance of CFs and stations against contractual agreements and KPIs and maintain related official documentation (see section 3.1). The HO should support the efficient and coherent work flows and operations between CFs and NFs operations.

3.3.4 Development and management of downstream services of ACTRIS

The HO shall manage the **downstream service provision** by ensuring contractual service provision (for example with Copernicus), and developing other service provision with partners to create investments and impact built on the ACTRIS data and services.

The HO need to be responsible for overseeing the labelling and validation process for the National Facilities, observational and exploratory platforms, during Implementation Phase of ACTRIS.

As part of operative responsibilities, the HO shall regularly inform and consult the national contacts about the activities in the organisation and developments in the RI to manage the community engagement and effective operations. The HO should provide support for sustainability, information distribution, outreach and promotion. HO need to collect the NF annual reports and work plans, manages the labelling process, and applications to be new ACTRIS NF.

The HO shall allocate funds to support CF operations according to financial and work plan, collect annual reports and plans and provide timely information about the on-going developments in the national consortia and projects to ensure effective operations.

The HO should organise the archive of any operational documentations deemed necessary from NFs or CFs, such as protocols and Sops, self-assessment reports, KPI reports, etc.

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3.4 ACTRIS scientific and operations strategy development and establishment and management of external relations

This task interlinks with the previous main tasks and relates especially to the sustainability aspects scientific excellence and socio-economic impact.

3.4.1 Strategic Development of ACTRIS

The strategic planning is of highest importance for the success of the ACTRIS. To be able to adhere to the best governance practices requires that a well-defined strategy is in place and that the RI managers engage to the strategy. Adhering to the best practices, managing the development of the strategy and communicating it to the RI managers is on the responsibility of the HO. HO should ensure that clear and agreed work plans to execute the strategy are in place to guide the optimum decision-making in ACTRIS.

The HO should collect data to support the strategy-based decision-making. These data include user feedbacks on the service provision, continues monitoring reports on user needs, various performance indicators throughout the RI, and data on internal quality assurance processes and results and external evaluations.

Important task for HO is to follow the scientific development of climate and air quality research and actively participate on various science activities and events to understand the development needs and anticipate the changing user needs and take them into account in the RI service provision.

The HO should facilitate interaction and cooperation with international research infrastructures and organisations in order to develop strategies for the research infrastructure. This helps to formulate and coordinate long-term scientific development strategies of the RI to increase the socio-economic impact of the RI. In addition, HO should network and cooperate with other ESFRI infrastructures in developing common solutions, exchanging best practices and improving the European RI landscape.

Additionally, the HO shall be responsible in organising the management of the projects (e.g. H2020 projects) where ACTRIS ERIC is the coordinator. These projects can be part of strategic and operative development activities. Since these projects are not part of the ACTRIS ERIC core activities or core budget, they need separate arrangements and may require recruiting separate project staff inside the ACTRIS ERIC.

3.4.2 Coordinating and supporting communication and dissemination of ACTRIS

The HO should be responsible for developing a communication and outreach strategy for the RI in collaboration with CFs and NFs. The strategy includes also the coordination and development of the ACTRIS User Forum (see section 3.2) that promotes the dialogue between researchers and society and helps to gather valuable information on the potential users, their research interests, and needs. The User Forum need to serve to translate the atmospheric knowledge to what is needed to address societal challenges. The HO utilises social media tools to build ACTRIS community and to manage of public relations.

The aim of the communication and dissemination should be to increase general awareness of ACTRIS and the opportunities it provides, its products, services and in this way to increase the RI's socio-economic

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impact. The HO should coordinate the communication and outreach activities of the RI and also take care of the ACTRIS RI brand and visual outlook. The HO may use multiple means and tools to increase the awareness of the RI.

The HO should promote and organize the communication and outreach at the RI level by delivering timely information to the end user community for example by providing a web site, communication platform and information system, publishing internal documents, coordinating ACTRIS presence in media, publishing press releases, promotional or perspective articles in professional journals, and preparing outreach material.

Equally important, HO should enhance and facilitate the internal RI communication and seek the most efficient communications tools and means for internal RI communication.

3.4.3 Building and maintaining external relations

The HO as hosting the statutory seat of ACTRIS shall represent ACTRIS in all arenas, also beyond the science community, on the European and international levels and maintain formal interactions with national, European and global partners and stakeholders.

The HO shall be responsible for engaging new member countries through stakeholder liaison and country level communication. The development of pan-European wide NF network for observational platforms and engaging European high-quality exploratory platforms as a part of ACTRIS is one of the main targets of ACTRIS. HO should create and maintain liaisons and partnerships with new countries (not yet ACTRIS members) and their potential ACTRIS NF principle investigators and research performing organisations with the target of expanse the ACTRIS operations in Europe.

In addition to the new membership relations, HO shall regularly build and maintain connections to user communities, incl. innovation and private sector liaisons and service development, and promote activity the usage of the RI facilities and data, and product development and monitoring.

3.4.4 Enhancing innovations through private sector liaisons and collaboration

One of the HO responsibilities shall include awareness rising, building relationships, prospecting new business, and establishing partnership opportunities with industry, and to offer ACTRIS services to industrial actors e.g. in the form of NF visits and by define flexible business models adapted to users' needs (including open-access data, expert services and physical access to the infrastructure) for private sector actors.

4 Services and benefits for the user communities

The Head Office shall lead the development and implementation of the user strategy and the provision of services to the user communities. An ACTRIS user is a person, a team, or an institution using either ACTRIS data or any other ACTRIS service. ACTRIS users originate from academia, business, industry and public services, from ACTRIS member countries as well as from countries, which are not ACTRIS members, inside and outside Europe. Basically, the Head Office need to reach user communities with active relations, communication and dissemination activities and shall serve all users requesting ACTRIS services through SAMU.

Access to some ACTRIS services will be open and free, most importantly the access to ACTRIS data, data products, and digital tools provided by the Data Centre, which is the point of entry for free ACTRIS data services. Other access to ACTRIS services is considered competitive access based on capacity or excellence and will require a review process that should centrally managed by SAMU. SAMU is the single point of entry for user access to all TC services and to some specific services and data products provided by the Data Centre. Access is regulated by both the ACTRIS access policy and the ACTRIS data policy, respectively.

The ACTRIS Head Office shall be the central hub of ACTRIS that coordinates the operations of ACTRIS and enables services for generating and disseminating knowledge, boosting technological development, creating human capital and jobs for the benefit of society, and tackling environmental challenges. ACTRIS has multiple user communities that benefit from ACTRIS services. ACTRIS provides added value for the researchers, policy makers, private sector, ministries and funding organizations, educators and the Civil Society (e.g. general public, national and international media).

ACTRIS added value for scientists via quality-assured and open-access ACTRIS data; standardized operating procedures; instrument and procedure inter-comparisons; access to research platforms for conducting excellent research and creating new scientific knowledge; enhancement of research performance due to centralized access to ACTRIS data and specific services; increased possibilities for international collaboration, large-scale research projects and training opportunities; and technical support from CFs and on-site support from NFs. The Head Office shall coordinate, integrate and monitor the performance of ACTRIS to maintain the scope, sustainability and quality of the operations. High quality operations ensure high scientific output.

ACTRIS added value for policy makers by providing support for policy-driven networks established under EU-directives (local and European air-quality networks); development of new policies by provision of novel tools for validating the impact of regulation strategies and emission abatement policies through direct evaluation of atmospheric trends at regional / European scale; decision-making regarding environmental issues by provision of high-quality and long-term data for predicting climate scenarios from local and regional up to national and international level; atmospheric hazard (e.g. volcanic eruptions) management and risk mitigation via the knowledge base of ACTRIS expert teams and monitoring of extreme atmospheric events; and enhancing job creation indirectly (expert jobs, new business opportunities). HO shall collect and disseminate the results.

ACTRIS added value for the private sector via open-access data; expert services and physical access to the infrastructure for innovative research for the development of novel technologies and products and as a test bed for new technologies and instruments; development of quality assurance standards to support the technological development; and novel public-private collaborations leading to the establishment of spin-off and start-up companies. HO shall provide capacity to share information, liaise, and create opportunities to public-private collaboration.

ACTRIS added value for ministries and funding organizations by optimization of national investments in research infrastructures; providing better value for money via pan-European dimension and coordinated access to data and services; and by the establishment of a unique research infrastructure for atmospheric sciences within Europe to improve efficiency of operation and coordination among the European research institutions avoiding the duplication and fragmentation of research efforts. The HO is the main contact point, liaison and information source for the funding organisations about ACTRIS. HO shall find new funding sources for the operations and make a plan for the sustainability of the RI. The HO shall secure the funding organisations' commitment and through their engagement in the highest decision-making body.

ACTRIS added value for educators by offering training, exchange programmes and knowledge transfer, e.g. basic and advanced international courses on atmospheric composition and processes for Master's and PhD students; providing educational material; and offering expertise (e.g. expert visitors to schools of all levels). HO shall plan and coordinate the ACTRIS training and education portfolio, and find the best partners to organise them in a cost-effective way.

ACTRIS added value for to Civil Society (e.g. general public, national and international media) arises from improved weather, climate and air quality predictions due to novel scientific findings resulting from research using ACTRIS services; enhanced awareness on the environmental challenges that society is facing, e.g., climate change and air quality issues; and promotion of dialogue between researchers and society to translate scientific knowledge into practical applications. The task of the HO should be to efficiently disseminate the results using ACTRIS and to reach out to the society and politicians in order to make an impact.

List of identified ACTRIS User Communities:

- Atmospheric science research communities world-wide (climate and air-quality, observational/ experimental/ modelling/ satellite communities, national and international research programmes and organizations);
- Environmental science research communities and communities from other neighboring fields: hydro-marine, bio-ecosystem, geosciences, space physics, energy, health, and food domain, to study interactions and processes in across different disciplines;
- Instrument manufacturers and sensor industries for development, testing, prototyping and demonstration;
- Operational services, National weather services, climate services for model validation, weather and climate analysis and forecasting;
- Space agencies for validation and the development of new satellite missions;
- National and regional air quality monitoring networks and environmental protection agencies for air quality assessments and validation of air pollution models;

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- Policy makers and local/ regional/ national authorities for climate and air-quality related information for decision making and policy development.

5 Governance and management structure of the Head Office

5.1 Organisational structure requirements for Head Office

The activities of the Head Office should be organised in units, the foreseen unit structure should reflex the specific role of the HO, assuring that it complies with the requirements and obligations described in Section 3 of this document, and considering the general principles described in the *Baseline document for the concept of the Central Facilities*. The HO shall be organized so that it:

- has a well-defined structure of Units,
- has a well-defined decision-making process,
- is led by the Executive Director and Scientific Director, supported by the Unit Heads and staff in the HO Units,
- has clear, rational and cost-efficient task sharing between the Units,
- has a risk management strategy,
- hold the legal representation of ACTRIS as being the statutory seat for ACTRIS ERIC,
- Directors have RI Committee as an advisory and support body for the strategic development, ensuring the RI operations and facilitating the implementation of ACTRIS GA decisions. HO shall support the work of RI Committee.

The HO should be organized in four units reflecting the main functional categories described above. The foreseen units are Service and Access Management Unit, ERIC Management Unit, RI operations Unit, Development and Relations Unit (Fig. 1). Each unit has its specific functions (see Fig 2).

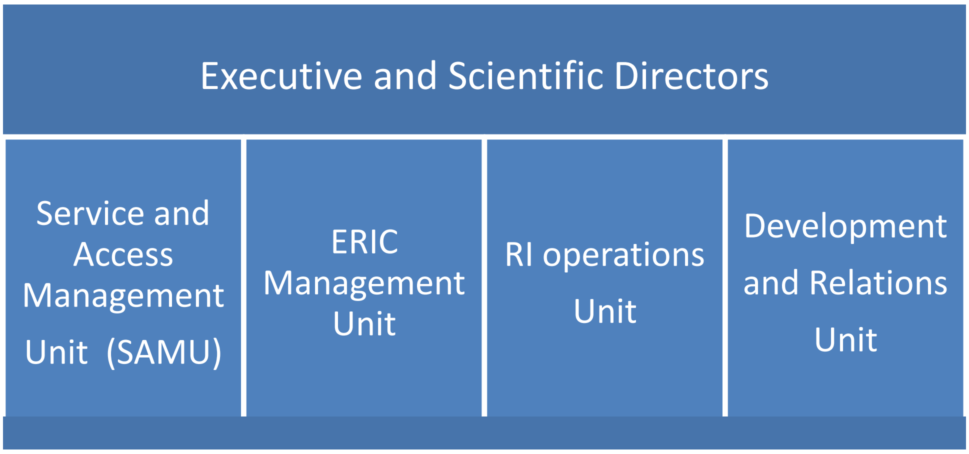

Figure 1. Proposed Units of the Head Office according to identified and needed functionalities.

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Service and Access Management Unit (SAMU) should be the single entry point for users requesting services. The SAMU shall optimize access to physical and technical services provided by ACTRIS Topical Centres and selected National Facilities.

ERIC Management Unit should manage the ACTRIS ERIC organisation tasks and runs all the day-to-day administrative tasks, such as administration, finances, legalities, and assessments of the RI performance. It should ensure that the RI is operating sustainably in terms of finances, RI operations follow the laws and regulations and established policies that are implemented in the RI.

RI Operations Unit should manage the internal operations of the RI, ensure the technical development of the RI and enhance the down streams the service provision. RI Operation Unit should work in close connection with Topical Centres and the National Facilities.

Development and Relations Unit should be in charge of strategic planning and strategy development for ACTRIS, building and maintaining national, European and international level liaisons and partnership with user communities, other RIs and programmes, countries, stakeholders (incl. innovation liaisons and service development), and supporting awareness rising of ACTRIS within scientific communities, industry and private sector, civil society and decision makers. This Unit shall take care of communication and dissemination activities with all the necessary tools and means.

The Directors lead the Head Office and ensure synergies among the Units and ACTRIS CFs and NFs.

The Figure 2 summaries the identified tasks and activities (functions) identified for the Head Office in the section 3 and their connections to the specific units.

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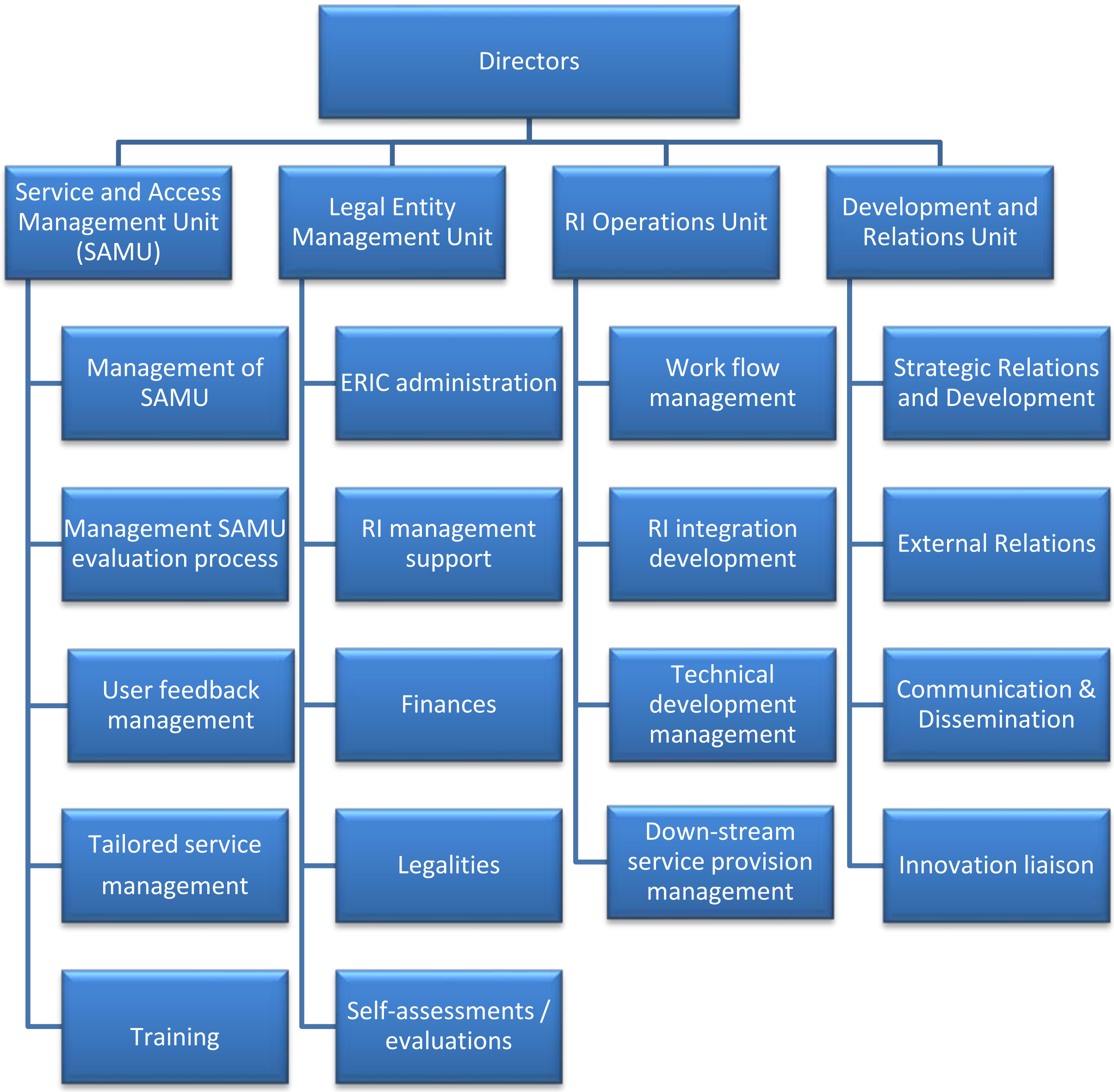

Figure 2. The identified functions of the units of Head Office.

5.2 Management body of the Head Office

Executive and Scientific Directors are leading the Head Office and the entire ACTRIS ERIC. The Directors shall have a HO Management body to support their work. The HO Management body shall include the Directors, the Heads of Units and the legal adviser of ACTRIS ERIC. The HO Management body shall have regular meetings to ensure the coherence of the HO work and that all the HO tasks are completed with available resources.

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5.3 Head Office linkages to NFs and other CFs

The role and linkages to the other ACTRIS CFs (Data Centre and Topical Centres) are integral part of the day-to-day work of the Head Office as it shall coordinate, oversee and support all the ACTRIS internal activities and access and service management of ACTRIS. In the section 3 and 4 the interlinkages between HO and other CFs and NFs are described.

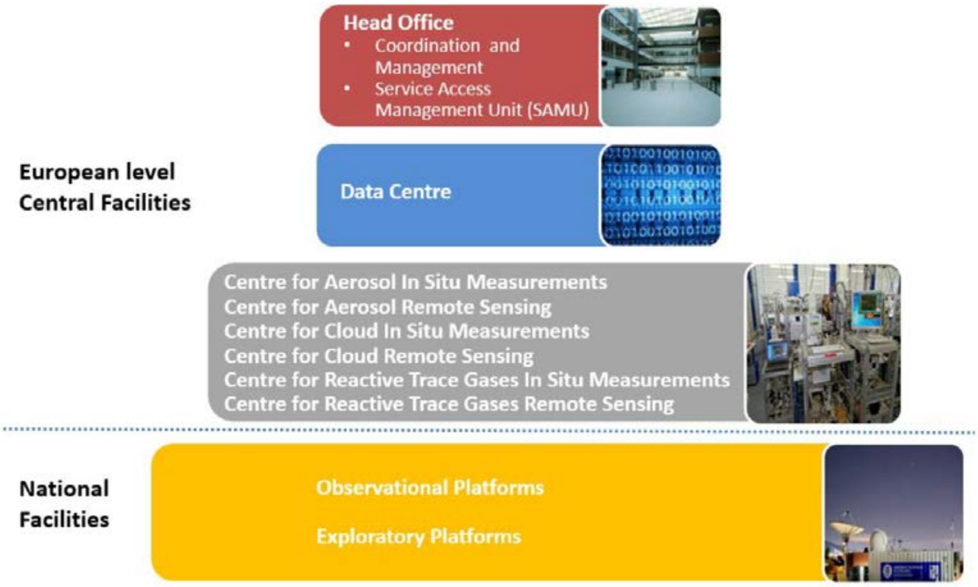

Figure 3. The structure of ACTRIS. Head Office coordinate all the ACTRIS activities.

5.4 Head Office link to ACTRIS ERIC governance

The ACTRIS governance framework for the legal entity 2021 onwards is presented in Figure 4. The legal entity of ACTRIS shall include the following bodies: the General Assembly, Science and Innovation Advisory Board, Ethical Advisory Board, Financial Committee, and Executive Director (as a legal representative of ACTRIS ERIC) and Scientific Director, Board of Directors (depending of the whether other CF directors are part of ACTRIS ERIC) and supported by the ACTRIS Research Infrastructure Committee, and National Facilities Assembly. Also, the engagement with the user community shall be done in the form of Science and User Forum. The role of the different governance bodies are mainly related to decision making (GA), advising and support in decision making and implementation of the decisions. To ensure the execution of the decisions and obtaining timely advises, the Head Office shall facilitate the communication with different bodies by having a contact point to each external body (Table 1).

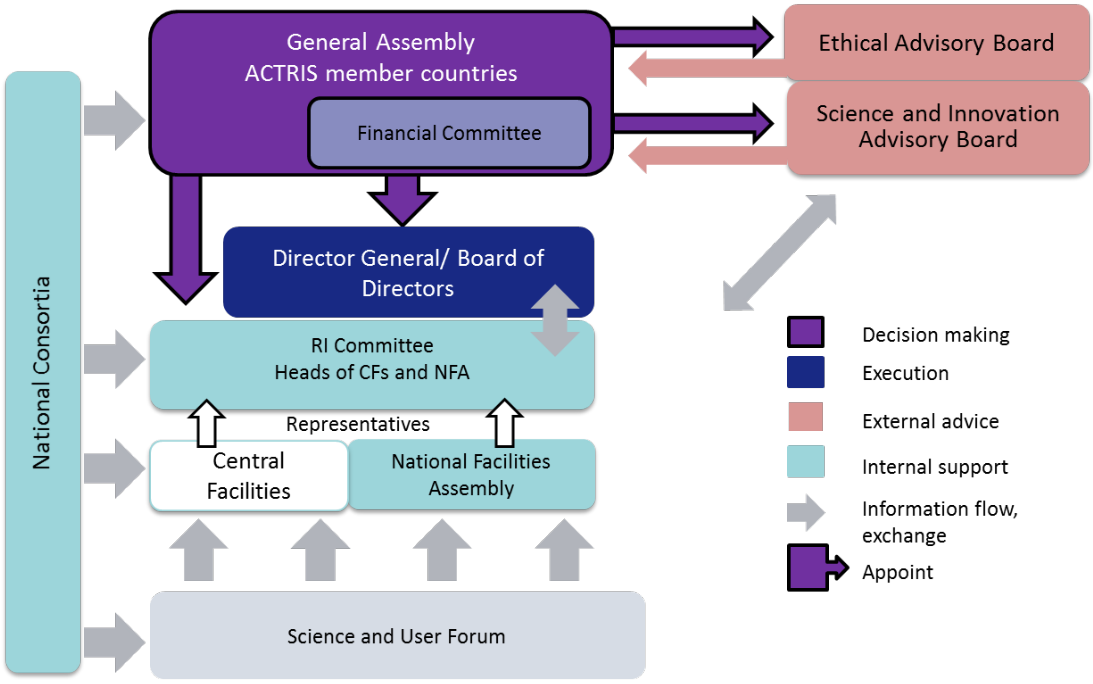

Figure 4. Plan for the ACTRIS governance framework 2021 onwards when ACTRIS ERIC is expected to be in place. General Assembly consists of the representatives of the ACTRIS ERIC member and observer countries and is the highest decision making body of the ACTRIS ERIC, but it also decides on the strategic issues of the whole research infrastructure. Executive Director of ACTRIS ERIC has the executive power and the legal representation. Scientific Director is in charge the scientific liaisons and development of ACTRIS strategy. Depending on whether the other CF directors are part of ACTRIS ERIC, ACTRIS ERIC can have can have a Board of Directors to implement the GA decisions. HO support the work of the ACTRIS ERIC bodies.

Table 1. ACTRIS ERIC external bodies and their roles, and contact point in Head Office.

GOVERNANCE BODY	ROLE	CONTACT POINT IN HEAD OFFICE
GENERAL ASSEMBLY (GA)	Decides the overall direction and supervision of ACTRIS Decides the strategic orientation of the RI, structure and budget of the ACTRIS legal entity, and termination of ACTRIS	Executive Director and Scientific Director (+ Board of Directors)
FINANCIAL COMMITTEE	Gives advice on financial matters related with the management and administration of ACTRIS	Executive Director

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		with Head of Management Unit
SCIENCE AND INNOVATION ADVISORY BOARD (SIAB)	Gives advises on topics related to science, innovation and management Gives feedback and make recommendations to develop ACTRIS research infrastructure activities Monitors the scientific and operative quality of the ACTRIS research infrastructure	Scientific Director with Head of Development and relations
NATIONAL CONSORTIA	Coordinate and implement national level ACTRIS operations	Head of RI Operation with Head of Management Unit
SCIENCE AND USER FORUM	Gives consultation about the science and technology development and future needs and directions via virtual and physical activities	Scientific Director with Head of SAMU and Head of Development and Relations Unit
RI COMMITTEE	Gives consultation (when requested) to matters related to the ACTRIS research infrastructure operations to ensure consistency, coherence and sustainability of the operations of the research infrastructure	Executive Director and Scientific Director (+ Board of Directors) with Head of RI Operations Unit
ETHICAL ADVISORY BOARD	Gives advice on issues such as research ethics, data integrity, code of conduct, conflict of interest, equality, representation Give its recommendations to the General Assembly when needed	Executive Director and Scientific Director with Head of Management Unit

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6 Requirements for the Head Office

6.1 General requirements

In order to be labelled as Head Office, the HO applicant shall:

- Commit for long-term operation, at least 5-10 years starting with the next year after the implementation of the legal entity,
- Set-up an appropriate structure of Units, to ensure an adequate functionality of the HO, cost-effective operation, and scalability with respect to the user demands and advancement of the state-of-the art methodology,
- Demonstrate the capacity (in terms of material and personnel resources), to ensure the provision of the needed services and organisational support, as described in section 3.
- Provide a feasible implementation and operation plan for the first five years, starting with the next year after the selection as Head Office and seat of the legal entity,
- Commit to provide a minimum amount of support for users, as described in Section 3 and 4.
- Commit to provide the organisational support, as described in Section 3.

6.2 Technical requirements

6.2.1 Facilities

For the operation of HO there no need of specific facilities besides the adequate office space, meeting rooms and efficient network connections, telecommunication and regular office tools, as well as back office services (IT support/Office management), and adequate administrative support tools .

6.2.2 Human resources

The Head Office shall have staff with strong expertise in managing large research infrastructures and disseminating its impact and interacting with and attracting users. For the full operative phase the personnel need is estimated to be for the Head Office 14 FTE; 2 FTE for directors and 3 FTE for each HO Unit (in total 12 FTE). The Table 2 identifies the required skills and expected experience of the HO staff. In addition to the required skills and expected experience, there are certain transversal skills required from all HO staff, such as HO staff shall have experience in working in the international environment, experience on coordination, have excellent communication skills and good management skills.

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Table 2. Foreseen staff profiles and capacity for the Head Office in its operative phase.

	PMs per year (fully operational phase, 2025	Skill level, general task description	Experience in years
Executive Director	12	Qualified senior management professional in executive role, solid experience in successfully leading organizations and/or distributed networks, esp. in the field of distributed RIs in nature of natural sciences, minor emphasis on science	>10
Scientific Director	12	Qualified and merited senior scientist in the field of ACTRIS, also understanding on managerial issues of RIs but with less emphasis.	>10
Head of SAMU	12	Qualified senior management specialist, with scientific background as well as experience in the organization of processes, management of teams, access and services. Lead the management of access services and evaluation processes	> 5
Officer (access management, evaluations)	12	Qualified officer with background in administration & management, organizational skills, experience in monitoring, access and services provision	>3
Officer (user feedback, user needs, training)	12	Qualified officer with background in administration & management, organizational skills, experience in monitoring, access and services provision	>3
Assistant (SAMU)	1.2	Back office assistant, support for SAMU, Assistant with background in administration & management as well as	>3

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		organizational, monitoring and communication (social media) skills	
Head of MGT Unit	12	Qualified senior management specialist on RI and organizational matters; responsible for the day-to-day management of the legal entity. Contributes to the financial tasks of HO	>5
Officer (legal)	3	Senior lawyer, knowledge on constitutional, employment and tax issues of the seat country laws, regulations and rules; can be outsourced	>5
Officer (financial)	6	Financial professional experienced with the budgetary issues and account management, works together with Head MGT	>5
Officer (self-assessment and evaluations)	6	Experienced in quality management, monitor and collect information on KPIs and organizes the evaluations and draft the assessment reports	>5
Assistant	12	Back office assistant, support for the directors, professional administrative management skills	>3
Head of RI Operations	12	Qualified senior RI operations specialist understanding the work flows and interlinkages between RI components and RI operations, is familiar with distributed RIs and technological requirements in ACTRIS. Lead the work on optimizing the RI operations and ensures the integrations of operations.	>5

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Officer (integration)	6	System engineering and data management skills, knowledge of the field of ACTRIS and operative services	>5
Officer (workflow)	12	Experience on system engineering, management of workflows, knowledge of the field of ACTRIS	>5
Officer (tech development, downstream activities)	6	Experience on technical development and industry collaboration & technology transfer, knowledge of the field of ACTRIS	>5
Head of Development and Relations Unit	12	Experience in strategic planning and liaisons and public relations, holds a degree in Earth /environmental sciences. Have skills in foresight activities and development processes, knowledge of the field of ACTRIS	>5
Officer communications	12	Experience in communications and PR, experience in outreach and dissemination activities	>5
Officer (innovations)	6	Experience in private sector collaboration, technology transfer and marketing	>5

6.2.3 Other requirements

The Head Office shall have task to organise the following issues for the whole ACTRIS ERIC:

- The ACTRIS ERIC needs to take the insurance for the ACTRIS ERIC legal entity in all those countries where it is operating.
- The ACTRIS ERIC needs to organize the payroll and financial system in all those countries where it is operating.
- The ACTRIS ERIC requires legal advice in all the countries where it is operating, the main work load being in the country of the legal seat.

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7 Basic criteria for the selection of the Head Office

The applications to host the Head Office are evaluated against a set of criteria covering:

- Ability and readiness to manage and **host the legal entity**
- The **level of commitment** for long-term operation
- The **capacity** to provide the organisational support and the services described in sections 3 and 4.
  - The availability of the necessary facilities and management tools
  - The availability for recruiting the needed human resources (FTE, expertise)
- The **efficiency** in providing the organisational support and the services
  - The feasibility of the implementation plan (costs, resources, timeline)
  - The feasibility of the operation plan (methodology, costs of activities)
- The level of maturity
  - Status of the development of the Units
  - Adequacy of the organisational structure and management
  - Risk management strategy

These criteria will be detailed in the associated call documents.

8 Obligations of the Head Office

8.1 General obligations

The Head Office shall be responsible for establishing and improving the Quality Management System for the ACTRIS. This task will include organising self-assessments and consultation, monitoring KPIs and risks, providing guidance on quality management to the CFs and NFs, employ benchmarking and best practices to support planning and development of quality management.

The following general obligations shall apply to the Head Office while operational:

- To organize its activities in a cost-efficient way, timely, and with high quality,
- To actively participate in the governance and sustainable development of ACTRIS,
- To manage the access of users to ACTRIS services, according to the access policy, availability of time, and material resources,
- To provide organisational support to ACTRIS CF and NF, according to the identified needs, agreed schedules, and procedures,
- To manage ACTRIS document management and archiving systems
- To implement efficient user interaction activities by:
  - Organizing workshops, to interact with the users (User Forum),
  - Collecting user feedbacks,
  - Maintaining the ACTRIS website,
- To document its activities, services and access provided, key performance indicators, and finances

- To collect and document from the whole ACTRIS level the key performance indicators and impacts, and provide this information to the General Assembly and European Commission,
    - To contribute to minimize and assess the uncertainties related to data and data products, according to their role and in collaboration with each other.

The HO is responsible for managing and developing a system where the Pan-European level performance indicators (KPIs) of ACTRIS are collected, analysed and reported to the IAC as part of the Quality Management System with the aim to reduce costs, improve the quality of the RI, measure effectiveness of training activities and improve timing and productivity of operations. These RI level KPIs are to be selected by the ACTRIS ERIC executive in consultation with the RI Committee (or any working group dedicated to this), and finally decided by the General Assembly.

8.2 More specific obligations

8.2.1 .Obligations to the General Assembly and other governance bodies

The Head Office acts as a secretariat for the General Assembly involving all duties related to organising and preparing its meetings, meeting documentation and decision minutes and follow-up. Regular annual legal tasks include e.g. annual accounting process of the legal entity. The Head Office supports the Executive in its work towards the General Assembly.

- preparing all documents regarding the legal entity: budget, long term financial plan, work plan (legally binding)
- giving an overview of the RI level work plan and budget and financial information (not legally binding on those parts that are not part of the legal entity)

The HO also supports other bodies:

- Scientific and Innovation advisory board,
- ethical advisory board,
- RI Committee

More detailed description of the facilitation of the ACTRIS ERIC governance bodies are given in section 3.

8.2.2 Obligations towards the ACTRIS National Facilities and Central Facilities

Technical obligations of the Head Office refer to the management, and different governance related tools, standard information collection tools and reporting tools. E.g., the HO shall be responsible for organizing the system where the CFs can directly report their annual activities, performance indicators, finances and risks.

For those CFs that are part of the legal entity:

- All legal responsibilities regarding financing, staff payroll, insurances

For all CFs:

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- Collection of annual work plans and reports and financial plans and financial reports from each Central Facility.
- Allocation of the budget according to the General Assembly decision and financial rules to each CF.
- Providing information on national ACTRIS developments to the CFs to enable the planning of work and resources.
- Collection of KPIs from CFs
- Overseeing the ethical issues, IPR

For CF and NF:

- Managing the access process and interaction with the NF and CF (capacity/feasibility check, organise calls, evaluation, selection, implementing the user access, reporting) for the CF and NF services (SAMU)

SAMU and the Data Centre shall establish a specific link so that the ACTRIS single access point also points to all services at the Data Centre.

Head Office should organize knowledge transfer and training sessions with the CFs and NFs to support the implementation of guidelines, procedures, and quality control of the management. Head Office should strengthen the involvement of industry using specific training for RI users, including industry users.

The Head Office provides support for sustainability, information distribution, outreach and promotion of the NFs. It collects NF annual reports and work plans and manages of the labelling process during the implementation, and applications for new ACTRIS NF. The Head Office is promoting strengthening the fund raising on the national level and sustains national contact person communication.

8.2.3 Technical obligations towards the ACTRIS users

SAMU shall be the main and unique interface between the ACTRIS users and all services offered by the ACTRIS CF and NF. It shall maintain and advertise the ACTRIS service portfolio, promote and inform the users on the opportunities for access, communicate with and support users for any needs and requests, coordinate the access and review process, disseminate the access output and provide access to results and publications, and collect the user feedback.

SAMU shall commit to provide a minimum amount of user services as described in section 4.

- o Definition of the user strategy and common protocols for user access; ACTRIS User web tool/virtual platform, service and access management…
- o Science conferences, access to the RI (SAMU) for conducting excellent research, training, education, fostering new activities/projects,

The Head Office organizes the Science and User Forum interactive platform and also organizes science conferences.

SAMU has the following obligations towards users:

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- to implement clear, simple and fair access procedures
- to familiarize users with these procedures
- to promote and duly inform users on access opportunities selecting the most appropriate communication channel or medium
- to plan, schedule, organize and manage the peer review process
- to promote measures to facilitate the smooth operations during the access
- to make every possible effort to solve any issue that may arise during the review process and/or the access

8.3 Evaluation of the activity of the Head Office

In general, the performance of the Head Office is measured by the success in maintaining the sustainability of the ACTRIS, which is the strategically the main objective of the Head Office. (The sustainability criteria are: scientific excellence, successful user strategy, efficient governance and management (incl. human resources), financial sustainability, technological development and upgrading of the RI, innovation, data management, measuring the socio-economic impacts, and accounting for risks).

The performance indicators for the HO are connected to the core mission of the HO and they can be grouped in to the following points.

- Quality Management
- Human Resources
- Community building, visibility (leading to socio economic impact)
- Cost efficiency
- Success of the training
- Success of the user strategy (SAMU)

Once established and operational, the Head Office shall be annually evaluated for its performances against a set of KPIs that will be revised by the executive of the ACTRIS ERIC and finally decided by the General Assembly. It has to be remembered that the HO in part of the ERIC and it is responsible for providing performance indicators for the whole RI. The basic task of the HO is to ensure the sustainability of the whole RI and the KPIs have to reflect the main objectives. Some of the KPIs mentioned in Table 3 are not only on the responsibility of the Head Office, but will be candidates for the indicators of the whole RI.

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Table 3. KPIs against which the HO will be annually evaluated, taking into consideration general and technical obligations.

Index	Comment	Source of information	Type of data	Frequency
Quality Management				
Number of countries and international organizations that are Members or Observers of ACTRIS ERIC		HO	numerical	yearly
Ratio of number of governance bodies established and planned or needed according the statutes of ACTRIS ERIC	Monitored by the end of the Implementation Phase	HO	numerical	yearly
Number of new released standards, guidelines, policies as outcomes of the ACTRIS ERIC governance, Working Groups or Head Office	Includes internal rules and procedures, terms of references approved by the executive, published policies and strategies approved by the General Assembly, published quality criteria of the RI operations	HO	numerical	yearly
Number of Central Facilities that filled out the quality self-assessment survey	Reflects the success of the QM process and motivation	HO and CFs	numerical	yearly
Number of dissemination events (both physical or online – trainings, webinars, etc.) related to QM		HO	numerical	yearly
Number of MoUs ACTRIS ERIC has signed with other research infrastructures and organisations		HO	numerical	yearly

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Human resources				
Proportion of ACTRIS ERIC personnel recruited from 100% needs evaluated in concept(s)	Monitored by the end of the Implementation Phase	HO	percentage	yearly
Staff satisfaction of the ACTRIS ERIC	work place questionnaire	HO	semi-quantitative	every second year
Number of projects focused on mobility (such as COST), involving ACTRIS ERIC or at least National or Central Facilities from two ACTRIS ERIC members or observers		HO and CFs	numerical	yearly
Number and nature of activities taken specifically in order to improve the gender equality in ACTRIS ERIC and the whole ACTRIS	Can include e.g. approval of the Gender Equality Plan by the General Assembly, training events and consultations	HO and CFs	semi-quantitative	yearly
Community building, visibility				
Number of visit of ACTRIS web pages		HO	numerical	
Number of press release		HO and CFs and NFs	numerical	yearly
Number of presentations given at international events on ACTRIS/relating to ACTRIS/using ACTRIS data		HO and CFs and NFs	numerical	yearly
Number of commented recommendations, guidance documents, directives, such as WMO, Council of Europe, OECD,	Related to policy relevance and policy impact	HO and CFs	numerical	yearly

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IPCC, etc. on behalf of ACTRIS				
Number of subscribers in the e-newsletter or website		HO	numerical	yearly
Financial success				
Deviation from the annual ERIC/HO budget (??)		HO	numerical	yearly
Proportion of external sources to overall budget of ACTRIS ERIC such as H2020 projects, etc., not included the ERIC core budget		HO	percentage	yearly
Success of the training				
Number of applications (or participants) to training, education and experience sharing events related to SAMU/RI services	Need to measure what is the impact of the training, how many deems it useful and come back to ACTRIS, see Success of user strategy	HO	numerical	yearly
Applications to HO or HO/SAMU training events		HO	numerical	yearly
Success of the user strategy				
Number of *services provided (made available for the users) by the ACTRIS ERIC on Pan-European level. *Each service must be declared as a service and must be clearly defined,		HO	numerical	yearly

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also in terms of its target user group(s)				
Number of recognized individual users using services	Data collected per service, user groups, and aggregated across all the services	HO	numerical	half-yearly
Ratio between SAMU requests accomplished and reported, and total number of SAMU requests		HO	numerical	yearly
Number of members participating in the User Forum activities (representing various types of users and stakeholders)		HO	numerical	yearly
User satisfaction	Questionnaires related to user satisfaction should be attached to all user reports	HO	semi-quantitative	yearly

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9 Glossary

ACTRIS data - are the ACTRIS variables resulting from measurements that fully comply with the standard operating procedures (SOP), measurement recommendations, and quality guidelines established within ACTRIS.

- **ACTRIS level 0 data:** Raw sensor output, either mV or physical units. Native resolution, metadata necessary for next level.
- **ACTRIS level 1 data:** Calibrated and quality assured data with minimum level of quality control.
- **ACTRIS level 2 data:** Approved and fully quality controlled ACTRIS data product or geophysical variable.
- **ACTRIS level 3 data:** Elaborated ACTRIS data products derived by post-processing of ACTRIS Level 0 -1 -2 data, and data from other sources. The data can be gridded or not.
- **ACTRIS syntheses product** (*Proper name to be defined later*)**:** Data product from e.g. research activities**,** not under direct ACTRIS responsibility, but ACTRIS offer repository and access.

ACTRIS Data Centre (DC) - the Central Facility responsible for ACTRIS data curation, preservation, and distribution of data, value-added products and tools**,** and hosting the ACTRIS data portal.

ACTRIS data originator - entity operating instruments at a National Facility or Topical Centre, resulting in ACTRIS data and delivering ACTRIS data to the Data Centre.

ACTRIS data provider - the Data Centre offering the ACTRIS data and value-added data products and tools to users.

ACTRIS digital tools and services - tailored codes and software for processing and visualization of ACTRIS data, production of ACTRIS data products, and for data analysis and research.

ACTRIS exploratory platform - National Facility (simulation chambers, laboratories, or mobile facilities) operating on campaign basis and delivering dedicated data to the Data Centre.

ACTRIS General Assembly (GA) - a council of ministry- and funding organization representatives of ACTRIS members after ACTRIS legal entity has been established, superior decision-making body of ACTRIS.

ACTRIS Head Office (HO) - a Central Facility coordinating and representing ACTRIS, and holding the statutory seat.

ACTRIS label - earmarks a data set or a measurement site as ACTRIS data or ACTRIS National Facility.

ACTRIS observational platform – ACTRIS National Facility performing long-term, regular observations and delivering standardized data to the Data Centre.

ACTRIS Topical Centres (TCs) – a Central Facility offering services and operation support for QA/QC of measurements and data (including training, calibration, QA/QC tools, and development of standard operation and evaluation procedures)

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ACTRIS variables - the measured atmospheric variables as described in the ACTRIS Data Management Plan[1].

Central Facility (CF) - a European level ACTRIS component that offers ACTRIS data or other ACTRIS services to users as well as operation support to ACTRIS National Facilities.

Central Facility Unit – part of a Central Facility located at, and operated by a research performing organization (RPO) or by ACTRIS ERIC.

CF Director – the person responsible for the coordination and representation of a Central Facility.

CF Unit Head – the person responsible for the coordination and representation of a Central Facility unit.

CF Management Board – consists of the CF Unit Heads and the CF Director; this board manages the Central Facility.

Data curation - the activity that stores, manages and ensures access to all persistent data sets produced within the infrastructure.

Data traceability - an unbroken chain of uniquely identified process steps leading from raw data to any kind of processed data, where identification of process steps follows the data.

In situ measurements - measured or sampled air and instrument are at the same location and in physical contact. In the context of ACTRIS, in situ measurements of aerosol, cloud, and reactive-trace-gas properties are performed at observational sites near the Earth surface, on mobile surface-based or airborne platforms, and in atmospheric simulation chambers and laboratories.

Interim ACTRIS Council - a council of ministry- and funding organization representatives of ACTRIS members before ACTRIS legal entity has been established (during the ACTRIS Preparation and Transition Phase), superior decision-making body of ACTRIS.

Measurement traceability - an unbroken chain of comparisons relating an instrument's measurements to a known standard, in the ideal case SI units.

National Facility (NF) - an observational or exploratory platform providing data and/or physical access to the platform within ACTRIS.

Quality assurance and control: Quality assurance is process oriented and focuses on defect prevention; quality control is product oriented and focuses on defect identification:

- **Quality Assurance (QA):** The process or set of processes used to ensure the quality of a product (e.g. data series, instrument, sample, measured value of a variable, etc.),
- **Quality Control (QC):** The process and activities of ensuring products and services meet the expectations.

[1] The ACTRIS data management plan and list of variables were approved by ACTRIS-2 scientific steering committee, October 2015. These documents are expected to be refined during ACTRIS-PPP (WP5).

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Remote sensing - measured air and instrument are not at the same location and not in physical contact. In the context of ACTRIS, active and passive atmospheric remote-sensing techniques for the observation of aerosols, clouds, and trace gases are applied at observational sites and on mobile surface-based or airborne platforms.

RI committee – consists of up to two representatives from each Central Facility and [three] representatives from the National Facilities Assembly; the RI committee supports the (Interim) Director or Board of Directors in operating the RI.

Service and Access Management Unit (SAMU) - a part of ACTRIS Head Office facilitating the access to ACTRIS services.

User - a person, a team, or an institution making use of ACTRIS data or other ACTRIS services, including access to ACTRIS facilities.

10 Reference documents

ACTRIS PPP materials:

D1.1. Governance and Management structure

D2.1. Legal Entity Analysis

D 9.1 Communication and Dissemination Strategy

ACTRIS Central Facility Baseline document

Interim ACTRIS Council materials:

ACTRIS_IAC_03_04a_Concept and Services.pdf

ACTRIS_IAC_03_07a_Central Facility Descriptions.pdf

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Section 2

Concept of ACTRIS Data Centre

ACTRIS PPP WP 4 task 4.1

22.2.2018

Public

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1 Purpose of the document

This document describes the relevance, mission, requirements and obligations of the ACTRIS Data Centre.

2 Description and role of the ACTRIS Data Centre

2.1 Framework

The ACTRIS Data Centre (ACTRIS DC) is the Central Facility responsible for ACTRIS data curation[1], preservation, and distribution of data, value-added products and digital tools.

ACTRIS data are ACTRIS variables resulting from measurements that fully comply with the standard operating procedures (SOP), measurement recommendations, and quality guidelines established within ACTRIS under the responsibility of the Topical Centres (TCs). The following documents describe the complete concept within which the ACTRIS DC is embedded:

- **The ACTRIS framework** is described in the following documents:
    - ACTRIS ESFRI proposal
    - ACTRIS-PPP project
    - ACTRIS Stakeholder Handbook
    - ACTRIS Science Case document
- **The general rules and principles for the ACTRIS Central Facilities** are described in the Baseline document for the Concepts of ACTRIS Central Facilities.
- **The measurements techniques operated by the ACTRIS National Facilities** for which the data curation and access should be offered:
    - Technical concepts and requirements for ACTRIS Observational Platforms
    - Technical concepts and requirements for ACTRIS Exploratory Platforms

All ACTRIS measurement variables provided by the ACTRIS Observational Platforms are listed in Annex 1, associated with relevant information regarding methodologies, and other information. This is more than 150 variables, all produced through a data flow chain from level 0 to level 2. ACTRIS Level 3 are elaborated ACTRIS data products derived by post-processing of ACTRIS Level 0 -1 -2 data, and possibly data from other sources such as models, satellite observations or complementary data bases. A tentative list of ACTRIS Level 3 data offered by ACTRIS DC is included in annex II. The ACTRIS data levels are described in Figure 1.

[1] Data curation is defined in the Glossary at page 52

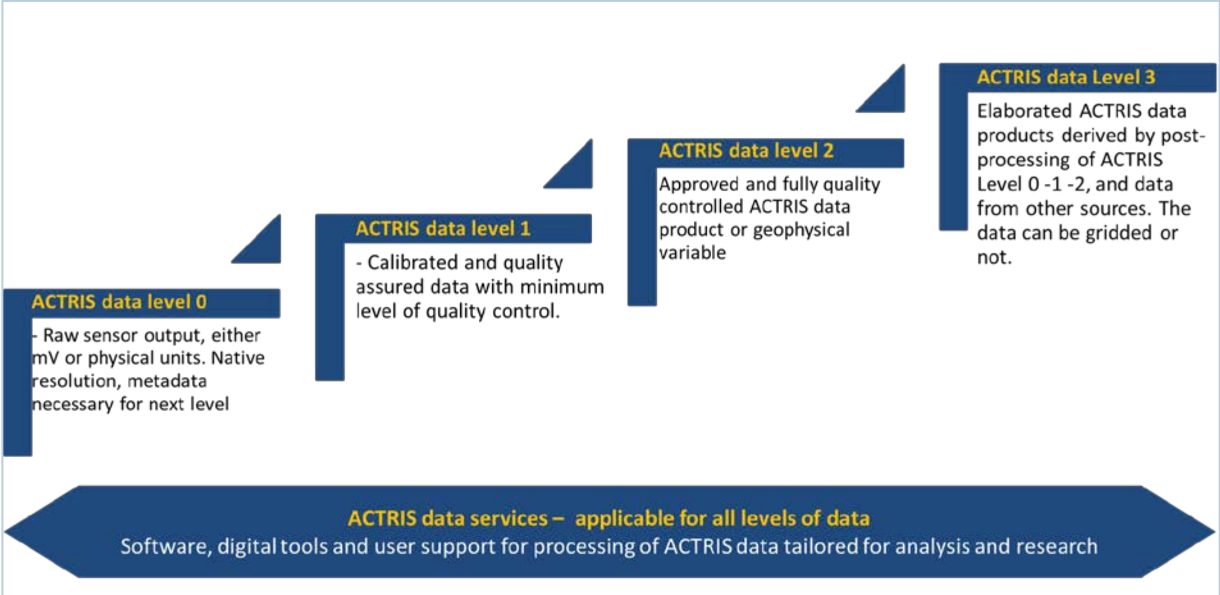

Figure 1: Definition of ACTRIS data levels applicable to all variables. ACTRIS digital tools can apply to all levels.

2.2 Scientific relevance, main tasks and structure of the data centre

The role and tasks of the ACTRIS Data Centre are multi-fold as the DC will offer a wide suite of services related to ACTRIS data, data products, and digital tools. These must include:

- Long-term archiving and preservation of ACTRIS level 1 to level 3 data and data products,
- Access to ACTRIS data, data products, and digital tools through a single point of entry, the ACTRIS data user interface
- Documentation of data, data flow, citation service, and data attribution, including version control, data traceability, and interoperability,
- Data curation and support for campaigns and dedicated research projects and initiatives, external or internal to ACTRIS.

To meet the needs of NFs, TCs and users of ACTRIS data, ACTRIS DC will offer 5 mandatory core data services:

I. **Data Curation**

ACTRIS DC must offer repositories and long term archive and preservation of ACTRIS data and data products.

II. **Access to level 0 – level 3 data**

ACTRIS DC must offer access to data, data products and digital tools through a single entry point, the ACTRIS Data Centre web interface.

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III. Documentation

ACTRIS DC must offer documentation of data through meta data, data flow, citation service (Digital object identifier) and data attribution.

IV. Data products and digital tools

ACTRIS DC must produce advanced data products and implement data production tools for advanced data products.

V. User community support and services

ACTRIS DC must offer training, help desk, tutorials, for data producers and users, including support to regional and global networks

The numerous measurement methodologies applied within ACTRIS (described in *"Technical concepts and requirements for ACTRIS Observational Platforms"*[2]*),* and listed in Annex I, result in a considerable diversity of data collected; ACTRIS provides advanced data and data products requiring a complex and well described data curation system. In accordance with these requirements, the ACTRIS Data Centre is foreseen to consist of a set of data centre units, each meeting the specific requirements and needs for the diversity of the remote and in situ data, about 50 atmospheric variables, where the trace gases are grouped. Counting all different traces gases, the numbers of variables and components is more than 150 in total, excluding auxiliary data. Annex I includes the ACTRIS variables from observational platforms associated with the measurement methodologies within ACTRIS. Additionally, ACTRIS level 3 products are offered, listed in Annex II.

For an ACTRIS DC consisting of a set of units, each ACTRIS topical DC unit must be responsible for the data curation of the their specific subset of data, and linked to the corresponding topic centre (TC) with clearly defined roles to facilitate efficient work flow, and to ensure adequate and complementary competence and required quality at all levels of the data flow. Independent of any DC units, all ACTRIS level 1-2-3 data are required to be available and accessible through a single entry point, the ACTRIS Data Centre web interface. Figure 2 is a schematic diagram displaying the potential architecture of the ACTRIS Data Centre, with the requisite links and interactions with TCs and NFs. The structure and architecture proposed is based on more than 15 years of experience with curation of ACTRIS datatypes through a list of EU projects (ACTRIS-2, ACTRIS-FP7, EUSAAR, CREATE, EARLINET, EARLINET-ASOS, CLOUDNET, EUROCHAMP, etc.) and also within EMEP, GAW-WDCA, GAW-WDCRG.

[2] Refer to Deliverable *D5.1: Documentation on technical concepts and requirements for ACTRIS Observational Platforms.*

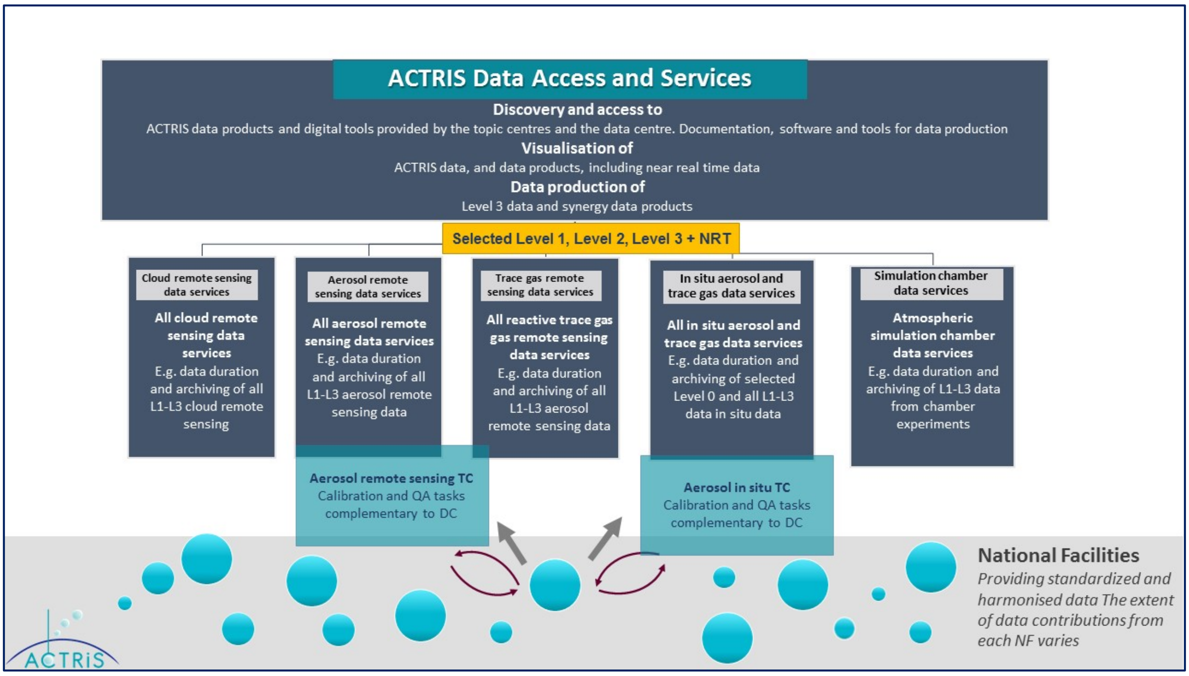

Figure 2: Schematic diagram of a potential architecture of the ACTRIS Data Centre, with examples of proper interactions between the TC and NF. The blue circles illustrate the NFs of various extent. There may be multiple access interface and levels depending on the need.

As indicated in Figure 2, the blue circles are symbols for NFs. Depending on the observational components included at the NF (see the general Principle #1 in "*D5.1: Documentation on technical concepts and requirements for ACTRIS Observational Platforms*") NFs must interact with the various components of- the DC, and submit data, and also interact with various required TCs, before data submission.

In case of distributed data nodes, each topical DC node requires an interface to the overarching ACTRIS Data Centre user interface, where all Level 2 and level 3 data will be identifiable and accessible, together with level 1 data (e.g. RRT data) when these are available, and relevant. This requires that data are documented by a comprehensive metadata throughout the whole data curation chain, where the metadata suite conforms to standards (e.g. ISO19115 and INSPIRE). The documentation includes references to standardized operation procedures, this requires close interactions and clearly defined workflows and procedures with the TCs.

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2.3 ACTRIS Data Centre mission

The mission of the ACTRIS Data Centre is to compile, archive and provide access to well documented and traceable ACTRIS measurement data and data products, including digital tools for visualisation, data analysis and research. As a tool for science, the highest priorities for the ACTRIS DC are to maintain and increase the availability of ACTRIS data and data products relevant to climate and air quality research for all interested users. National and international climate and air quality assessments for National and International Environmental agencies are also based on ACTRIS data and are the ultimate user of ACTRIS data and data products. Additionally, the data centre shall provide training and customized services including tools, tutorials, documentation for the NFs and ACTRIS data originators.

3 Data service support provided to ACTRIS National Facilities

The ACTRIS Data Centre is required to provide operation support to NFs in form of procedures, tools and data production, data quality assurance, data quality control, and data curation. The operation support related to data production and quality control follows predefined and standardized procedures and tools developed by ACTRIS DC in close collaboration with TCs. ACTRIS DC will offer training for each NF related to tasks such as data production, quality control tools meta data requirements, data submissions and data flow.

The operation support offered to NFs shall include the data resulting from measurement techniques described in technical centre concept documents, also listed in A*nnex I* for the various variables.

ACTRIS DC is obliged to put in place and offer to NFs the specific operation support marked with * in this document. Other operation support described in this document is not mandatory for the data centre, but is recommended or can be associated to access managed by SAMU and potentially a fee.

The operation support may be scheduled or on request. Participation in scheduled activities is mandatory for NFs. Measurements not following the mandatory actions are not considered as ACTRIS-conformant and do not yield ACTRIS data.

3.1 Required data curation services provided by the ACTRIS Data Centre

The ACTRIS DC is responsible for data curation of all ACTRIS variables; if the ACTRIS DC is distributed across a number of nodes, then each DC node is responsible for the curation of the associated subset of well-defined variables, so that the DC as a whole covers all ACTRIS variables. All data centre units responsible for data curation of ACTRIS data have to offer the following service for data curation of data from NF, both observational and exploratory platforms:

- Long-term sustainable archive for ACTRIS level 2 data provided by NFs with regular, frequent back up, at least weekly, ideally every night, dependent on data type, and described in the following sections,
- Organise and set up procedures for long-term archive of ACTRIS level 0 and selected level 1 data from the NFs with regular, back up

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- Back up of level 2 and level 3 data and data products to a different location,
- Development and implementation of data production tools (software and digital tools) for generating the required data levels,
- Implementation of data quality control tools and procedures developed in DC or TCs,
- Portal for standardised submission of data by NF operators to DC,
- Standardised sanity and consistency checks of data submitted through submission service,
- Development and maintenance of tools for quality control of data, including implementation of new quality assurance criteria defined by TCs,
- Tools for performing quality controls homogeneously at NF,
- Implementation of data flow for new instruments from NF to DC in collaboration with TCs.
- Automatic and centralized processing tools for achieving quality assured and real real time (RRT) data from observational NF platforms at network level.
- Data curation of data from the topical centres for internal use for documenting provenance and QA/QC, and for external users as reference data

3.1.1 Data curation service and tools for ACTRIS in situ aerosol, cloud, and trace gas data

All ACTRIS in situ[3] aerosol, cloud, and trace gas variables are listed in Annex 1, associated with their instrument type and potential for real-real-time (RRT) data. Measurements of atmospheric aerosol-, cloud and gas variables at ACTRIS NFs that represent the in situ conditions need to be organised in 2 groups: *online and offline observations*

- **Online observations**: Air stream enters the station or instrument enclosure through an inlet, and is led to the instrument itself. The measurement is conducted and reported by the instrument as the sample passes through the instrument. Instrument-side quality assurance measures consist of on- or off-site comparisons to standard instruments or primary standards. RRT data provision is possible
- **Offline observations**: Air stream enters the station or enclosure through an inlet, and is conducted to a sample medium. The sample medium either stores the whole sample, or extracts a part of the sample and stores it. The sample medium is transported to an analysis facility, where it also has been pre-treated before exposure. At the analysis facility, the sample undergoes the steps of preparation and analysis to yield actual variable. Quality assurance concerns the field side (field blanks) as well as the analysis side of the process (round-robin analysis). RRT data provision is not possible.

There might be combinations of these, where the offline analysis process has been streamlined enough to fit an online time schedule.

[3] See Glossary

The ACTRIS data levels are described in Figure 1. A more detailed description of data levels for in situ data is following, in agreement with the general description:

- **Level 0**: raw data as produced by the instrument, all main and instrument status parameters provided by instrument, brought to a common, well-defined data format. Discovery, use, provenance, and configuration metadata attached, including all information needed for further data production, as far as known at stations level (e.g. QC metadata). Content is instrument model specific, time resolution as native to the instrument, reference conditions of temperature and pressure conditions as provided by instrument.
- **Level 1**: Produced from level 0 data to contain the physical property to be observed, including measures of uncertainty. Instrument status parameters, QC measurements and invalid data removed, quality control and post-calibrations applied. Time resolution native to instrument. Content specific for measured property, standard conditions of temperature and pressure.
- **Level 2**: Produced from level 1 data to contain data averaged to a homogeneous time resolution, typically 1 h. Includes measure of atmospheric variability, content specific for measured property.

1.1.1.1 Data curation service of online ACTRIS in situ data

Data curation of online ACTRIS in situ data starts with the raw data stream coming from the instrument. Already at the station, the raw data stream is transcribed to a homogeneous level 0 format, and annotated with discovery, use, provenance, and configuration metadata. The level 0 data are uploaded to the ACTRIS DC at a real-real-time (RRT) schedule (latest 3 h after measurement) to facilitate rapid discovery of potential high/low episodes, detections of errors, and to provide RRT data for operational services.

Next in the data production flow, the data receives quality control (QC). Two QC options are foreseen:

1. **Automatic QC**: inspection of data by an algorithm for outliers, spikes, and automatically identifiable instrument malfunctions. The data are flagged accordingly. Automatic QC is typically applied for RRT data.
2. **Manual QC**: inspection of data by an identified person under the responsibility of the NF. The QC includes at least tests for outliers (with location-specific threshold values), spikes, episodes (e.g. atmospheric transport, local / regional contamination), instrument malfunctions, and verification of correctly applied instrument QC, e.g. calibrations. The data are flagged accordingly. Manual QC is applied at least at an annual frequency.

As a general rule in ACTRIS in situ data QC, only data subject to instrument malfunctions are flagged as invalid. Data with episodes are flagged as such, but not as invalid, to avoid limiting data use only to certain use cases. From this point in the data curation workflow, data level designations are to distinguish between data having received automatic QC or also undergone manual QC of the data.

The workflow for ACTRIS surface in situ data production offers an option for a review process during data QC. For this purpose, the level 0 data QCed by the NF are made available to a review process in a machine-to-machine interface, where the review process is administered by the responsible TC. The TC organises the review process and defines the review criteria. The DC assists in the process by providing a web-based issue tracker where the review process is traceably documented for each dataset by assigning QC tasks to the NF responsible for the dataset. Successful completion of the review process is documented in the QC metadata.

The QCed level 0 data are the basis for producing level 1 data. This production step includes calculation of the final physical property from raw signals, application of corrections and post-calibrations, measures of uncertainty, removal of periods with invalid or calibration data, and inclusion of metadata on instrument QA measures conducted by the TC, where the QA measure metadata is maintained by the TC.

The production step from data level 1 to data level 2 comprises averaging of the data to a common time resolution, usually hourly, where invalid data is disregarded in the averaging process, and episode flags occurring in the averaging period are copied to the average value. Also included are flags for data coverage during the averaging period, and measures of atmospheric variability during the averaging period.

Finally, level 2 data are inserted into the ACTRIS surface in situ data repository, and public and available to all users. Immediately before, data are subjected to a final QC, covering syntactic and semantic correctness of metadata, syntactic correctness of data, parameter dependent completeness of metadata, and completeness and correctness of framework associations. By inserting the data into the repository, the data are released and published in the release channels of the ACTRIS surface in situ repository (web-interface, data and metadata machine-to-machine interfaces) as well as the ACTRIS data user interface.

1.1.1.2 Data curation service of offline ACTRIS in situ data

For measurements using the offline workflow for ACTRIS surface in situ data, data production starts with the sample medium. At the NF central lab, the sample medium is pre-treated, i.e. prepared for being exposed. Depending on the requirements of the measurement method, pre-treatment may include pre-heating, impregnation, weighing-in, pre-cleaning, or other methods of conditioning. The pre-treatment is documented by a protocol, where the NF is responsible for correct documentation.

Following pre-treatment, the sample medium is exposed to air sample at the NFs field site. The step is documented by a protocol, including e.g. medium ID, exposure begin and end time, sample amount collected, exposure standard protocol ID, and others. The NF is responsible for correctly assembling this documentation.

After exposure and transporting the sample medium back to the NF's central lab, the sample medium is prepared for analysis. This step may comprise weighing-out, medium extraction, partitioning of sample medium, or other steps as required by the method. The corresponding protocol, assembled under the responsibility of the NF, may contain parameters like medium ID, preparation time, preparation protocol, numerical preparation results, or others.

Finally, the sample extracted from the sample medium is analysed at the NF. The pertaining protocol, assembled responsibly by the NF, contains parameters such as sample medium ID, extract ID, analysis, device type and ID, numerical analysis results, and others.

All protocols of sample medium and sample extract treatment generated in the workflow are stored in machine-readable form in a sample and analysis database. Operation of this database is to meet long-term archive standards, e.g. intervals of upgrading database hard- and software, and frequent schedule for on- and off-site backups.

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The NF is responsible for producing the final level 2 data product of the workflow by using the results of all 4 sample medium and sample extract treatment steps. Besides the concentration of the desired atmospheric property and standard level 2 metadata, the data product contains metadata such as sample medium and extract ID, standard procedures used, special condition flags, and others.

3.1.1.1 Data services and tools offered to NF for in situ data production and quality control

In order to improve data quality and assist the NF in data production, the ACTRIS surface in situ data centre unit have to offer services and data control tool, and development of required tools and procedure for data submission and production. The in situ data centre unit need to offer;

- Online portal for standardised submission of data by the NF operators to the in situ data centre unit,
- Check of meta data formats upon data submission
- Traceable documentation of data QC processes by review, accessible to NF, TC and DC
- File and meta data production tool
- Standardised sanity and consistency checks of data submitted through submission portal
- Software and digital tools for generating required data levels,
    - Development and implementation of data production tools (L0 – L1 – L2) for selected types of data
- Implementation of data quality control tools and procedures developed at the DC or TCs
- Development and maintenance of tools for quality control of data, including implementation of new quality assurance criteria defined by TCs,
- Tools for performing manual quality controls in a homogeneous way at the NF,
- For the RRT branch of the online ACTRIS surface in situ data workflow, a service for testing thresholds of incoming data and instrument parameters with connected e-mail alert service, facilitating early detection and mitigation of instrument problems at the ACTRIS NFs
- For the RRT branch of the online ACTRIS surface in situ data workflow, a service for testing physical consistency between observations (closure). The reports of this service are sent to the responsible NFs in scheduled intervals.

1.1.1.3 General Principles for ACTRIS in situ Data curation

The relation between the various data products, pre-products, and processing steps of both online and offline ACTRIS surface in situ data workflow is depicted in the corresponding workflow diagram (see Annex III). The details concerning implementation of these workflows for individual ACTRIS variables are specified in the pertaining, variable specific data management plan and implementation plan. This implementation plan describes the data and metadata items contained in each data level, data format used, the individual operations performed in each production step between data levels, as well as data and metadata items contained in each sample handling protocol (offline workflow). The content of the data management plan and implementation plans is determined by the responsible TC in collaboration with the in situ data centre unit.

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All data products, pre-products, and sample handling protocols, as well as all software and algorithms used in production steps, version controlled, archived following long-term archive standards, and identified in each version. Persons involved in manual data production steps are identified, as well as entity responsible for the production step. For establishing traceability, the data products and pre-products contain references to the identifiers of all (pre-)products, production tools, persons and entities involved in the whole production chain leading up to the (pre-)product.

To facilitate harmonised data products and quality, the ACTRIS DC is responsible for ensuring that all instances of a specific data production step operated in the ACTRIS network uses the same identified version at any given time. To the same end, the DC provides tools for conducting standardised manual data QC under the responsibility of the NFs. As a low-barrier tool, the surface in situ data centre unit offers a web-based data submission portal allowing interactive checks of data submissions, as well as conducting the submission upon successful check. The test include syntactic and semantic correctness and consistency of metadata and data, as well as standardised tests for outliers and spikes.

In the workflows, the TCs are responsible for QA of instruments and analysis methods in the network, and also responsible for specifying QC procedures conducted in the network, for data QC in collaboration with the surface in situ DC unit. Examples for instrument and analysis QA measures are on-site comparisons to a standard, centralised off-site comparisons, and laboratory round-robin exercises. Together with the responsible data centre unit, the TCs are responsible for specifying data and metadata items documenting these QA measures in a harmonised way. The TCs are also responsible for collecting the data and metadata items when conducting QA measures, and storing them in a QA result database in machine-readable form. From here, the QA measure results are joined with ACTRIS variable data during data production. Based on the generic data production workflows described above, the ACTRIS surface in situ DC node supports implementation of data workflows for new surface in situ variables as agreed by the consortium

3.1.1.2 Potential campaign service for ACTRIS in situ data

The data centre need to offer a service for campaigns at the NF sites. A general procedure needs to be offered for this through SAMU, described in section 4.7 on page 33.

3.1.2 Data curation service and tools of ACTRIS aerosol remote sensing data

All ACTRIS aerosol profile variables are listed in Annex I, associated with instrument type and potential for real-real-time (RRT) data. ACTRIS DC must provide support to the aerosol profile data originator for centralized data processing through the common standardized automatic analysis software developed in previous projects toward the ACTRIS RI, the Single Calculus Chain (SCC). The Single Calculus Chain (SCC) is an open source software for analysing aerosol LIDAR data to obtain aerosol optical property profiles from raw data. The SCC is an official EARLINET developed tool to accomplish the fundamental need of any coordinated LIDAR network to have an optimized and automatic tool providing high-quality aerosol property profiles. Main concepts at the base of the SCC are automatization and full traceability of quality-assured aerosol optical products.

Two other algorithms are also implemented in ACTRIS DC:

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- The AERONET-ACTRIS processing stream, which process the photometer data from ACTRIS European sites. It produces the radiances (almucantar, principal plane, polarized principal plane) and the aerosol optical depth. All this processing stream is fully controlled inside the ACTRIS RI.
- The GARRLiC (Generalized Aerosol Retrieval from Radiometer and Lidar Combined data), which simultaneously inverts coincident LIDAR and radiometer observations to retrieve aerosol optical and physical properties (profile and column).

The data curation workflows is suitable for the provision in RRT and RRT, following the same steps and procedures of the standard processing. RRT/RRT delivery of not fully quality assured data can be possible for stations if the steps for collecting, transferring and submitting data to the processing suite are fully automatized.

The ACTRIS data levels is described in Figure 1. A more detailed description of data levels for aerosol profile data is following, in agreement with the general description:

- **Level 0**: raw data as produced by the instrument, all main and instrument status parameters provided by instrument, brought to a common, well-defined data format. Discovery, use, provenance, and configuration metadata attached, including all information needed for further data production, as far as known at stations level (e.g. QC metadata). Time and temporal resolution as native to the instrument.
- **Level 1**: not fully quality controlled data. This level of data contains both pre-processed LIDAR data, i.e. a step in between the raw signal (Level 0 data stored at each station) and the optical properties, and optical properties themselves. At this level, some instrumental corrections are already implemented and annotated into the data for both pre-processed data and optical properties. The instrumental corrections are based on the inputs reported in an agreed machine readable format by the TC and provided to DC.
- **Level 2**: fully quality controlled data generated from Level 1 data. At this level, all QC are completed and fully reported into the data. Instrumental corrections and annotation are completed: quality assurance of the instrument is complete based on scheduled intercomparison and check-up of the instruments. On the other hand the feedback mechanism of QC could suggest further specific instrumental check, on which basis new technical annotations/corrections were needed and annotated in this fully QC data level. Fully QC aerosol optical properties are reported as well in this level: for these products Level 2 pre-processed data are used and the needed inputs in terms of atmospheric density and temperature if needed are updated using reanalysis models.

1.1.1.4 Data curation service of ACTRIS aerosol profile data

Raw data collected at the NF in the original acquisition data format are transcribed in a homogeneous and agreed netCDF data format to the aerosol remote sensing processing suite at the ACTRIS DC. All information needed for the steps forward in the processing chain are annotated into the file.

The raw data are submitted to the SCC by the Data Originator through **SCC web interface**. Through the SCC interface, Data Originator can interact with the SCC database, which is a relational database which handles the large number of input parameters needed for the retrievals of aerosol optical products from LIDAR signal. Two different types of parameters are needed: experimental (which are mainly used to correct instrumental effects) and configurational (which define the way to apply a particular analysis procedure). This information is the outcome of the QA and is provided to the DC by the CARS. The SCC web interface here and at the other processing steps, allows the monitoring of the processing status of each measurement.

After the configuration set-up for the processing the raw signals are processed through the **Pre-processor module (ELPP: EARLINET Lidar Pre-Processor).** The ELPP module implements the corrections to be applied to the raw LIDAR signals before they can be used to derive aerosol optical properties. Following the QA procedures, some instrumental effects are corrected. Level 1 pre-processed data are stored in internal SCC archive and on ACTRIS DC.

Level 1 pre-processed data are then processed through the **Optical processor module (ELDA: EARLINET Lidar Data Analyser).** ELDA enables the retrieval of particle backscatter coefficients, the calculation of particle extinction coefficient and finally the computation of particle and volume linear depolarization profiles, multi-wavelength and layer products. All the optical products are written in netCDF files in the agreed DC format and constitute the Level 1 processed data.

For aerosol remote sensing NFs which are also equipped with microwave radiometer and cloud radar, the level 1 pre-processed data are also an input data for the cloud profile data unit.

Then the data are submitted to the ACTRIS aerosol remote sensing DC database. **On fly QC procedures** run directly during the submission phase. These procedures control that the file content respect to the file structure as agreed. Additional scientific controls check that all mandatory products are reported into the files. All data passing the on-fly QC are uploaded on the DC as Level 1 products. **Off-line QC procedures** are run systematically every 3 months. The data originator receives feedback of the outcome of the QC. This feedback mechanism potentially allow to discover and address instrumental issues, with links to the TC. All the data compliant to all the QC requirements (both pre-processed and processed data) are made available as Level 2 data.

Finally, the ACTRIS DC have to offer different products resulting from the processing at DC itself of Level 2 LIDAR and photometer data collected at the aerosol remote sensing NFs. The ACTRIS datacentre offers in this way the possibility to ACTRIS users to access among the others to profiles of aerosol volume concentration profiles which is potentially of great interest for different users, like modellers, and local, national and international authorities.

3.1.2.1 Data services and tools offered to NF for aerosol profile data production and quality control

In order to improve data quality and assist the NF in data production, the ACTRIS aerosol remote sensing data unit offers services and data control tool, and development of required tools and procedure for data submission and production. The ACTRIS aerosol remote sensing data unit needs to offer;

- Online portal for standardised submission of data by the NF operators to the aerosol profile data centre unit,
- Automatic check of meta data formats upon data submission
- Automatic standardised sanity and consistency checks of data submitted through submission portal
- Implementation of data quality control tools and procedures developed at the DC or TCs

- Development and maintenance of tools for quality control of data, including implementation of new quality assurance/control criteria defined by TCs,
- Feedback mechanisms about QC to Data originator
- Processing suite for the processing of aerosol LIDAR data for the retrieval of all the described above products
- Development and maintenance of processing chain for aerosol LIDAR data, including implementation of new products in agreement with TCs,

1.1.1.5 General Principles for ACTRIS aerosol profiles Data curation

The relation between the various data products, pre-products, and processing steps of both ACTRIS aerosol profile data workflow is depicted in the corresponding workflow diagram (see Annex III). The details concerning implementation of these workflows for individual ACTRIS variables are specified in the pertaining, variable specific data managements plan and implementation plan. This implementation plan describes the data and metadata items contained in each data level, data format used, the individual operations performed in each production step between data levels, as well as data and metadata items contained in each sample handling protocol. The content of the data managements plan and implementation plans is determined by the responsible TC in collaboration with the aerosol profiles data centre unit.

All data products, pre-products, and sample handling protocols, as well as all software and algorithms used in production steps, version controlled, archived following long-term archive standards, and identified in each version. Persons involved in data production steps are identified, as well as entity responsible for the production step. For establishing traceability, the data products and pre-products contain references to the identifiers of all (pre-)products, production tools, persons and entities involved in the whole production chain leading up to the (pre-)product.

To facilitate harmonised data products and quality, the ACTRIS DC is responsible for ensuring that all instances of a specific data production step operated in the ACTRIS network uses the same identified version at any given time. To the same end, the DC provides tools for conducting standardised manual data QC under the responsibility of the NFs. As a low-barrier tool, the surface in situ data centre unit offers a web-based data submission portal allowing interactive checks of data submissions, as well as conducting the submission upon successful check. The test include syntactic and semantic correctness and consistency of metadata and data, as well as standardised tests for outliers and spikes.

In the workflows, the TCs are responsible for QA of instruments and analysis methods in the network, and also responsible for specifying QC procedures conducted in the network, for data QC in collaboration with aerosol profiles DC unit. Examples for instrument and analysis QA measures are on-site comparisons to a reference instrument and on-site tests. Together with the responsible data centre unit, the TCs are responsible for specifying data and metadata items documenting these QA measures in a harmonised way. The TCs are also responsible for collecting the data and metadata items when conducting QA measures, and storing them in a QA result database in machine-readable form. From here, the QA measure results are joined with ACTRIS variable data during data production.

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Based on the generic data production workflows described above, the ACTRIS aerosol profile DC node supports implementation of data workflows for new aerosol profiling variables as agreed by the consortium

3.1.2.2 Potential campaign service for ACTRIS aerosol profiles data

The data centre need to offer a service for campaigns at the NF sites. A general procedure needs to be offered for this through SAMU, described in section 4.7 on page 33.

3.1.3 Data curation service and tools of ACTRIS cloud remote sensing data

All ACTRIS cloud profile variables are listed in Annex I, associated with their combination of instrument types, and the potential for being produced in rear-real-time (RRT) or real-real-time (RRT). The ACTRIS DC shall provide to the cloud profile data originator support for centralized data processing through the common standardized automated processing software developed in previous projects for the ACTRIS RI, the Cloudnet processing scheme. The Cloudnet processing scheme is open source software designed for combining cloud radar and LIDAR observations in order to obtain vertical profiles of cloud parameters. The Cloudnet scheme provides the necessary tools for full traceability of harmonized data processing, automated quality control and product generation.

The data curation workflow (reported in Annex 3) follows the automated standard processing and enables RRT and RRT delivery of cloud profile variables.

The ACTRIS data levels are described in Figure 1. A more detailed description of data levels pertaining to cloud profile data follow, in agreement with the general description:

- Level 0: raw data as produced by the instrument, including instrument status parameters provided by instrument, brought to a common, well-defined data format. Discovery, use, provenance, and configuration metadata attached, including all information needed for further data production, as far as is known at station level (e.g. QC metadata). Time and temporal resolution as native to the instrument.
- Level 1: processing of Level 0 instrument data, 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 synergistic product 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 retrieval algorithms, as well as providing the underlying target identification for retrievals to operate on.
- Level 2: Cloud variables generated from Level 1 data, including uncertainties and product status.

3.1.3.1 Data curation service of ACTRIS cloud profile data

Raw data collected at the NF in the original data acquisition format are transcribed to an agreed harmonized netCDF data format suitable for ingestion by the Cloudnet processing scheme. Data from each instrument is pre-processed separately to identify and remove artefacts, and a calibration factor applied as required, supplied by the responsible TC. The pre-processed single-instrument level 0 data are made available for review and possible re-calibration by the responsible TC. The TC organises the review process, defines the review criteria, and performs re-calibration if required. All information necessary for the Cloudnet processing chain to operate is checked or included at this stage.

After configuration set up for the specific instrument combination, the pre-processed instrument data is then combined using the target categorisation module of the Cloudnet processing scheme to produce the level 1 data. This module also calculates and applies radar attenuation parameters, together with a quality status reflecting the instrument performance and the impact of the atmospheric conditions on the measurements.

Level 2 products are generated from the level 1 synthesis product with all uncertainties, quality status, and metadata propagated from level 1. Cloud remote sensing NFs which are also equipped with aerosol profiling capabilities can then generate additional synthesis products combining cloud remote sensing products with level 1 aerosol remote sensing data.

Level 3 climatological and composite datasets are obtained using Level 2 cloud products through monthly and yearly aggregation. Datasets are composited by seasonal, diurnal, precipitation, omega-at-500 mb (vertical motion) and other suitable parameters. Metrics containing mean values and the distribution are reported. Level 3 datasets are also used in numerical weather prediction (NWP) and climate model evaluation.

The entire processing chain, from level 0 to level 3 (including model evaluation), can operate in two QC streams:

1. **Automatic QC**: algorithmic inspection of data for outliers, spikes, and automatically identifiable instrument malfunctions. Instruments receive automated or the previous manual calibration values. This stream is used for RRT/RRTdata.
2. **Manual QC**: inspection of data by an identified person under the responsibility of the NF. The additional manual QC includes extra tests for specific instrument and atmospheric issues that may be location-specific (radio interference, fog, and insects) and verification of instrument QC such as re-calibration. Manual QC is applied at least at an annual frequency.

3.1.3.2 Data services and tools offered to NF for cloud profile data production and quality control

In order to improve data quality and assist the NF in data production, the ACTRIS cloud remote sensing data unit offers data tools and services, and the development of the required tools and procedures for data submission and production. The ACTRIS cloud remote sensing data unit shall offer;

- Online portal for standardised submission of data by the NF operators to the cloud profile data centre unit,
- Standardised sanity and consistency checks of data on submission
- Implementation of data quality control tools and procedures developed at the DC or TCs
- Development and maintenance of tools for quality control of data, including implementation of new quality assurance/control criteria defined by TCs,
- Mechanisms to feedback data QC issues to Data originator
- Processing suite for the retrieval of all cloud products (L0 - L1 - L2)
- Development and maintenance of processing chain for cloud remote sensing data, including implementation of new products in agreement with TCs

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3.1.3.3 General Principles for ACTRIS cloud profile data curation

The relationship between the various instruments and processing steps in the ACTRIS cloud profile data workflow is depicted in the corresponding workflow diagram (see Annex III). The details concerning implementation of these workflows for individual ACTRIS variables are specified in the pertaining, variable-specific data management plan and implementation plan. This implementation plan describes the data and metadata items contained in each data level, the data format used, the individual operations performed at each production step at every data level, and the items contained in each sample handling protocol. The content of the data management plan and implementation plan is determined by the responsible TC in collaboration with the cloud profile data centre unit.

All data products, pre-products, and sample handling protocols, as well as all software and algorithms used in production steps, version controlled, archived following long-term archive standards, and identified in each version. Persons involved in data production steps are identified, as well as entity responsible for the production step. For establishing traceability, the data products and pre-products contain references to the identifiers of all instruments, (pre-)products, production tools, persons and entities involved in the whole production chain leading up to the (pre-)product.

To facilitate harmonised data products and quality, the ACTRIS DC is responsible for ensuring that all instances of a specific data production step operated in the ACTRIS network uses an identifiable version at any given time. To the same end, the DC provides tools for conducting standardised manual data QC under the responsibility of the NFs. including syntactic and semantic correctness and consistency of metadata and data, as well as standardised tests for outliers and spikes.

In the workflow, the TCs are responsible for QA of instruments and analysis methods in the network, and also responsible for specifying QC procedures conducted in the network, for data QC in collaboration with the cloud profile DC unit. Examples for instrument and analysis QA measures are routine calibration, and on-site comparisons to a reference instrument. Together with the responsible data centre unit, the TCs are responsible for specifying data and metadata items documenting these QA measures in a harmonised way. The TCs are also responsible for collecting the data and metadata items when conducting QA measures, and storing them in a QA result database in machine-readable form. From here, the QA measure results and calibrations are joined with ACTRIS variable data during data production.

Based on the generic data production workflows described above, the ACTRIS cloud profile DC node supports implementation of data workflows for new cloud profiling variables as agreed by the consortium

3.1.3.4 Potential campaign service for ACTRIS cloud profile data

The data centre need to offer a service for campaigns at the NF sites. A general procedure needs to be offered for this through SAMU, described in section 4.7 on page 33.

3.1.4 Data curation service and tools for ACTRIS trace gas remote sensing data

Trace gas remote sensing data can be issued from four types of instruments: FTIR, UV-VIS, SAOZ and LIDAR and produced by using a specific data production chain. According to the type of instrument the data production is performed either by NFs or TCs while ACTRIS DC must be in charge of data curation for Level 2 data as well as tools and services for data producers and users. The required ACTRIS data workflow for these data and variables are still under discussion between TC, DC and requirements to NF. This work will proceed and clarification of the requirements to the DC will be made in 2018.

3.1.5 Data curation service of ACTRIS atmospheric simulation chamber data

3.1.5.1 Overview of the data production chain of ACTRIS atmospheric simulation chamber data

Data produced by simulation chamber experiments are diverse and are organized within three databases:

- The Database of Atmospheric Simulation Chamber Studies (DASCS): This database provides a compilation of experimental and modelled data obtained from experiments in simulation chambers. These experiments can be used to further understanding of the atmospheric processes involved in air pollution and climate change, as well as their impact on health and cultural heritage. These data are highly useful for the development and the validation of atmospheric models.
- The Library of Analytical Resources (LAR): This database provides infrared, UV and mass spectra of atmospheric key species as well as mass spectra of derivatives at mid to high resolutions. Most of the spectra are calibrated to allow for quantification of species. The specificity of this library is that it focuses on atmospheric species and provides spectra of complex molecules which cannot be found elsewhere, some of them being synthesized as they are not commercially available.
- The Library of Advanced Data Products (LADP): This database provides different types of mature and high level products of chamber experiments which are very useful for researchers working on atmospheric observations, as well as atmospheric model development and validation. It includes data products for the development of chemical mechanisms in atmospheric models and for the retrieval of satellite data and for radiative transfer modelling as well as tools to generate oxidation schemes which are very useful to interpret field measurements as well as laboratory studies.

Following the ACTRIS data levels described in Figure 1, a more detailed description of data levels for atmospheric simulation chamber data is as follows:

- **Level 0:** raw data as provided by the instruments, with metadata attached. These data are typically time series of measured parameters during the course of the experiment.
- **Level 1:** Time series of the targeted properties (for example trace gas concentration, aerosol mass …). These data are obtained from level 0 data after calibration of the instrument. For base instrumentation, calibrations are performed at the TC or following procedure recommended by the TC. For specific instrumentation, for which there is no standard procedure provided by TC, calibrations are performed at the NF following their own procedure.
- **Level 2:** Approved and fully quality controlled time series of the targeted properties. This quality control includes data gathering from different instruments and check for internal consistency and disregard of invalid data. Chambers characteristics, experimental protocol and metadata are attached. These data are produced by NF and are made available in the DASCS.
- **Level 2.5:** Approved and fully quality controlled time series of the targeted properties after corrections for wall losses and dilution have been applied. Chambers characteristics, experimental protocol and

metadata are attached. These data are produced by NF after level 2 data processing and are made available in the DASCS.

- **Level 3:** Approved and fully quality controlled advanced data products (rate constants, cross sections, SOA yields, complex refractive index of aerosols …). These data are produced by NF after level 2.5 data processing and are made available in the LAR and in the LADP.

The complete data workflow for these data levels is depicted as diagram in Annex 7. It should be noticed that unlike other data centre units, all the data processing is performed by NFs while the data centre unit is in charge of data curation for Level 2 to Level 3 data as well as tools and services for data providers and data users. The detailed list of ACTRIS measurement variables as well as level 3 data products provided by the ACTRIS Exploratory Platforms, i.e. by simulation chambers, has not been fully established so far and will be provided in a second step.

3.1.5.2 Data curation services for ACTRIS atmospheric simulation chamber data

Curation of Level 2 to Level 3 data is ensured by ACTRIS DC. The data curation service need to bring together all the processes that applied to datasets from the moment they enter the data centre. The important steps in the curation of atmospheric chamber data are as follows:

- **Identification**: When entering the data centre, each dataset is assigned a unique identifier (uuid). This identifier is usually a 16 character long meaningless code. It need to follow it in all curation processes.
- **Cataloguing**: Each dataset is associated with a metadata record that provides the usual information (abstract, title, contact, etc.) This catalogue implements a certain number of standards: it can be requested via the CSW protocol and its content is compliant to ISO 19115 standards.
- **Version control**: The different versions of the same dataset are kept in the data centre. Submitting a new version involves providing a description and a motivation of the changes performed. All of these elements are kept in the metadata file to provide a precise history of the data.
- **Backup and Archiving:** A daily backup mechanism is put in place. This mechanism allows performing a quick data recovery in case of human error in the handling of data files. In addition, a more complex archiving mechanism based on the use of multiple remote sites and regular integrity checking processes is also set up. It ensures that the contents of the files in the data centre do not change because of storage media issues.
- **Quality control**: The quality of data centre data sets is ensured by the establishment of a repository portal. An automatic tool checks for the quality of the metadata (mandatory fields, controlled vocabulary). The use of shared formats by the community (EDF, JDX ...) ensures the homogeneity of the data. In addition, verification scripts are used at the time of filing. Finally, the data centre provides the NF with validated libraries that make it easy to produce the requested formats.

3.1.5.3 Tools and services provided for simulation chamber data production and usage

Services are a set of value-added processes for both the data provider and the data user. The main services for atmospheric chamber data are as follows:

- Online portal for standardized submission of data by the NF,
- Standardized sanity and consistency checks of data on submission,

- **Data Object Identifier (DOI)**: A DOI is automatically associated with each dataset to facilitate its quotation in an article. For this, its suffix must be a short and insignificant chain. So it is not the uuid, but the data centre keeps the correspondence between these two values up to date. The landing page of this DOI is the metadata record describing the dataset. All DOI metadata provided to DataCite comes from the metadata record.
- **Data preview**: In order to allow the user a better data discovery, data preview mechanisms are set up.
- **Data access**: The different datasets are downloadable in their different versions.
- **Usage Report**: A report is regularly sent to the data producers. This report describes the number and origin of downloads of the different datasets that the producer has deposited in the data centre.
- **Change alert**: A user can sign up to be notified of different changes in a dataset.

3.2 Estimation of the need

The table show the estimated number of annual data sets from the NFs, and the associated need for data storage for the various types of data.

	Number of annual data sets			Data volume		
	Now	by 2025		Now	by 2025	
		Min.	Max.		Min.	Max.
ACTRIS in situ aerosol data	60	50	120	18 000 MB	15 000 MB	50 000 MB
ACTRIS in situ cloud data	0	35	105	0	1 GB	3 GB
ACTRIS in situ trace gas data	27	30	60	300 MB	200 MB	400 MB
ACTRIS aerosol remote sensing data	28	30	70	4 GB	2.5 TB	25 TB
ACTRIS cloud remote sensing data	9	9	15	5 TB	15 TB	30 TB
ACTRIS trace gas remote sensing data	57	60	80	400 MB	400 MB	550 MB
ACTRIS Atmospheric simulation chamber data	160	150	250	1 GB	3 GB	10 GB

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3.3 ACTRIS Data provenance, attribution, and traceability

The term "provenance" has originally been used in the context of archiving historical objects, where it describes the documentation of the production process if known, the history of ownership and the places and conditions of storage.

In data science, "provenance" is used for the process of documenting individual executions of a workflow to the point that each step can be reproduced. Thus, provenance is the tool for establishing traceability. Documenting provenance has at least 3 important applications:

1) Attributing the contributions to the workflow to the entities involved in the workflow
2) Making the workflow product traceable
3) Tracing errors in the workflow and removing them by re-executing the workflow.

To document provenance in a workflow, each component used in the workflow need to be uniquely identified by persistent identifiers (PIDs). This applies to:

- Humans, e.g. identified by their ORCID.
- Legal entities. Candidate identifier systems for legal entities such as funding agencies and affiliations are the International Standard Name Identifier (ISNI), the Ringgold system, and OrgIDs.
- Final data products, identified by their Digital Object Identifier (DOI).
- Algorithms, software, instruments, data and instrument quality assurance and quality control reports, and data pre-products, identified by a general PID. Candidate PID systems include the Handle System, Persistent URLs (PURLs), and the European persistent identifier consortium (ePIC) system.

All algorithms, software, data and instrument quality assurance and quality control reports, and data pre- and final products used or produced anywhere in ACTRIS data production workflows will be archived in suitable repositories. These repositories must be accessible by referencing their PIDs, and meet the need for long-term archive standards. For keeping the PID references unique, these repositories must have version control.

It is required that all data pre-products, algorithms, software, legal entities, instruments, and relevant data and instrument quality management documents used in the production of a data pre- or final product is referenced in the metadata by their PIDs. This is achieved by means of a data provenance framework. In this respect, ACTRIS shall use the recommendations and experience gained in ENVRI. A provenance framework describes the elements in a workflow as resources such as "artefacts" (immutable pieces of state), processes, and entities controlling these processes. These are put into relations such as "used" (a process used some artefact), "wasControlledBy" (an agent controlled some process), "wasGeneratedBy" (a process generated an artefact), "wasDerivedFrom" (an artefact was derived from another artefact) and "wasTriggeredBy" (a process was triggered by another process). Potential relevant data provenance frameworks include:

- The Open Provenance Model (OPM)
- The PROV model

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Each potential ACTRIS DC node needs to select and implements provenance documentation by annotating each connection in its data production workflow with the respective relation defined in the provenance framework.

3.4 Operation support for knowledge transfer and training

3.4.1 Training of instrument operators and data submitters

ACRTIS DC must offer training of data producers and scientists at ACTRIS NFs for:

- Experienced data producers and scientists facing a potential upgrade of their instrument, exchange on instrument methodologies or extension of the NF with more and additional instruments recommended within ACTRIS
- New operators that need to learn and comply with the protocols and procedures valid for reporting of ACTRIS data
- Availability of new SOPs, QA procedures and tools, and/or data evaluation procedures and plausibility tests
- New types or QC tools and versions available, or revised versions of existing QC tools

The training shall be organized on various channels:

- The data centre shall offer opportunities for focused training sessions on pre-defined data types ((e.g. remote sensing/in situ) and topics (e.g. RRT/QA data, reporting procedures and tools, meta data, flagging, application of QC tools etc.)
- Transfer of expertise during online exercises and workshops
- Documentation, procedures, tutorials and tools available on the data centre website for e.g. data QC and submission,
- Guidance for NFs in setting up data flows to DC unit
- Help desk for data submission and reporting periods
- Data centre participation on summer/winter school for students and scientists and during large comprehensive campaigns

3.4.2 Consultancy for setting-up new data flow from new sites or new instrument at existing sites

New measurement techniques, technological products and methods are developed by the TC in collaboration with the NFs. Depending on the situation, ACTRIS DC may recommend to the ACTRIS RI Committee to decide on the implementation of such new techniques at the RI level. The data centre needs to offer assistants to the NF in setting up data stream from new measurement techniques, if this is embraced by ACTRIS RI Committee and need to be implemented as part of the National Facilities and the ACTRIS labels.

3.5 Access to documentation for ACTRIS standards and data flow

Documentation generated in ACTRIS data curation procedures includes quality management concepts and reports, data management concepts and workflows, operating procedures, quality control reports and others. Many of these documents are referenced in the metadata of the various data products. It is required that all documents and reports are stored in a versioned document repository for long-term archiving, and identified by a PID (persistent identifier). Documents are distinguished between open access and RI internal, where access conditions to the open access documents are defined in the access policy. As a general rule, at least all documents referenced in the metadata of the data product need to have open access.

Open access documents and internal documents include:

- Standard operating procedures
- Data quality control reports
- Instrument quality control reports
- Data and instrument quality assurance concepts
- NF, CF, and DC concept documents
- Workflow implementations plans

4 Services provided to ACTRIS users

An ACTRIS user is a person, a team, or an institution using either ACTRIS data or any other ACTRIS service. ACTRIS users originate from academia, business, industry and public services, from ACTRIS member countries and from countries which are not ACTRIS members, both inside and outside Europe.

As a tool for science, the highest priority for the ACTRIS Data Centre is to maintain and increase the availability of ACTRIS data and data products relevant to climate and air quality research for all interested users. National and international climate and air quality assessments are employing ACTRIS data, and are the ultimate user of ACTRIS data and data products. Level 3 data offering ACTRIS data with other available data is highly valuable for a wide community. Most of the level 3 data products developed in the framework of ACTRIS shall be derived from a combination of multi-source and/or multi-temporal parameters and variables: synergetic retrieval from different instruments, combination of ground-based data, and satellite and model data. They can also be derived from an advanced processing of data obtained from simulation chamber experiments. Annex II list the level 3 data. This section includes a brief description of each of the products planned, sorted the subcategories. The ACTRIS Data Centre aim to put in place and offer to all users the specific level 3 products marked with * in this document, from year 1. The rest can be implemented later, depending on support and expressed user needs.

4.1 Estimation of the need

Type of ACTRIS user	Number of users to which ACTRIS DC is providing services per year		
	Now	by 2025	
		Min.	Max.
Academia, Business, Industry, Public services	600	400	4000

Based on current statistics, academic users are likely to be more than 80%, and governmental and intergovernmental bodies constitute around 3-5 %.

4.2 Access to ACTRIS data and digital tools

ACTRIS DC shall offer access to data, data products and digital tools through a single entry point, the ACTRIS data user interface. As a tool for science, the highest priority for the ACTRIS Data Centre will be to provide access to ACTRIS data and data products relevant to climate and air quality research for all interested users. Access to some ACTRIS services is open and free, most importantly the access to ACTRIS data, data products, and digital tools provided by the DC. Other access to ACTRIS services is considered competitive access based on capacity or excellence and require a review process that will be centrally managed by the HO/SAMU. SAMU is the single point of entry for user access to all TC services and to some specific services and data products provided by the DC. Access is regulated by both the ACTRIS access policy and the ACTRIS data policy, respectively.

4.2.1 Access to ACTRIS level 0

It is required that access to level 0 data need to be upon specific requests and regulated by a license, depending on the variables and tailored to the various types of data. Level 0 data encompass huge data volumes, and shall be archived in accordance with the requirements related to this. This ensures full traceability of ACTRIS data, in a flexible system meeting the specific needs for the various data types.

4.2.2 Access to ACTRIS level 1

It is required that access to level 1 data can be regulated by variable, but is restricted by default. Level 1 data do not need to be accessible directly through the ACTRIS data user interface, with the exception of RRT and RRT data products. All level 1 data shall be discoverable and accessible by the machine-to-machine interfaces according to their access policy. The level 1 data access policy for each ACTRIS variable is specified in Annex I. For restricted level 1 data, ACTRIS will offer common license models, taking into account that there may be different needs for RRT/NRT data, which are specified in the data policy.

4.2.3 Access to ACTRIS level 2

It is required that access to all ACTRIS level 2 data shall be open, free and offered through the ACTRIS data user interface. The access shall follow the FAIR principles (see section 3.3).

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4.2.4 Access to ACTRIS level 3 and to specific data products on demand

It is required that access to standard ACTRIS level 3 data shall be open, free and offered through the ACTRIS data user interface. The access shall follow the FAIR principles (see section 3.3).

It is also required that ACTRIS offer access to specific tailboard data products and tools on demand. This is considered as competitive access and can be based on capacity or excellence. SAMU is the single point of entry for user access to all TC services and to some specific services and data products provided by the DC. This will require a review process that is centrally managed by the HO/SAMU.

4.2.5 Access to digital tools

It is required that the ACTRIS data user interface offers access to digital tools for data production, quality control and analysis. Access to selected tools can be regulated, depending on the application, and SAMU will organise and manage the access. ACTRIS will also offer a common license for digital tools.

4.3 Production of level 3 data solely based on ACTRIS observations from NF

4.3.1 Aerosol surface in situ data – combination of variables and instruments

ACTRIS DC shall produce different products resulting from the processing at DC itself of atmospheric aerosol variables measured in situ at ACTRIS NFs. ACTRIS DC will offer several products resulting from combining data provided by different in situ instruments. The use cases comprise QC at NFs by means of closure (comparison of same variable obtained by different measurements or retrievals), and verification of climate and air quality model results. The targeted aerosol variables comprise physical (full-range particle number size distribution, PM mass concentrations derived from particle size distribution) and optical ones (extinction and scattering coefficients, single scattering albedo, all dry-state), as well as data compilations.

4.3.2 Aerosol remote sensing data – combination of variables and instruments

ACTRIS DC shall produce different products resulting from the processing at DC itself of Level 2 LIDAR and photometer data collected at the aerosol remote sensing NFs. Such products include profiles of aerosol volume concentration, potentially of great interest for modellers, and local, national and international authorities.

4.3.3 Data products from simulation chamber experiments

ACTRIS DC shall provide level 3 data products derived from simulation chamber experiments. These advanced data products are used for researchers working on atmospheric observations as well as atmospheric model development and validation. They include products for the development of chemical mechanisms in atmospheric models, products for the retrieval of satellite and for radiative transfer modelling, e.g. rate constants for gas and condensed phase reactions, mass extinction coefficients of aerosols, absorption cross sections and Secondary Organic Aerosol yields.

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These data are produced by exploratory NF after level 2.5 data processing. ACTRIS DC offers data curation service and long term archive. It can also provide tools for data visualisation and treatment. Level 3 data from exploratory platforms are not shown in annex II.

4.3.4 ReOBS - long-term (> 10 years) multi-parameter product

ACTRIS DC shall produce long-term (> 10 years) multi-parameter, homogenized and harmonized datasets following the ReOBS approach for all variables available in annex I. ReOBS refers to a scientific approach that aims to aggregate and harmonize all geophysical variables available at a given ACTRIS NF on a regular temporal scale (typically hourly) over a long time period (decadal and beyond). ReOBS long term data are Re-calibrated, Re-quality controlled, Re-expertized, Re-averaged, Re-formatted, and Re-nomenclatured. The resulting harmonized dataset is a unique resource to support multiannual and multi-variables studies combining atmospheric dynamics and thermodynamics, radiation, clouds, aerosols, and reactive trace gases from ground-based observations.

While individual datasets from ACTRIS NF observations exist, the application of synergy between different types of observations is currently under-used because of complexity in the exploitation of multi-variable datasets and diversity inherent to calibration, quality control, treatment, format, temporal averaging, and metadata. The use of synergy shall be as users will have access to ReOBS datasets.

The ReOBS approach must be tightly connected to other tools and services offered by the DC. For example, the ReOBS approach will utilize gap filling tools (see section 4.5.4). ReOBS datasets enhance the capacity of the DC to provide model evaluation services, and shall serve these users. Pilot products will be available from year 1, the number of NFs will gradually increase.

4.3.5 Climatology products for ACTRIS variables @National Facilities across Europe

ACTRIS DC shall produce climatology products updated yearly suitable for both the scientific community and authorities and policy makers. These include monthly and seasonal means of selected ACTRIS variables based on the compiled level 2 observations of aerosol in situ, aerosol profiles, trace gas in situ data. The products will utilize the data production tools described in section 4.5.2. See annex II for more details.

4.3.6 Source apportionment of submicron organic aerosols in Europe

ACTRIS DC shall offer products including long-term trends and seasonal variation of the most important organic aerosols (OA) source signatures in Europe. A source apportionment tool (e.g., based on Multilinear Engine (ME2)) can be used for a factorial analysis of level 2 datasets. This approach identifies organic factor profiles and their resulting long-term trends. The TC for aerosol in situ measurements has to make available the necessary products including metadata.

4.3.7 Volatile Organic Compounds (VOC) source attribution in Europe

ACTRIS DC shall offer products including long-term trends and seasonal variation of the most important VOC source signatures in Europe using a receptor oriented approach. A source apportionment tool (e.g. Positive Matrix Factorization-PMF) can be used for factorial analysis of level2 datasets for selected of

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variables resulting in two output datasets describing the chemical profiles of the factor and a time series of the factor contribution. Products must be updated regularly, e.g. Yearly updated.

4.3.8 Cloud occurrence @ cloud in situ National Facilities

The ACTRIS DC will produce monthly updates of cloud occurrence at ACTRIS observational platforms with cloud in situ instrumentation. The analysis will be based on level 2 data of the cloud liquid water content and will include both highly time resolved data series of cloud free and cloudy conditions as well as monthly and yearly statistics of cloud coverage at the stations. These products will be needed for the interpretation of other in situ measurements at the same stations and may also be used to constrain and further improve cloud, weather and climate models. Long-term series of cloud occurrence at several stations in Europe will also contribute to identify trends in regional weather and climate systems.

4.4 Production of ACTRIS level 3 data and tools through multi-source data integration services, employing external ground based measurement data

4.4.1 Bridge to external ground-based observational data relevant for ACTRIS

ACTRIS DC shall provide access to external data holdings and repositories of ground-based observations commonly used by ACTRIS users, valuable when combined with ACTRIS data. This functionality shall facilitate contextual analysis, inter-comparison, and validation purposes, and is required to produce derived products using multi-instrument synergetic retrieval algorithms. These regional and global networks and initiatives include EMEP, GAW, AERONET and NDACC.

4.4.2 Collocation service of data from regional and global networks

ACTRIS DC shall offer comprehensive data products combining ACTRIS data with data from regional and global networks, based on the functionality described in section 4.4.1. ACTRIS DC will offer yearly updates of benchmark data products adding complementary data from GAW and EMEP together with ACTRIS data e.g. ACTRIS variables presented together with PM and/or sulphate at the ACTRIS National Facilities. This will also provide data sets with global coverage, employing ACTRIS methods on data from sites outside Europe. The selection of variables can be made upon user requests, regulated through review process controlled by SAMU. See annex II for more details.

4.4.3 Aerosol remote sensing data – combination of variables and instruments from global networks

ACTRIS DC shall provide level 3 products derived from the standard AERONET products. Based on NASA algorithms, including AERONET Level 1 (Synergy or Single) data: Spectral refractive indexes, spectral extinction/absorption AOD, single scattering albedo, spectral LIDAR ratio, Ångström exponent, volume size distribution and spherical fraction. Furthermore, ACTRIS DC shall offer Direct Sun/Moon Extinction Aerosol Optical Depth (column) from AERONET, and Column Water Vapour Content.

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4.4.4 PM retrieval @GAW sites globally

ACTRIS DC will utilize ACTRIS procedures and data to develop a methodology for estimating particulate mass at GAW sites, not yet generally available, through a combination of nephelometer measurements and size distribution. This will be used at all GAW sites to enable a yearly updated global PM product, together with complementary variables also included in ACTRIS. See annex II for more details.

4.4.5 Satellite data – combined with ground based ACTRIS data

ACTRIS DC shall provide access to external open data holdings of satellite measurements and retrievals commonly used by ACTRIS users combined with ACTRIS data, for contextual analysis, inter-comparison, or to produce derived products using multi-instrument synergetic retrieval algorithms. These external data bases include major product suites from the A-Train satellites (Terra/MODIS, Aqua/MODIS, PARASOL, CALIPSO, CloudSat, Aura/OMI, and Terra/MISR), Envisat/AATSR, IASI, and MSG/SEVIRI.

Due to the complexity of the geometry and orbital pattern of satellite sensors, the data centre will provide collocation tools capable to subset satellite data spatially and temporally with ACTRIS ground-based measurements.

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4.5 Production of ACTRIS level 3 data products involving regional and global model data

4.5.1 Aerosol and Gas trend assessment

ACTRIS DC shall produce and provide level 3 products based on ACTRIS level 2 data comprising:

- best estimates of trends in atmospheric composition of components covered by ACTRIS
- display of complementary multi-annual information from models and/or satellites from hindcasts or reanalysis
- web visualisation of trends at individual stations as well as for regions
- regular biennial trend assessments based on updated information

4.5.2 Data Interpretation and Outlier Identification Tool

ACTRIS DC shall offer automated assessments of ACTRIS data quality using assimilation model products, model climatologies and satellite data for intercomparison with ACTRIS data. The centre should in particular:

- Collocate model data such that outliers in ACTRIS data products become apparent and can be investigated further
- Provide a visualization and download tool to allow data interpretation with model information (e.g. meteorological parameters, non-observable atmospheric chemistry parameters, source contributions from sectors or regions)

4.5.3 Optimal interpolation and Gap filling tool

ACTRIS DC must produce tools that enable the merging of observational and model data to produce continuous data products both in space and time. In particular it should:

- Fill gaps in incomplete time series, profiles of ACTRIS data products to allow for the production of climatologies, trends, spatial distribution
- Allow for the optimal interpolation or assimilation of data into assimilation systems, and provide access to the assimilation products derived

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4.5.4 Model Evaluation Service

ACTRIS DC must produce and provide level 3 data and services based on ACTRIS level 2 data for enabling model evaluation. In particular the centre should:

- foster the preparation of specific model evaluation benchmark datasets, with appropriate documentation
- provide web services for interactive model evaluation e.g. AeroCom, CMIP, ICAP, SDSWAS and NWP models based on ACTRIS data
- make available advanced visualization of model data comparisons on all levels, with free access to users
- automate model evaluation to provide fast feedback to model development

4.5.5 Transport modelling products for assessment of source regions at the NFs

ACTRIS DC must produce inversion products built on backward transport modelling and tools to enable backward modelling operationally and automatically on a regular basis, e.g. monthly, for every site and platform. The results (both data and plots) should be made publicly available via an ACTRIS access interface so that they are readily accessible and can be used in the interpretation of the most recent measurement data.

4.5.6 Alert Service for National Facilities

ACTRIS DC must offer tools for exploiting the potential of current chemical weather forecasting systems to help national facilities and campaigns in resource efficient management of measurement capacity. Alerts shall be send to interested users and experimental campaign managers based on variable criteria (e.g. dust plumes, winter inversions or clean air approaching).

4.6 Production of level 3 data ACTRIS data products from simulation chamber experiments

ACTRIS DC is required to provide level 3 data products derived from simulation chamber experiments. These advanced data products will be used by researchers working on atmospheric observations and atmospheric model development and validation. This includes products for the development of chemical processes in atmospheric models, products for satellite retrievals and for radiative transfer modelling, e.g. rate constants for gas and condensed phase reactions, mass extinction coefficients of aerosols, absorption cross sections and Secondary Organic Aerosol yields.

These data are produced by NF after level 2.5 data processing. ACTRIS DC will offer the data curation service and long term archive and can also provide tools for data visualisation and treatment. Level 3 data from exploratory platforms are not shown in annex II.

4.7 Service to campaigns

ACTRIS DC need to provide appropriate service and support related to campaigns. Application and access to this service will be a part of a review process managed by SAMU. Services may be offered free or for a fee, depending on the request, and the work foreseen. The following sections outline the possible campaign services that may be provided.

4.7.1 Digital tools and products for campaign support

For campaigns, the ACTRIS data centre will offer a centralised support website for providing relevant services, once agreements and contracts have been established.

4.7.1.1 Campaign dashboard

During intense observation periods, scientists require up-to-date information from multiple sources in order to schedule their measurements. These data are heterogeneous: images, documents, web services (e.g. OGC services), sensor and model data files. The website shall automatically harvest and compile in near real time all required data in a global dashboard. Manual upload of data will also be possible.

In addition, added value services may be provided such as

- trajectory forecast, flight plan tools,
- back trajectories for source regions and source analysis

4.7.1.2 Data curation and archive of campaign data

ACTRIS DC may offer data curation service and long term archive of data from campaigns. Application and access to this service will be a part of a review process managed by SAMU. Services may be offered free or for a fee, depending on the request, and the work foreseen.

Datasets acquired during the campaign must follow the ACTRIS data lifecycle:

- Identification (DOI)
- Cataloguing and harvesting
- Data discovery (including data preview)
- Public distribution according to ACTRIS Data policy
- Data usage statistics
- Long term preservation

However, the DC requires the tools necessary to offer to setup a specific website. It will be mainly dedicated to the campaign community and will offer extra features for the data providers:

- Metadata edition
- Dataset upload
- Restricted distribution of not-validated data during the post campaign period
- User management

CMS features (news publication, statics pages, document upload)

4.8 User community support and services

As a tool for science, the highest priorities for the ACTRIS Data Centre is to compile data, and maintain and increase the availability of ACTRIS data and data products relevant to climate and air quality research for all interested users.

4.8.1 ACTRIS Data provenance, attribution, and traceability

In an effort to spread good practise for attribution of data production efforts and traceability of data, ACTRIS offer the same routines to the user community for documenting data provenance as those used internally described in section 3.3 .

4.8.2 Support to regional and global networks and related initiatives

ACTRIS will support international frameworks in the field of air quality and climate change, e.g., GAW, EMEP, GALION, and GCOS, and further utilize and add value to satellite based atmospheric observations. It is a requirement that the ACTRIS data centre supports GAW and the EMEP program by contributing with required scientific and technological expertise in relation to atmospheric observations, and will also offer tools and data curation facilities to improve and ensure the harmonization and standardization of data and meta-data. This will ensure impacts and harmonization on both a regional and global scale. Specifically, it is required that ACTRIS support ongoing efforts made by the EMEP Chemical Coordinating Centre, and of the EMEP Task Force on Measurements and Modelling, as well as relevant bodies and institutions engaged in Global Atmosphere Watch (i.e. http://www.wmo.int/pages/prog/arep/gaw).

4.8.3 Interoperability and link to other RIs and initiatives

Interoperability in ACTRIS shall be guided by the FAIR Data Principles Findable, Accessible, Interoperable, Re-Usable laid out by the FORCE11 community. In ACTRIS, these will be implemented by the following measures:

Findable: All ACTRIS data shall be uniquely identified by DOIs (identification requirement). ACTRIS data shall be accompanied by a comprehensive set of metadata including discovery, quality, uncertainty, and production process metadata, including a complete provenance record (rich metadata requirement). ACTRIS data have to be registered with domain relevant higher level frameworks facilitating their discovery for re-use, which includes the European Open Science Cloud (EOSC), the Global Earth Observation System of Systems (GEOSS), the WMO Integrated Global Observing System (WIGOS), and the EU Copernicus Atmospheric Services (CAMS) (indexing requirement). Mutual data discovery also includes the European atmospheric RIs IAGOS and ICOS.

Accessible: ACTRIS data and metadata shall be accessible by domain-specific standardised machine-to-machine interfaces. Metadata can be served via the OAI-PMH protocol. Data shall be served via e.g. the OPeNDAP and OGC protocols. A World Wide Web Consortium (W3C) endorsed SPARQL endpoint can be considered. By definition, ACTRIS data DOIs point to the human- and machine-readable interfaces of the dataset.

Interoperable: The metadata interface deploys the standardised, community specific and WMO endorsed metadata profiles of the WMO Information System (WIS) and WIGOS, with vocabularies of the Climate and Forecast (CF) conventions and WIGOS. The data services make use of the NetCDF format, which is commonly used in the atmospheric community.

Re-usable: Use of an open-access data policy, combined with a full documentation of provenance, and meeting community standards in data and metadata services and formats, ensures the re-usability of ACTRIS data.

4.8.4 Knowledge transfer and training on the use of data products and tools

ACTRIS DC offers services devoted to the transfer of knowledge addressed to the heterogeneous expected user community: from scientists to local authorities and citizens at large.

Fostering the international scientific cooperation, training activities addressed to scientific community about the use of offered data production and processing tools are offered. Additionally, tutorials about the use and the correct interpretation of ACTRIS data from Lev1 to Lev 3 are offered. The tutorials shall be specifically addressed to the different communities, so replying to the specific needs related to the background expertise and knowledge of the different users.

5 Organization and management structure of the ACTRIS Data Centre

All ACTRIS Central Facilities (CFs) shall be organized according to the role of the specific CF, ensuring that the CF complies with the requirements and obligations described in section 6 and 8 of this document, and considering the general principles described in the *Baseline document for the concept of the Central Facilities*. The ACTRIS Data Centre (ACTRIS DC) shall be organized such that:

- It has a well-defined structure of Units,
- It has a well-defined links, procedures and structure for interaction between any DC Units, and TCs and NFs
- It has a well-defined decision-making process,
- It is coordinated by a CF Director and managed by a CF Management Board, which consists of the CF Director and the CF Unit Heads,
- It has clear and cost-efficient task sharing between the Units,
- It has a risk management strategy,
- It participates in the ACTRIS decision making by sending representative(s) to the ACTRIS legal entity bodies, e.g. to the RI committee.

6 Requirements for the ACTRIS Data Centre

6.1 General requirements for Central Facilities

ACTRIS Data Centre shall:

- Commit for long-term operation (at least 10 years)
- Ensure appropriate links between the various activities to ensure a robust, cost-effective and functional data centre,
- Document the capacity in terms of material and personnel resources, to ensure the provision of the requested services and operation support, as described in section 6.2

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- Provide a feasible implementation and operation plan for the first five years, starting with the first year after the selection as CF.

6.2 Specific requirements for ACTRIS Data Centre

ACTRIS DC must comply with these requirements:

- Answer to specific needs for data curation for the methodologies applied by ACTRIS NF;
- Provide virtual access to ACTRIS data, services and tools via the ACTRIS data user interface
- If the ACTRIS Data Centre is distributed across different nodes, demonstrate close interaction between the nodes.
- Employ standardized nomenclature Climate and Forecast Metadata nomenclature (CF)
- Implement standardised meta data exchange protocols across the RI to ensure interoperability with other RIs and frameworks (e.g. WIGOS, GEOSS, and EOSC).
- Offer access to measurement data compliant with FAIR principles (FORCE11)
- Offer legally binding license systems to regulate the conditions of use and facilitate open data access common over the infrastructure
- Commit to provide the mandatory operation support to the ACTRIS NFs, as described in section 3
- Commit to provide mandatory core services listed in section 4 to the ACTRIS internal and external users
- Commit to provide the mandatory operation support to the ACTRIS NFs, as described in section 3.
- Commit to provide user services, as described in section 4
- Commit to offering virtual access to data and services to ACTRIS users as close to 24/7 as possible.
- Operate a secure and robust ICT infrastructure.
- Implement an information security policy

The information security policy must detail the measures taken to ensure data security by protecting data from being destroyed by either accidents or through deliberate actions by unauthorised users (cyberattacks). Data protection includes security procedures and backup procedures. In particular, the backup procedures must contain the following:

- Well-defined regular and frequent back up schedule
- Off-line backup requiring manual interaction
- Off-site data protection, where the archive is in a different location to the operational servers
- A disaster recovery plan

All data must be stored in such a way to:

- ensure the long term archival of all data products and pre-products produced in the associated workflow
- ensure long term archival of all QA and QC documents produced and referenced in the metadata
- ensure long term archival of any value-added services and references related to the data products

- ensure consistency and unambiguousness of data and metadata, harmonised across the RI and, if applicable, with other relevant frameworks
- enable traceability of changes in the archive (deletions, updates, corrections) and reproducibility of historic data holdings

ACTRIS data curation requests the following operational requirements

- Ensure sufficient availability of the system, , above 90% of the time is the ambition
- Monitoring of databases, data flows and system performance. Downtimes of components must be detected and escalated to technical staff automatically.
- Availability and response times of the web interface
- Detect backlogs and errors in submitted files.
- Analyse critical system components and define backup schedules for the different components. Typically, daily backups should be available.

6.2.1 Additional requirements of ACTRIS in situ aerosol, cloud and trace gas data services

ACTRIS in situ data curation requests the following additional operational requirement:

- Monitoring of databases and system:
    - Performance of the RRT dataflow

The ACTRIS in situ data curation and data base system must scale to handle

- Ca. 1000 QA files submitted per year (ca. 30 GiB)
- In addition, ca 30-50 RRT instruments is scheduled to submit approximately 300 000 files yearly.
- Overall, approximately 100-200 unique users use the system's web interface for data submission, about 1000-1500 unique users access data.
- Typically, between 1000 and 3000 instruments years of data are accessed per month.

The data archive for level 2 data is suited for a relational database system keeping all metadata and measurement data in one database. The data model is specialized for in situ time series. The database should support historic storage of data, so that the full history of changes can be traced at any time. Historic data content can be reproduced even if the data have been deleted or updated (corrected) in the archive.

The database is hosted on a dedicated database server. The web interface can be implemented with e.g. dot.net web application that accesses the archive database directly. The web application can e.g. use AJAX technology to achieve a more dynamic user experience.

The web application can be hosted on a dedicated web server. The data curation tasks, including the data ingestion, are performed using command line tools to interface with the database system. A dedicated Linux server is reserved for those tasks. For the RRT dataflow, a customized dataflow control software is used.

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6.2.2 Additional requirements of ACTRIS aerosol remote sensing data services

ACTRIS aerosol remote sensing data curation request the following additional operational requirement:

- Implementation of the Single Calculus Chain (SCC); the automatic and traceable processing tool for the analysis of Level 0 up to Level 1 products.

The ACTRIS aerosol remote sensing data curation and data base system must scale to handle

- about 150000 Level 0 files be submitted per year (ca. 4 TB)
- about 500 unique users use the system's web interface for data submission, about 1000-1500 unique users access data.
- about 500 unique SCC users

The data archive for level 1 and level 2 data is suited for a relational database system keeping all metadata and measurement data in one database. The database should support historic storage of data, so that the full history of changes can be traced at any time. Historic data content can be reproduced even if the data have been deleted or updated (corrected) in the archive.

The database is hosted on a dedicated database server. The web interface can be implemented PHP, Java or Python web application that accesses the archive database directly.

The web application should be hosted on a dedicated web server. The data curation tasks, including the data ingestion, are performed using both web (graphical) interface and via API allowing command line tools to interface with the database system.

The SCC should be implemented at least on three different dedicated servers: one hosting the SCC database where all the processing parameters are collected and used in the analysis; a second one running and coordinating all the SCC calculus modules; and finally a third server on which the SCC web interface is implemented.

The servers hosting the SCC should be designed to allow the automatic generation of RRT and RRT Level 1 products.

6.2.3 Additional requirements of ACTRIS cloud remote sensing data services

ACTRIS cloud remote sensing data curation request the following operational requirements:

- Monitoring of databases and system:
    - Performance of the NRT dataflow
    - Performance of the NRT NWP model data flow
- Implementation of the Cloudnet processing scheme producing Level 1 and 2 products from Level 0 data, together with full traceability.

The ACTRIS cloud remote sensing data curation and database system must scale to handle

- about 50000 Level 0 files submitted per year (ca. 5 TB) rising to 10 TB per year once Doppler spectra are stored.
- About 50000 Level 1 and 2 files stored per year (ca. 5 TB)

The data volume required for storing Level 1 and 2 data suits a file-based system which interacts with a relational database containing pertinent metadata for discovery and version control. The database and file system should be hosted on a dedicated server, with data ingestion in NRT through a separate dedicated FTP/SFTP server. The Cloudnet processing scheme should be implemented on a dedicated Linux server, with fast (high bandwidth) access to the database/fileserver. This server also performs the data curation tasks, including the single instrument data pre-processing and interfaces with the database server.

The web application should be hosted on a separate dedicated web server, with access to the data via a web API, which can be written in PHP and/or Python.

The servers hosting the cloud remote sensing database infrastructure should be designed to allow the automatic generation of NRT and RRT Level 1 and 2 products.

6.2.4 Additional requirements of ACTRIS trace gas remote sensing data

The volume of the prosed data sets is currently less than 1GB so that the data curation and database system do not need special requirements. The data processing scheme requires a dedicated server, with fast (high bandwidth) access to the database/fileserver. More clarifications and requirements will be made in 2018.

6.2.5 Additional of requirements of ACTRIS atmospheric simulation chamber data services

1.1.1.6 Facilities and requirements related to repositories and data curation

The ACTRIS atmospheric simulation chamber data are organized within three databases as described in section 3.5.1.1. The data products are stored in their own data model and original data formats. The database administration must trace the statistics of the database consultation.

The ACTRIS atmospheric simulation chamber data curation and database system must scale to manage all the data products collected during the time of the project and after (150 to 250 data sets – ca. 10 GB).

The web application is hosted on a dedicated web server, the data curation tasks including the data and metadata ingestion are performed using dedicated graphical web interfaces. A neutral client-side technology (web components, http://fr.wikipedia.fr/wiki/Composants_web) which allows developing custom rich html tags has been used to develop these interfaces. Concerning the data and metadata products, they are hosted on a dedicated database server (historical data and updates). Through the web interface, web applications permit to access the databases directly using RESTful requests.

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6.2.6 Additional requirements to the ACTRIS data user interface and access service

In contrast to lower data levels, level 3 data products may have arbitrary data structure and file formats. Thus, it is not required that these data products are stored in one unified data model, but rather in their original file formats. It is required that the data are accessible through the ACTRIS data user interface.

The archiving of these data files and the administration of their metadata must be performed in appropriate systems. In particular, the administration of DOIs and the related metadata are crucial:

- A suitable document archiving system / publishing system to archive the products
- Minting of DOI's, registration including all necessary metadata
- Provide landing pages for DOI's
- Provide data access through DOI landing page

The architecture needs to:

- Ensure sufficient availability of the system and data products
- Ensure regular back up of the archive (daily), keep off-site backups, and develop disaster recovery plans.

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6.3 Expected human resources

Operating the ACTRIS Data Centre requires in total about 20 persons (Full Time Equivalent) with complementary skills and a broad background. The expected minimum human resources for offering the planned services are shown in Fig. 3 and listed in the table below, associated with the expected expertise required for fulfilling the various data centre services envisaged.

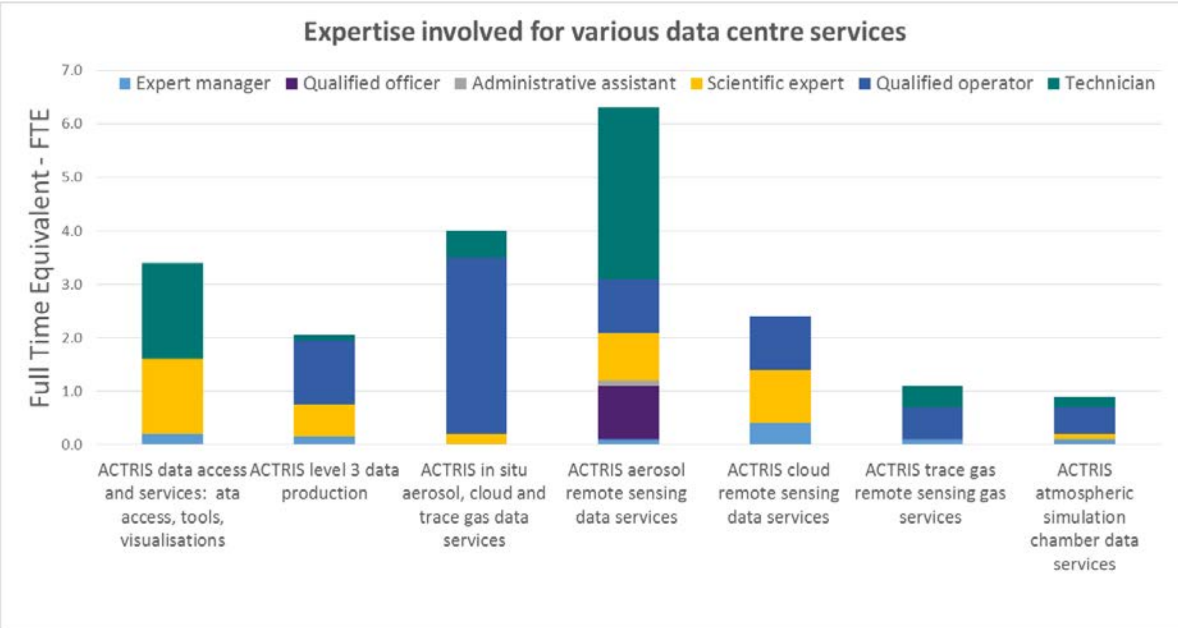

Figure 3: Expertise required for the various data centre services during operational phase, as described in section 3 and 4.

Table 1: The expected minimum human resources and expertise required to offer the planned operational services.

	Management & administration staff			Scientific & technical staff		
	Expert manager	**Qualified officer**	**Administrative assistant**	**Scientific expert**	**Qualified operator**	**Technician**
ACTRIS data access and services: data access, tools, visualisations	0.2	0.0	0.0	1.4	0.0	1.8
ACTRIS level 3 data combining various data and sources	0.2	0.0	0.0	0.6	1.2	0.1

ACTRIS in situ aerosol , cloud and trace gas services	0.0	0.0	0.0	0.2	3.3	0.5
ACTRIS aerosol remote sensing data services	0.1	1.0	0.1	0.9	1.0	3.2
ACTRIS cloud remote sensing data services	0.4	0.0	0.0	1.0	1.0	0.0
ACTRIS trace gas remote sensing data	0.1	0.0	0.0	0.0	0.6	0.4
ACTRIS atmospheric simulation chamber data services	0.1	0.0	0.0	0.1	0.5	0.2

7 Basic criteria for the selection of the ACTRIS Data Centre

Applications to host the ACTRIS Data Centre shall be evaluated against a set of criteria covering:

- The **level of commitment** for long-term operation
- The **capacity** to provide the operational support and the services described in sections 3 and 4
    - The availability of the necessary infrastructure and equipment
    - The availability of human resources (no., expertise)
- The **efficiency** in providing operational support and the services
    - The feasibility of the implementation plan (costs, resources, timeline)
    - The feasibility of the operation plan (methodology, costs per service)
- The **level of maturity**
    - Adequacy of the decision-making
    - Risk management strategy

These criteria will be detailed in the associated call documents.

8 Obligations of the ACTRIS Data Centre

8.1 General obligations

The following general obligations shall apply to the ACTRIS Data Centre. The ACTRIS DC is obliged:

- To organize its activities in a cost-efficient way, timely, and with high quality,
- To actively participate in the governance and sustainable development of ACTRIS,
- To provide services to users, according to the access procedures, and data policy
- To provide operation support to NFs, according to identified needs, agreed schedules, and procedures,
- To implement efficient user interaction activities by:
    - Organizing workshops, to interact with users,
    - Collecting user feed-back,
    - Maintaining CF and ACTRIS websites,
- To document its activities, data offered and accesses provided, key performance indicators, and finances, and provide this information to the HO,
- To contribute to minimize and assess the uncertainties related to data and data products, according to their role and in collaboration with each other.

8.2 Technical obligations

The ACTRIS Data Centre and its potential units are obliged to put in place and offer the specific operation support marked with * in this document, section 3 and section 4. Other operation support described in this document is not mandatory for the data centre, but recommended.

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8.2.1 Obligations towards the ACTRIS National Facilities

Technical obligations of the ACTRIS Data Centre towards the ACTRIS National Facilities refer strictly to the data curation of data and measurements described in this concept document and in *Technical concepts and requirements for ACTRIS Observational Platforms.* New techniques / instrument types are only accepted as ACTRIS instruments after the approval of the RI Committee and after the development of the associated QA procedures by the relevant CF. The operation of other techniques at the NFs does not imply obligation for the ACTRIS Data Centre to provide services or support.

8.2.1.1 Guidelines, quality control of data and procedures

The ACTRIS Data Centre is responsible for the quality control procedures applied to ACTRIS data and shall offer access to the guidelines for ACTRIS measurements conducted at the NFs. A full overview of all variables is included in Annex I, together with their associated TC. TCs develop and perform instrument QA, the DC develops and performs QC of submitted data. The procedures and routines and criteria for acceptance is defined in collaboration with the TC and DC.

8.2.1.2 Assessment of performances

The ACTRIS Data Centre is mandated to assist the related NFs and TC in the quality control of the measurements and data, by:

- Ensuring access to level 0 to level 3 data products
- Ensuring traceability of level 0 to level 3 data products
- Organizing regular exercises to assess the quality and control of the data
- Providing feedback on QC procedures and outcome to the NF

These activities require direct involvement of both NFs and TCs, and NFs should participate in these activities according to the plan proposed by the ACTRIS Data Centre and agreed together with the ACTRIS Scientific Advisory Board (SAB).

8.2.1.3 Transfer of knowledge and training

In addition to the training organized for the implementation of guidelines, procedures, and tools developed in support of the quality control of the measurements, the DC will organize training sessions with NFs for data submissions, metadata inclusion, flagging of data, the use of tools and software for QC. NFs should participate in these activities according to the plan proposed by the ACTRIS Data Centre and agreed together with the ACTRIS Scientific Advisory Board (SAB).

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8.2.2 Obligations towards the ACTRIS Topical Centres

The general share of responsibilities between the topical centres and the ACTRIS Data Centre is described in detail in the TC concept documents. ACTRIS DC shall ensure the implementation of a structure for interlinks, interactions, and collaboration. A proposed structure of a data centre with distributed nodes are illustrated in the figure below. An ACTRIS Data Expert team involving representatives from the DC, TC and NF is required to ensure the interactions. The team should be directed by the data centre leader.

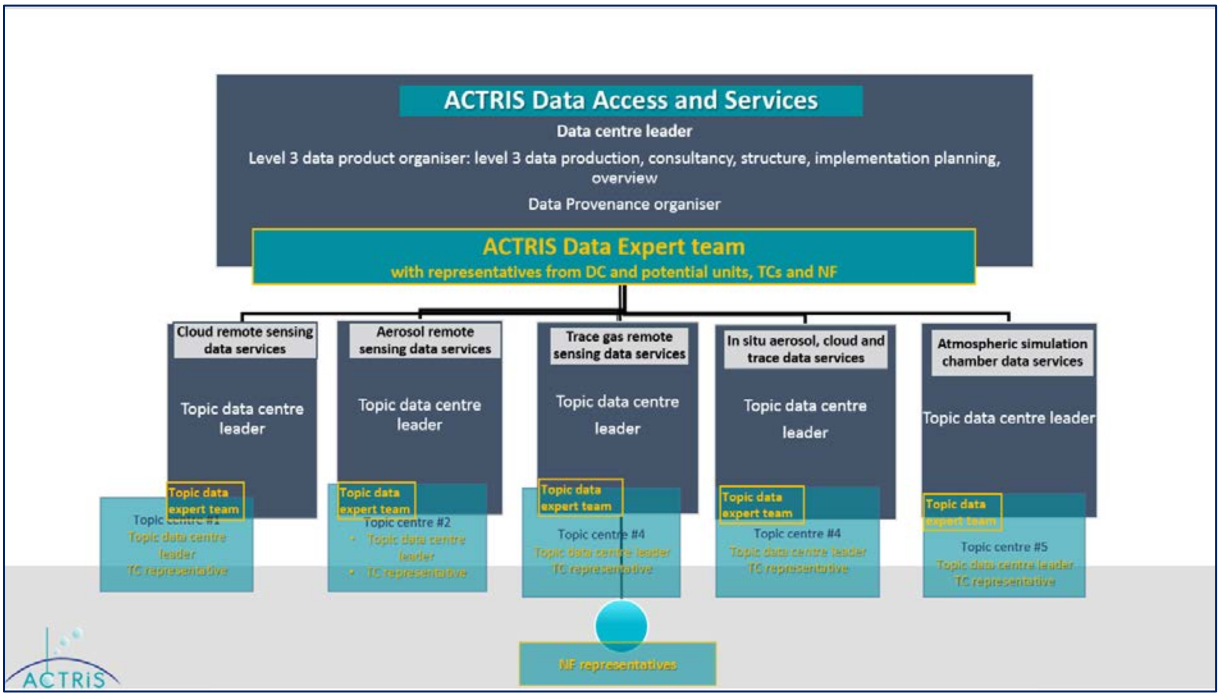

Figure 4: Schematic diagram of a structure for a distributed data centre ensuring interlinks, interactions, and collaboration within the ACTRIS Data Centre with the TC and NF, and for the integration and harmonisation across the RI. A Data Expert team is required to ensure the interactions between potential units and TCs.

8.3 Evaluation of ACTRIS Data Centre activities

The ACTRIS Data Centre performance will be evaluated annually with respect to Key Performance Indicators (KPIs), taking into consideration the general and technical obligations that have been described within this document. In the case of Data Centre distributed amongst several nodes, there will be completed a KPI form for each data centre unit.

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Criteria	Indicator	Planned value	Achieved value	Percentage of achievement[4]	Weight
	GENERAL SCORE				
Usefulness for ACTRIS NFs	**CRITERIA TOTAL SCORE**				**35%**
	Online and accessible tools for the NFs 24/7				
	Archiving of annual data from ACTRIS NFs compared to submitted data to the DC				
	Response time by help and support desk				
	Average score of satisfaction received from NFs *Including utility and timeliness of the activities for support*				
Usefulness for ACTRIS users	**CRITERIA TOTAL SCORE**				**35%**
	Online and accessible level 2 and level 3 data 24/7				
	No. of annual level 2 data sets offered to external users				
	Monitor if the documentation made available for the users are accessible findable and used.				
	Average score of satisfaction received from ACTRIS users *Including utility and timeliness of the services performed*				
Impact on science &	**CRITERIA TOTAL SCORE**				**20%**
	Download of level 2 from the ACTRIS data user interface				
	Download of level 3 from the ACTRIS data user interface				
	Machine-to-machine data delivery of annual level 2 data sets				
	Machine-to-machine data delivery of level 3 data sets				
Integrati	**CRITERIA TOTAL SCORE**				**10%**
	No. of participations to ACTRIS committees and boards				

[4] With regard to the planned and approved values

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	No. of activities performed in collaboration with other TCs (joint SOPs, joint workshops, etc.)				
	Average score of satisfaction received from ACTRIS TC for the contribution to documentation and access to data products and tools				
	Average score of satisfaction received from ACTRIS HO for the quality and readiness of the reports				

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Glossary

ACTRIS data - are the ACTRIS variables resulting from measurements that fully comply with the standard operating procedures (SOP), measurement recommendations, and quality guidelines established within ACTRIS.

- **ACTRIS level 0 data:** Raw sensor output, either mV or physical units. Native resolution, metadata necessary for next level.
- **ACTRIS level 1 data:** Calibrated and quality assured data with minimum level of quality control.
- **ACTRIS level 2 data:** Approved and fully quality controlled ACTRIS data product or geophysical variable.
- **ACTRIS level 3 data:** Elaborated ACTRIS data products derived by post-processing of ACTRIS Level 0 - 1 -2 data, and data from other sources. The data can be gridded or not.
- **ACTRIS synthesis product** (*Proper name to be defined later*)**:** Data product from e.g. research activities**,** not under direct ACTRIS responsibility, but ACTRIS offer repository and access.

ACTRIS Data Centre (DC) - the Central Facility responsible for ACTRIS data curation, preservation, and distribution of data, value-added products and tools**,** and for hosting the ACTRIS data user interface.

ACTRIS data originator - entity operating instruments at a National Facility or Topical Centre, resulting in ACTRIS data and delivering ACTRIS data to the Data Centre.

ACTRIS data provider - the Data Centre offering ACTRIS data and value-added data products and tools to users.

ACTRIS digital tools and services - tailored codes and software for processing and visualization of ACTRIS data, production of ACTRIS data products, and for data analysis and research.

ACTRIS exploratory platform - National Facility (simulation chambers, laboratories, or mobile facilities) operating on a campaign basis and delivering dedicated data to the Data Centre.

ACTRIS General Assembly (GA) - the council of ministry- and funding organization representatives of ACTRIS members once the ACTRIS legal entity has been established, superior decision-making body of ACTRIS.

ACTRIS Head Office (HO) - a Central Facility coordinating and representing ACTRIS, and holding the statutory seat.

ACTRIS label - earmarks a data set or a measurement site as ACTRIS data or ACTRIS National Facility.

ACTRIS observational platform – ACTRIS National Facility performing long-term, regular observations and delivering standardized data to the Data Centre.

ACTRIS Topical Centres (TCs) – a Central Facility offering services and operation support for QA/QC of measurements and data (including training, calibration, QA/QC tools, and development of standard operation and evaluation procedures)

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ACTRIS variables - the measured atmospheric variables as described in the ACTRIS Data Management Plan[5].

Central Facility (CF) - a European level ACTRIS component that offers ACTRIS data or other ACTRIS services to users as well as operation support to ACTRIS National Facilities.

Central Facility Unit – part of a Central Facility located at, and operated by a research performing organization (RPO) or by ACTRIS ERIC.

CF Director – the person responsible for the coordination and representation of a Central Facility.

CF Unit Head – the person responsible for the coordination and representation of a Central Facility unit.

CF Management Board – consists of the CF Unit Heads and the CF Director; this board manages the Central Facility.

Data curation - the activity that stores, manages and ensures access to all persistent data sets produced within the infrastructure.

Data traceability - an unbroken chain of uniquely identified process steps leading from raw data to any kind of processed data, where identification of process steps follows the data.

In situ measurements - measured or sampled air and instrument are at the same location and in physical contact. In the context of ACTRIS, in situ measurements of aerosol, cloud, and reactive-trace-gas properties are performed at observational sites near the Earth surface, on mobile surface-based or airborne platforms, and in atmospheric simulation chambers and laboratories.

Interim ACTRIS Council - a council of ministry- and funding organization representatives of ACTRIS members before ACTRIS legal entity has been established (during the ACTRIS Preparation and Transition Phase), superior decision-making body of ACTRIS.

Measurement traceability - an unbroken chain of comparisons relating an instrument's measurements to a known standard, SI units in the ideal case.

National Facility (NF) - an observational or exploratory platform providing data and/or physical access to the platform within ACTRIS.

Quality assurance and control: Quality assurance is process oriented and focuses on defect prevention; quality control is product oriented and focuses on defect identification:

- **Quality Assurance (QA):** The process or set of processes used to ensure the quality of a product (e.g. data series, instrument, sample, measured value of a variable, etc.),
- **Quality Control (QC):** The process and activities of ensuring products and services meet the expectations.

Remote sensing - measured air and instrument are not at the same location and not in physical contact. In the context of ACTRIS, active and passive atmospheric remote-sensing techniques for the

[5]The ACTRIS data management plan and list of variables were approved by ACTRIS-2 scientific steering committee, October 2015. These documents are expected to be refined during ACTRIS-PPP (WP5).

observation of aerosols, clouds, and trace gases are applied at observational sites and on mobile surface-based or airborne platforms.

RI committee – consists of up to two representatives from each Central Facility and [three] representatives from the National Facilities Assembly; the RI committee supports the (Interim) Director or Board of Directors in operating the RI.

Service and Access Management Unit (SAMU) - a part of ACTRIS Head Office facilitating the access to ACTRIS services.

User - a person, a team, or an institution making use of ACTRIS data or other ACTRIS services, including access to ACTRIS facilities.

Reference documents

ACTRIS-PPP proposal

ACTRIS Data Management Plan, approved by ACTRIS-2 SSC 23 October 2015

ACTRIS Concept Documents

ISO 10012:2003: Measurement management systems — Requirements for measurement processes and measuring equipment

ISO 9000:2015: Quality management systems—Fundamentals and vocabulary

Annex I: Catalogue with ACTRIS variables and detailed description

Full version of the file and detailed information for each variable is available from here until 1 March 2018:

https://folk.nilu.no/~richard/actris-ri-variables/Appendix_I_ACTRIS-RI_variables_21February2018.xlsx

Annex I: Catalogue with ACTRIS L1-L2 data from observational NF	Colour codes for measurement techniques	
	Variable produced from a single measurement technique	
	Variable produced from synergy of measurement techniques	
	Variable produced from synergy of measurement techniques where combinations are possible	

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ACTRIS variable	NF requirements Mandatory - M Specializing - S Optimum - O	Data level	Associated Topical Centre	Data producer	RRT-O= operational in RRT now RRT-S = scheduled from 2020	Time resolution	Integrating Nephelometer	Mobility Particle	Aerodynamic & Optical Particle Size	Absorption Photometer	Condensation Particle	Scanning PSM, (N)AIS, N-MPSS	Particle Size Magnifier (PSM)	Cloud Condensation Nuclei Counter	Filter sampling	Thermal-optical analyser	Offline filter-based	Aerosol Mass Spectrometer	X-Ray Fluorescence, Particle Induced X-ray
Aerosol in situ																			
Particle light scattering and backscattering coefficients	M	L0, L1, L2	CAIS	NF	NRT-O	1h	■												
Particle number size distribution - mobility diameter	M	L0, L1, L2	CAIS	NF	NRT-O	1h		■											
Particle number size distribution - optical and aerodynamic diameter	S	L0, L1, L2	CAIS	NF	NRT-S	1h			■										
Particle light absorption coefficient and equivalent black carbon concentration	M	L0, L1, L2	CAIS	NF	NRT-O	1h				■									
Particle number concentration	S	L0, L1, L2	CAIS	NF	NRT-S	1h					■								

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ACTRIS variable	NF requirements Mandatory - M Specializing - S Optimum - O	Data level	Associated Topical Centre	Data producer	RRT-O= operational in RRT now RRT-S = scheduled from 2020	Time resolution	Integrating Nephelometer	Mobility Particle	Aerodynamic & Optical Particle Size	Absorption Photometer	Condensation Particle	Scanning PSM, (N)AIS, N-MPSS	Particle Size Magnifier (PSM)	Cloud Condensation Nuclei Counter	Filter sampling	Thermal-optical analyser	Offline filter-based	Aerosol Mass Spectrometer	X-Ray Fluorescence, Particle Induced X-ray
Aerosol in situ																			
Nanoparticle number size distribution	S	L0, L1, L2	CAIS	NF	NRT-S	1h													
Nanoparticle number concentration	S	L0 ,L1, L2	CAIS	NF	NRT-S	1h													
Cloud condensation nuclei number concentration	S	L0, L1, L2	CAIS	NF	NRT-S	1h													
Mass concentration of particulate organic and elemental carbon	S	L2	CAIS	NF	-	<48h - 2/week													
Mass concentration of particulate organic tracers	S	L2	CAIS	NF	-	<48h - 2/week													

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ACTRIS variable	NF requirements Mandatory - M Specializing - S Optimum - O	Data level	Associated Topical Centre	Data producer	RRT-O= operational in RRT now RRT-S = scheduled from 2020	Time resolution	Integrating Nephelometer	Mobility Particle	Aerodynamic & Optical Particle Size	Absorption Photometer	Condensation Particle	Scanning PSM, (N)AIS, N-MPSS	Particle Size Magnifier (PSM)	Cloud Condensation Nuclei Counter	Filter sampling	Thermal-optical analyser	Offline filter-based	Aerosol Mass Spectrometer	X-Ray Fluorescence, Particle Induced X-ray
Aerosol in situ																			
Mass concentration of non-refractory particulate organics and inorganics	S	L2	CAIS	NF/TC	NRT-S	1h													
Mass concentration of particulate elements	S	L1, L2	CAIS	NF	-	<48h - 2/week													

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ACTRIS variable	NF requirements Mandatory - M Specializing - S Optimum - O	Data level	Associated Topical Centre	Data producer	RRT-O= operational in RRT now RRT-S = scheduled from 2020	Recommended time resolution	Mobility Particle Size Spectrometer	Condensation Particle Counter	Integrating Cloud Probe	Cloud Droplet Probe	Cloud Ice Probe	Aerosol Particle Sampler	Bulk collectors	INP instrument
Cloud in situ														
Liquid Water Content	M	L0, L1, L2	CIS	NF	NRT-S	1 min			■					
Droplet effective diameter	M	L0, L1, L2	CIS	NF	NRT-S	1 min			■					
Droplet number concentration	S	L0, L1, L2	CIS	NF	NRT-S	1 min				■				
Droplet size distribution	S	L0, L1, L2	CIS	NF	NRT-S	1 min				■				
Interstitial aerosol number concentration	S	L0, L1, L2	CIS	NF	NRT-S	1 Min		■						
Interstitial aerosol size distribution	S	L0, L1, L2	CIS	NF	NRT-S	20 min	■							
Total aerosol number concentration	S	L0, L1, L2	CIS	NF	NRT-S	1 Min		■						
Total aerosol size distribution	S	L0, L1, L2	CIS	NF	NRT-S	20 min	■							
Cloud residuals number concentration	O	L0, L1, L2	CIS	NF	NRT-S	10 min		■						

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ACTRIS variable	NF requirements Mandatory - M Specializing - S Optimum - O	Data level	Associated Topical Centre	Data producer	RRT-O= operational in RRT now RRT-S = scheduled from 2020	Recommended time resolution	Mobility Particle Size Spectrometer	Condensation Particle Counter	Integrating Cloud Probe	Cloud Droplet Probe	Cloud Ice Probe	Aerosol Particle Sampler	Bulk collectors	INP instrument
Cloud in situ														
Cloud residuals composition	O	L1, L2	CIS	NF	NRT-S	1 h								
Ice particle number concentration	S	L0, L1, L2	CIS	NF	NRT-S	1 min								
Ice particle size distribution	S	L0, L1, L2	CIS	NF	NRT-S	10 min								
Ice nucleating particle number concentration	S	L0, L1, L2	CIS	NF	NRT-S	1 h								
Ice nucleating particle temperature spectrum	S	L1, L2	CIS	NF	NRT-S	<= 24 h								
Bulk cloud water chemical composition	S	L1	CIS	NF	NRT-S	<= 24 h								

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ACTRIS variable	NF requirements Mandatory - M Specializing - S Optimum - O	Data level	Associated Topical Centre	Data producer	RRT-O= operational in RRT now RRT-S = scheduled from 2020	Time resolution	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	Of-line glass flask	NO-O3 chemiluminescence	Potentially other measurement technique supported by the TC	Cavity Attenuated Phase Shift Spectroscopy (CAPS)	CI-APi-TOF
Trace gases in situ																				
MHCs	M*, O	L0, L2	CGas-SiM	NF	NRT-S	1 h-2/week														
OVOCs	M*, O	L0, L2	CGas-SiM	NF	NRT-S	4 h-2/week														
Terpenes	M*, O	L0, L2	CGas-SiM	NF	-	1 h-2/week														
NO	M	L0, L1, L2	CGas-SiM	NF/TC	NRT-S	1h														
NO2	M	L0, L1, L2	CGas-SiM	NF/TC	NRT-S	1h														
Condensable vapours	O*, S	L2	CGas-SiM	NF/TC	NRT-S	10 min														

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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	Time resolution	Approx. height resolution	High-power aerosol LIDAR	Automatic sun/sky/lunar photometer	Automatic low-power aerosol LIDAR	Integrating Nephelometer	Mobility Particle Size Spectrometer	Aerodynamic & Optical Particle Size Spectrometer
Aerosol remote sensing												
Attenuated backscatter profile	M	CARS	DC	NRT-S	1h, 5/week	60 m						
Volume depolarization profile	M	CARS	DC	NRT-S	1h, 5/week	60 m						
Particle backscatter coefficient profile	M	CARS	DC	NRT-S	1h, 5/week	60 m						
Particle extinction coefficient profile	M	CARS	DC	NRT-S	1h, 5/week	60 m						
Lidar ratio profile	M	CARS	DC	NRT-S	1h, 5/week	60 m						
Ångström exponent profile	O	CARS	DC	NRT-S	1h, 5/week	60 m						
Backscatter-related Ångström exponent profile	O	CARS	DC	NRT-S	1h, 5/week	60 m						
Particle depolarization ratio profile	M	CARS	DC	NRT-S	1h, 5/week	60 m						
Particle layer geometrical properties (height and thickness)	M	CARS	DC	NRT-S	1h, 5/week	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	Time resolution	Approx. height resolution	High-power aerosol LIDAR	Automatic sun/sky/lunar photometer	Automatic low-power aerosol LIDAR	Integrating Nephelometer	Mobility Particle Size Spectrometer	Aerodynamic & Optical Particle Size Spectrometer
Aerosol remote sensing												
Particle layer optical properties: extinction, backscatter, LIDAR ratio, Ångström exponent, depolarization ratio, optical depth	M	CARS	DC	NRT-S	1h, 5/week	60 m						
Column integrated extinction	M	CARS	DC	NRT-S	1h, 5/week	60 m						
Planetary boundary layer height	O	CARS	DC	NRT-S	1h, 5/week	60 m						
Spectral Downward Sky Radiances	M	CARS	TC	NRT-O	1h	NA						
Direct Sun/Moon Extinction Aerosol Optical Depth (column)	M	CARS	TC	NRT-O	15min	NA						
Aerosol columnar properties	M	CARS	DC	NRT-S	1h	NA						
Aerosol profile microphysical and optical properties	M	CARS	DC	NRT-S	1h, 5/week	GARRLIC Resolution						

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ACTRIS variable	NF requirements Mandatory - M Specializing - S Optimum - O	Data level	Associated Topical Centre	Data producer	RRT-O= operational in RRT now RRT-S = scheduled from 2020	Recommended time resolution	Approx. height resolution for remote sensing data	Cloud radar	Doppler cloud radar	Lidar/ceilometer	Radiosonde	Microwave radiometer	Drop-counting raingauge	Disdrometer	NWP model input required
Cloud remote sensing															
Cloud/aerosol target classification	M	L2	CCRES	DC	NRT-O	30s	60m								
Drizzle drop size distribution	M	L2	CCRES	DC	NRT-O	30s	60m								
Drizzle water content	M	L2	CCRES	DC	NRT-O	30s	60m								
Drizzle water flux	M	L2	CCRES	DC	NRT-O	30s	60m								
Ice water content	M	L2	CCRES	DC	NRT-O	30s	60m								
Liquid water content	M	L2	CCRES	DC	NRT-O	30s	60m								
Liquid water path	M	L1,L2	CCRES	DC	NRT-O	30s	-								
Temperature profile	O	L1,L2	CCRES	DC	NRT-O	30s	variable								
Relative humidity profile	O	L1,L2	CCRES	DC	NRT-O	30s	variable								
Integrated water vapour path	O	L1,L2	CCRES	DC	NRT-O	30s	-								

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ACTRIS variable	NF requirements Mandatory - M Specializing - S Optimum - O	Data level	Associated Topical Centre	Data producer L1, L2	RRT-O= operational in RRT now RRT-S = scheduled from 2020	FTIR	UVVIS - ZS	UVVIS- MAXDOAS
Trace gases remote sensing					-			
Ozone partial columns		L2	RTGRSC		NRT-O			
Ozone column		L2	RTGRSC		NRT-O			
Formaldehyde column		L2	RTGRSC		NRT-O			
Formaldehyde lower tropospheric profile		L2	RTGRSC		NRT-O			
NO2 column	To be decided later	L2	RTGRSC	To be decided later	NRT-O			
NO2 lower tropospheric profile		L2	RTGRSC		NRT-O			
NH3 column		L2	RTGRSC		NRT-O			
C2H6 column		L2	RTGRSC		NRT-O			
SO2 lower tropospheric profile		L2	RTGRSC		NRT-O			
SO2 column		L2	RTGRSC		NRT-O			

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Annex II: ACTRIS level 3 data products

Full version of the file and all detailed information for each level 3 product is available from here until 1 March 2018:

https://folk.nilu.no/~richard/actris-ri-variables/Appendix_II_ACTRIS-RI_level3_variables_21February2018.xlsx

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ACTRIS level 3 data product name	Expected user community A= Academia B=Business and industry P= policy makers, authorities, etc.	Aerosol/ Cloud/ Trace gas	Profile: P Total column: C Near surface: S	ACTRIS L0-L2 data: Obs Model product - M Earth observation - EO	Required external data and source	Status O= operational from 2020. S= Support required from supporting projects
Column Water Vapour Content	A	Trace gas	C	Obs	ACTRIS L1 , AERONET	O
Climatology products for ACTRIS variables @ ACTRIS National Facilities across Europe	A, P	Aerosol/Trace gas	S, P	Obs	ACTRIS L2	S
Calculated Particle light scattering coefficients	A	aerosol	S	Obs	ACTRIS L2	O
Collocation service of data from contributing networks	A, P	aerosol	S	Obs	ACTRIS L2, EMEP	O
PM retrieval @GAW sites	A, P	aerosol	S	Obs	ACTRIS L2	S
Single Scattering Albedo @ACTRIS National Facilities	A, P	aerosol	S	Obs	ACTRIS L2	S
Calculated particle light extinction coefficient	A	aerosol	S	Obs	ACTRIS L2	S
Integrated full-range particle number size distribution	A	aerosol	S	Obs	ACTRIS L2	S
Source apportionment of submicron organic aerosols in Europe	A, P	Aerosol	S	Obs	ACTRIS L2	S
Volatile Organic Compounds (VOC) source attribution across Europe	A, P	Trace gas	S	Obs-M	ACTRIS L2	S
Cloud occurrence at cloud in situ observational platforms	A, P	Cloud	S	Obs	ACTRIS L2	O
Direct Sun/Moon Extinction Aerosol Optical Depth (column)	A	Aerosol	C	Obs	AERONET L1	O
Spectral Downward Sky Radiances	A	Aerosol	C	Obs	AERONET L1	O
Aerosol columnar properties	A	Aerosol	C	Obs	ACTRIS	S
ReOBS	A	Aerosol/ Cloud/ Trace gas	P, C, S	EO-Obs-M	ACTRIS L1, L2, AERONET, METEOSAT	S

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ACTRIS level 3 data product name	Expected user community A= Academia B=Business and industry P= policy makers, authorities, etc.	Aerosol/ Cloud/ Trace gas	Profile: P Total column: C Near surface: S	ACTRIS L0-L2 data: Obs Model product - M Earth observation - EO	Required external data and source	Status O= operational from 2020. S= Support required from supporting projects
Aerosol profile microphysical and optical properties	A	Aerosol	P	Obs	ACTRIS	S
Satellite data – combined with ground based ACTRIS data	A, P	Aerosol	P, C, S	EO-Obs	ACTRIS L2, MODIS, PARASOL, CALIPSO, CloudSat, OMI, MISR, Envisat/AATSR, IASI, MSG/SEVIRI	O
ACTRIS data products involving regional and global models						
Aerosol and Gas trend assessment	A, P	Aerosol/Trace gas	C,S	Obs-EO-M	ACTRIS L2, /AERONET/AEROCOM/CAMS	O
Data Interpretation and Outlier Identification Tool	A, P	Aerosol/Trace gas	S	Obs-M	EBAS/CAMS	O
Optimal interpolation and Gap filling tool	A	aerosol	P, C, S	Obs-M	ACTRIS L2/AEROCOM	S
Model Evaluation Service	A	aerosol, cloud	P, C, S	Obs-M	ACTRIS L2/AERONET/AEROCOM/ICAP/SDSWAS	O
NWP Model Evaluation Service	A	cloud	P, C, S	Obs-M	ACTRIS L2/NWP Models	O
Transport modelling products for assessment of source regions	A	Aerosol/Trace gas	P, C, S	M	ECMWF + FLEXPART	S
Alert Service for National Facilities	A	aerosol, cloud	P, C, S	M	CAMS/SDSWAS/CAP	S

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Annex III: ACTRIS workflow diagrams for data production

ACTRIS workflow diagrams depict the required interaction and distribution of work between NF - TC – DC as described in the Concepts of ACTRIS Central Facilities, and the description of NFs.

The diagrams will be available upon request to study the details.

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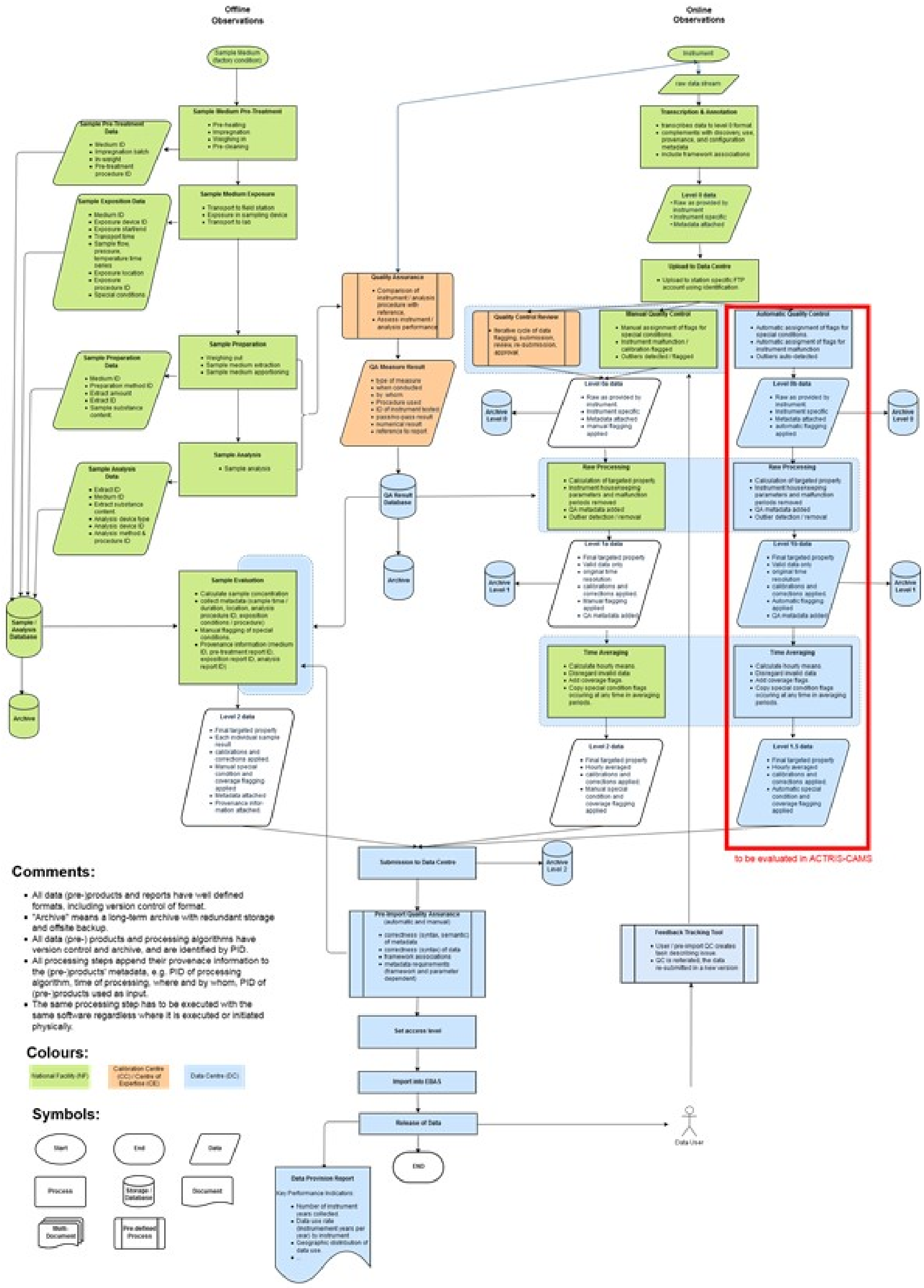
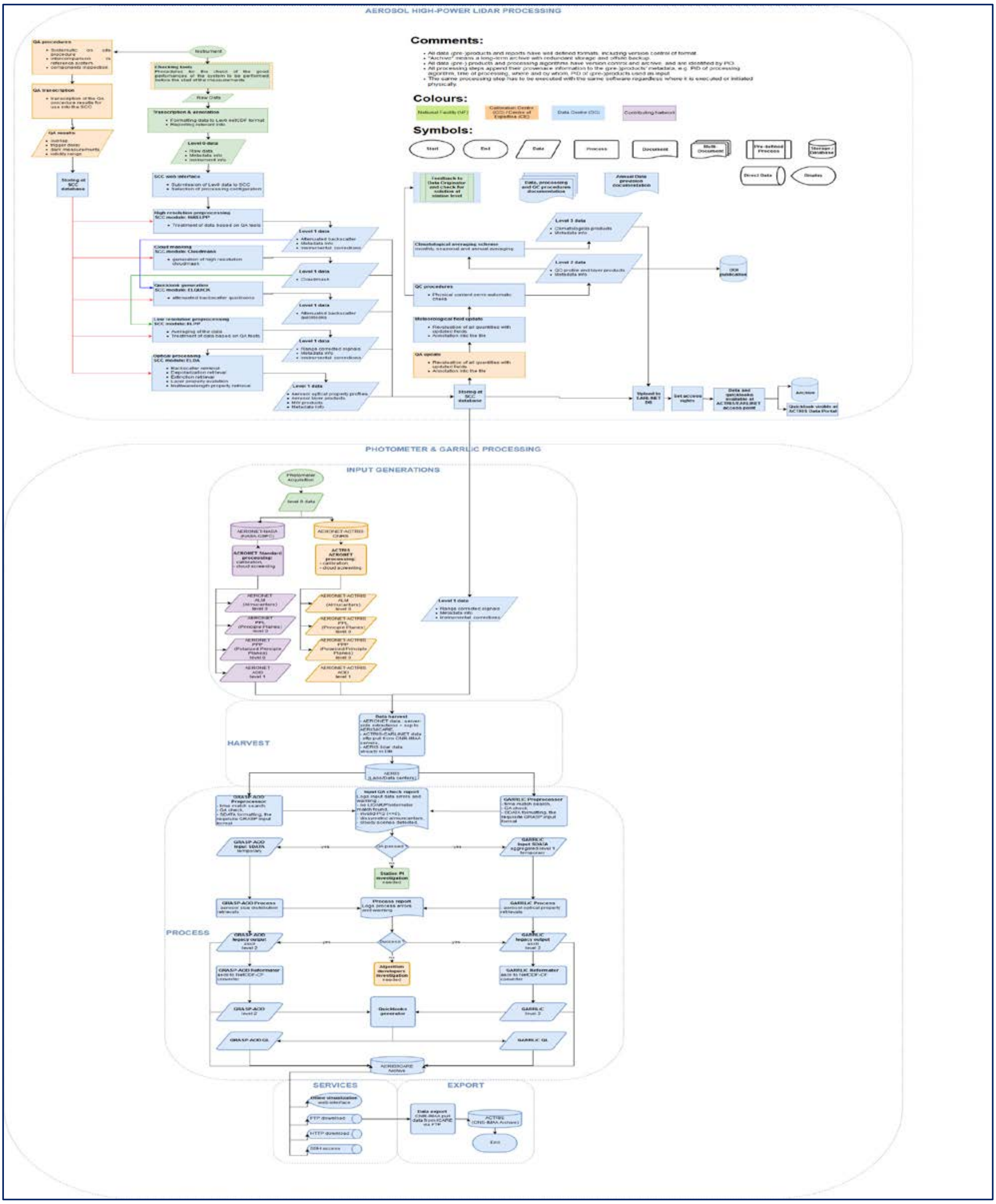
Draft ACTRIS in situ aerosol, cloud and trace gas data workflow

The picture can be downloaded from here for details: https://folk.nilu.no/~richard/actris-ri-variables/ until 1 March



Draft ACTRIS aerosol remote sensing data workflow

The picture can be downloaded from here for details: https://folk.nilu.no/~richard/actris-ri-variables/ until 1 March



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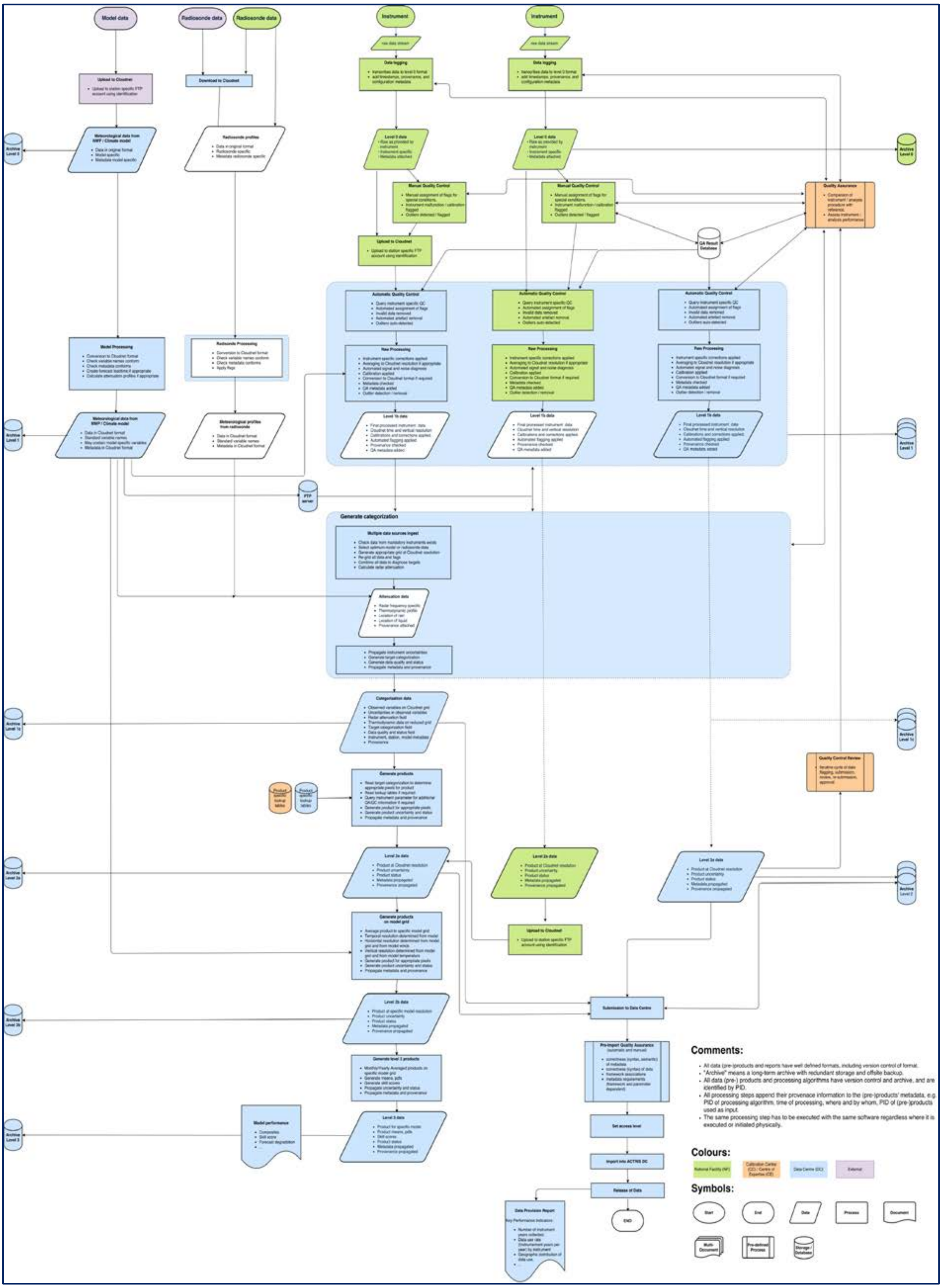
Draft ACTRIS cloud remote sensing data workflow

The picture can be downloaded from here for details: https://folk.nilu.no/~richard/actris-ri-variables/ until 1 March



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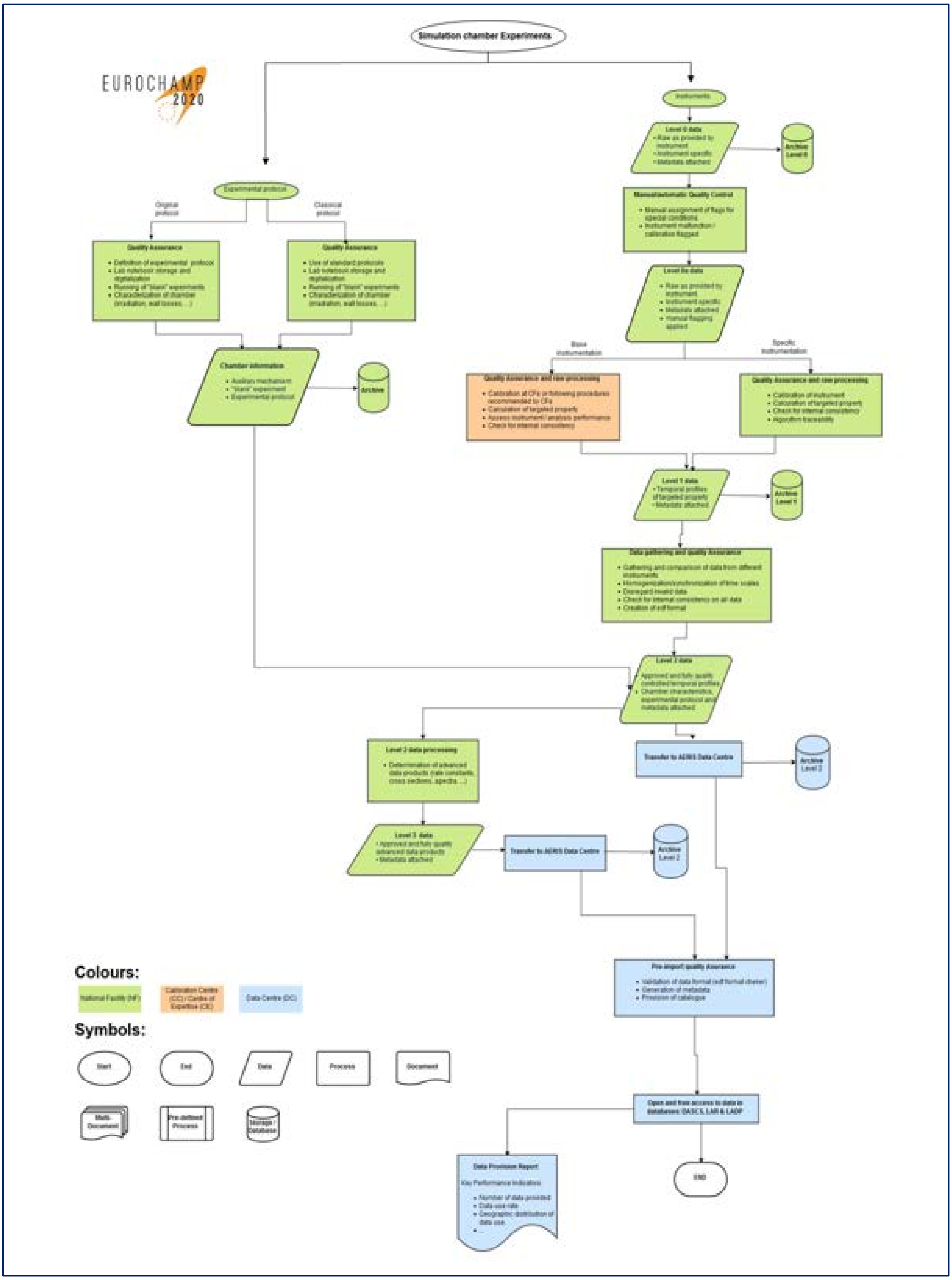
Draft ACTRIS atmospheric simulation chamber data workflow

The picture can be downloaded from here for details: https://folk.nilu.no/~richard/actris-ri-variables/ until 1 March



Section 3

Concept of the Centre for Aerosol In Situ Measurements

ACTRIS PPP WP 4 Task 4.1

26.2.2018

Public

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1 Purpose of the document

This document describes the relevance, mission, requirements and obligations of the ACTRIS Centre for Aerosol In Situ Measurements.

2 Description and role of the Centre for Aerosol In Situ Measurements

2.1 Framework

ACTRIS is the European platform for fostering the use of research data and data analysis tools in the field of atmospheric aerosols, clouds, and reactive trace gases. ACTRIS Central Facilities (CFs) represent the key operative entities of this Research Infrastructure (RI) and have a fundamental role as they provide services to the users according to the ACTRIS access policy as well as operation support to the National Facilities (NFs). CFs are operated at the European level and are part of the governance and decision-making structure of the RI. Each CF may have several operational Units that can be located in the same or different locations, and are operated by research performing organizations (RPOs) or by ACTRIS ERIC. The CFs link the NFs, i.e. the observational and exploratory platforms, which are operated at the national level and produce the majority of the ACTRIS measurement data.

The Centre for Aerosol In Situ Measurements is one of the six ACTRIS Topical Centres (TCs) organized around the main scientific themes of ACTRIS: aerosols, clouds, and reactive trace gases, each with a particular focus on either remote sensing or in situ measurement techniques.

2.2 Scientific relevance

Aerosol particles play an important role in atmospheric physics and chemistry. They contribute not only health effects, but also influence directly radiative climate forcing and indirectly by acting as cloud or ice nuclei. They are thus involved into the hydrological cycle, supply nutrients to oceanic and terrestrial ecosystems, influence heterogeneous atmospheric chemistry, lead to adverse health effects, and reduce visibility. In contrast to trace gases, which have "a" concentration, aerosol particles have multi-dimensional properties. First, aerosol particles cover a size range from 0.001 µm to approximately 100 µm, making them subject to size-dependent aerosol microphysical processes. Aerosol particles of a certain size may also have different shapes, leading to different particle surface areas, which is important, for instance, for heterogeneous chemical processes. Moreover, particles of the same size can have different chemical composition, and compounds in the particle can either be liquid or solid. Not all of these dimension can be currently accounted for by appropriate measurement techniques, but the most relevant ones with respect to climate forcing and air quality shall be measured at the ACTRIS aerosol in situ NFs. These are currently (2018):

- Particle number size distribution – mobility diameter (0.01 - 0.8 µm)
- Particle light scattering and backscattering coefficient (multi-wavelengths)
- Particle light absorption coefficient and equivalent black carbon concentration

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- Mass concentration of particulate organic and elemental carbon
- Particle number size distribution – optical and aerodynamic diameter (0.7 - 10 µm)
- Particle number concentration (> 0.01 µm)
- Mass concentration of particulate elements
- Mass concentration of particulate organic tracers
- Cloud condensation nuclei number concentration (at various supersaturations)
- Mass concentration of non-refractory particulate organics and inorganics
- Nanoparticle number concentration (< 0.01 µm)
- Nanoparticle number size distribution (0.001 - 0.02 µm)

Accordingly, operation support with respect to quality assurance and quality control (QA/QC) is needed for these variables in ACTRIS and this is described in this document.

The ACTRIS aerosol in situ observations already started to be established in the framework of the European projects CREATE (Construction, use and delivery of a European aerosol database, 2003 - 2005) and EUSAAR (European Supersites for Atmospheric Aerosol Research 2006 - 2011). In the ACTRIS-1 (2011 - 2015) and ACTRIS-2 (2015 - 2019) European projects this development was intensified, with a particular focus on harmonization, quality assurance and quality control. Now, in ACTRIS PPP (2017 - 2019) the definition and selection of aerosol in situ NFs and the respective TC shall be organized.

2.3 Mission

The mission of the Centre for Aerosol In Situ Measurements is to offer operation support to ACTRIS NFs operating instruments for the physical or chemical in situ characterization of atmospheric aerosol particles as well as for particle sampling and subsequent laboratory analysis of these particles.

Additionally, the Centre for Aerosol In Situ Measurements should offer specialized services for the above instruments and related ACTRIS variables, to ACTRIS users of various types: academia, business, industry, and public services.

3 Operation support provided to ACTRIS National Facilities

The operation support provided by the Centre for Aerosol In Situ Measurements comprises: a) procedures and tools for quality assurance and quality control of ACTRIS measurements and data, b) transfer of knowledge and training to ACTRIS operators, and c) improvements of measurement methodologies for aerosols, clouds, and reactive trace gases. The operation support is offered to the NFs for the measurement techniques described in this concept document, also listed in the *Technical concepts and requirements for ACTRIS Observational Platforms*.

The Centre for Aerosol In Situ Measurements is obliged to put in place and offer to NFs the specific operation support marked with ***** in this document. Other operation support described in this document is not mandatory for the TC, but recommended.

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The operation support can be scheduled or on request. Participation at the scheduled activities is mandatory for the NFs. Measurements not following the mandatory actions are not considered as ACTRIS-conform and do not yield ACTRIS data.

In addition, NFs may request operation support which is not scheduled, depending on the identified need. Specific operation support offered as scheduled or offered on request is detailed in *Annex: Provision of the operation support.* This annex shall be updated each time is necessary (e.g. development of new testing or calibration methods and tools).

The Centre for Aerosol In Situ Measurements should operate at the state-of-the-art, fostering the implementation of validated new techniques in ACTRIS. To sustain a high level of performance and to stimulate the advancement of new techniques and methodologies, the Centre for Aerosol In Situ Measurements contributes to expert collaboration networks.

3.1 Measurement techniques covered by the Centre for Aerosol In Situ Measurements, and related ACTRIS variables

3.1.1 Particle number size distribution - mobility diameter

A mobility particle size spectrometer (MPSS) is used to measure the particle number size distribution of the sub-micrometre size range from approximately 0.01 to 0.8 µm. The technology is well established and is commercially available, but there are also custom designed measurement systems. A MPSS is robust and designed for long-term operations. However, it need regular checks on-site to quality-assure the measurement. The MPSS includes also a Condensation Particle Counter (CPC), which ideally has to undergo frequent on-site checks. This is done by a Round-Robin test with CPCs, which are sent from station to station. Additionally, annual or biannual calibrations of the entire MPSS and the CPC against a reference instruments are required. In case the MPSS instrument performance is not controlled, MPSS might drift with time causing unnoticed biases in both particle sizing and particle number concentration of up to several ten percent.

3.1.2 Particle light scattering and backscattering coefficient

Currently (2018), an integrating nephelometer is used to determine the particle light scattering and backscattering coefficient, usually for the PM_{10} size range. The technology is well established and instruments are available from two manufacturers. Integrating nephelometers are robust and designed for long-term operations. Regular on-site gas calibrations are done with a frequency of at least once per three month to quality-assure the measurement. These calibrations are a common standard procedure already. Additionally, annual or biannual calibrations against a reference instrument are required. In case the nephelometer performance is not controlled, nephelometers might drift with time causing an unnoticed bias of up to several ten percent.

3.1.3 Particle light absorption coefficient and equivalent black carbon concentration

Generally, filter-based absorption photometers are used to determine the particle light absorption coefficient. The equivalent black carbon concentration mass concentration can be estimated from this.

Usually for regional site, the measurements are done for the PM10 size range, while for urban station also PM1 can be required. The technology is well established and different instruments are available covering different number of wavelengths. Absorption photometer are robust and designed for long-term operations. However, they need regular checks to quality-assure the measurement, especially in terms of cleaning. Additionally, annual or biannual calibrations against a reference instrument are required. In case the absorption photometer performance is not controlled, absorption photometers might drift with time causing an unnoticed bias of up to several ten percent.

3.1.4 Mass concentration of particulate organic and elemental carbon

Particulate organic and elemental carbon concentrations are determined from the thermal-optical analysis on atmospheric particulate matter deposited on filters. Thermal-optical analysers actually determine the mass of total carbon deposited on the filter. Total carbon is split in OC and EC by measuring the aerosol deposit light transmittance during the thermal analytical process. The measurement of OC and EC deposited on filters is described in the European standards EN 16909. It states that OC and EC shall be determined using the thermal protocol EUSAAR-2 (Cavalli et al., 2010), also described in EN16909. This protocol is currently used by most research performing organisations in Europe. However, the 14 inter-laboratory comparisons organised across Europe show that various instruments lead to different determination of total carbon and OC or EC content in the same filter. Support is therefore needed to determine systematic error (bias) or random error (variability) in the determination of the total carbon, OC and EC variables. The errors generally observed are about 10% for total carbon and 25% for EC. Feedback provided to the beneficiaries by the TC can help reduce systematic biases. At least, bias and variability communicated to the beneficiaries can be clearly associated to the final data products.

3.1.5 Particle number size distribution – optical and aerodynamic diameter

For the upper accumulation and coarse more size ranges, optical and aerodynamic particle size spectrometers (OPSS and APSS) are employed. The technology of the APSS is well established and is commercially available from one manufacturer. The APSS is robust and designed for long-term operations. There a different OPSS on the market, from which most could be used for long-term measurements. However, APSS and OPSS need regular checks on-site for sizing to quality-assure the measurement. Additionally, annual or biannual calibrations against a traceable standards and reference instruments are required. In case OPSS or APSS performance is not controlled, OPSS or APSS instruments might drift with time causing an unnoticed bias of up to several ten percent.

3.1.6 Particle number concentration

A condensation particle counter (CPC) is used to measure the particle number concentration for particle greater than 0.01 µm. The technology is well established and is commercially available from different manufacturers. The CPC is robust and designed for long-term operations. However, it need regular checks on-site to quality-assure the measurement, especially in terms of cleaning the saturator and the optics. Additionally, annual calibrations the CPC against a reference instrument are required. In case CPC performance, the counting efficiency, is not controlled, CPCs might drift with time causing an unnoticed bias of up to several ten percent.

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3.1.7 Mass concentration of particulate elements

Mass concentration of particulate elements and other elements are determined by several analytical techniques

- Particle Induced X-ray Emission (PIXE)
- Energy Dispersive X-Ray Fluorescence (ED-XRF)
- Inductively Coupled Plasma Mass Spectrometry (ICP-MS)
- Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-AES)

The quantification of particulate elements by these techniques depends on internal and/or external calibration. Trained practitioners are needed to produce high quality data that have passed various QA/QC measures. Previous inter-laboratory comparisons have shown that the various techniques can lead to different determination of aerosol elemental components in the same filter sample. Thus, feedback provided to the beneficiaries by the TC will reduce systematic biases. Audits in the form of inter-laboratory comparisons and Round-Robin tests with reference samples are needed to evaluate the performance of each single technique and/or experimental set-up.

3.1.8 Mass concentration of particulate organic tracers

Several analytical techniques are used to determine the Mass concentration of particulate organic tracers including:

- *Liquid Chromatography Mass Spectrometry (LC/MS):* (Ultra)- High-Performance Liquid Chromatography coupled to Hybrid Quadrupole-Orbitrap Mass Spectrometer (UHPLC/HRMS), High-Performance Liquid Chromatography Electrospray Ionization coupled to Time-of-Flight Mass Spectrometry (HPLC/ESI-TOFMS), Ultra-Performance Liquid Chromatography Electrospray Ionization coupled to Ion-Mobility Mass Spectrometer with a Time-of-Flight Mass Spectrometry (UPLC/ESI-IMS-QTOFMS)
- *Gas Chromatography Mass spectrometry (GC/MS):* Curie-Point-Pyrolysis Gas Chromatography with Mass Spectrometry (CPP-GCMS), standard GCMS applications with derivatisation procedures)
- Ion Chromatography Pulsed Amperometric Detection (IC/PAD)

The quantification of organic tracers by these techniques highly depends on internal and external calibration. Thus, well trained operators are needed to produce high quality data that has passed various QA/QC measures. Also audits in the form of inter-laboratory comparisons and Round-Robin test with reference compounds are needed to evaluate the performance of each single system.

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3.1.9 Cloud condensation nuclei number concentration

A cloud condensation nuclei counter (CCNC) is used to measure the Cloud condensation nuclei number concentration at different supersaturations and possibly as function of particle size. The technology is established and is commercially available from one manufacturers. The CCNC designed for long-term operations. However, it needs regular calibrations with a standard aerosol (every six month) on-site to quality-assure the measurement. Additionally, annual or biannual calibrations the CCNC against a reference instrument are required. In case CCNC performance is not controlled, CCNC flow might change with time causing an undefined supersaturation in the instrument and a bias in the measured number concentration.

3.1.10 Mass concentration of non-refractory particulate organics and inorganics

An Aerosol Chemical Speciation Monitor is designed for in situ measurement of non-refractory submicron (NR-PM1) aerosol chemical species, on a time-basis of typically 30 min. Measured species include nitrate, sulphate, ammonium, chloride and organic aerosols. Further data treatments are also allowing for source apportionment studies, notably of the organic fraction. It is based on a rather simple and robust technology, and its suitability for continuous monitoring has been demonstrated within ACTRIS in the last 6 years. However, its operation and data production required the involvement of experienced users. Indeed, several calibration steps must be completed regularly and non-trivial raw data correction procedures have to be performed carefully. Moreover, the instrument technology and data treatment tools (e.g., upgrade of key parts of the analyser, detection and adjustments of measurement artefacts, etc.) are still constantly evolving. It is then necessary to perform intercomparison campaigns and update best practice documents, in order to ensure accurate final data products. The uncertainty of the latter ones will notably depend on the availability of the TC unit to evaluate and harmonize the procedures raw data correction, notably including correction of measurement artefacts.

3.1.11 Nanoparticle number concentration

Atmospheric aerosol number concentration below 0.002 µm in size (Kulmala et al. 2012) is observed with a Particle Size Magnifier, which is a dual stage Condensation Particle Counter (Vanhanen et al. 2011). In the PSM the aerosol is turbulently mixed with air saturated with di-ethylene glycol, therefore creating a supersaturation high enough to activate even 0.001 µm ions, the nominal cut-off size being about 0.0015 µm. The 50% activation diameter can be varied between 0.001 and 0.0025 µm in mobility diameter by changing the mixing ratio of the saturator and sample flows. The PSM allows us to determine aerosol number concentrations between 0.001 to 0.0025 µm as well as their initial growth rate as a function of particle size (Lehtipalo et al. 2014). This will enable comparison between number concentration measurements with larger cut-off diameters. Similar instruments are now in the market by other manufacturers as well.

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3.1.12 Nanoparticle number size distribution

There is a need to extend the size range of ACTRIS MPPS systems (Wiedensohler et al. 2012) below 0.02 µm. Here we utilize a well-established ultra-fine DMPS system of Aalto et al. 2001. However, we will drive towards development by utilizing higher resolution differential mobility analysis in combination with higher flow rate condensation particle counter and minimized particle diffusion losses in the sampling line as illustrated in Kangasluoma et al. 2017 (submitted). This facilitates better counting statistics in low concentrations as well as more detailed size classification in sub-0.01 µm size range.

Neutral Cluster and Air Ion Spectrometer (NAIS) measures electrical mobility distribution of naturally charged and total nanoparticles in high time resolution utilizing two parallel DMA columns. The size range is 0.002 – 0.042 µm and 0.0008 – 0.042 µm for the neutral aerosols and ions, respectively. The NAIS is a robust, field-worthy instrument, which can be operated for extended periods unattended (Manninen et al. 2010).

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3.2 Estimation of the need

Numbers in the following table are based on QA/QC expert estimates and information by the countries how many NFs they potentially want to contribute to ACTRIS.

Variable	Number of NFs to which the TC is providing operation support		
	Now	by 2025	
		Min.	Max.
1. Particle number size distribution – mobility diameter	40	70	110
2. Particle light scattering and backscattering coefficient	40	70	110
3. Particle light absorption coefficient and equivalent black carbon concentration	50	70	110
4. Mass concentration of particulate organic and elemental carbon	20	30	55
5. Particle number size distribution - optical and aerodynamic diameter	10	30	55
6. Particle number concentration	10	30	55
7. Mass concentration of particulate elements	5	30	55
8. Mass concentration of particulate organic tracers	5	20	55
9. Cloud condensation nuclei number concentration	10	30	55
10. Mass concentration of non-refractory particulate organics and inorganics	20	15	40
11. Nanoparticle number concentration	5	20	40
12. Nanoparticle number size distribution	10	30	55

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3.3 Timeline for implementation of the mandatory operation support

Mode	Operation support	Type	Preparation phase	Implementation phase	Operation phase
			<2020	2020-2025	>2025
In situ measurements	Measurement guidelines	On request	Edition of SOPs for measurements for which they do not exist yet	Review and revision of existing SOPs	Review and revision of existing SOPs
	Instrument-specific calibration workshop at TC facility	Scheduled	Test of calibration exercises	Regular calibration exercises	Regular calibration exercises
	Site performance test with reference instruments operated at NFs	Scheduled	Decision on which kind of tests shall be carried out, provision of reference instruments, test exercises	Site performance tests with reference instruments	Site performance tests with reference instruments
In situ sampling	Laboratory intercomparison at NFs	Scheduled	Decision on which kind of Round-Robin tests shall be carried out, test exercises	Site performance tests with reference samples	Site performance tests with reference samples
In situ measurements or sampling	Training of operators and scientists	Scheduled	Decision on which kind of training shall be provided with which frequency, test exercises	Regular training according to schedule	Regular training according to schedule

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3.4 Operation support for quality assurance and quality control

3.4.1 Definition and establishment of standard operation procedures

3.4.1.1 Particle number size distribution – mobility diameter

Measurement guidelines to operate mobility particle size spectrometers for long-term atmospheric observations have been developed during EUSAAR and ACTRIS, These have been published in Wiedensohler et al. (2012) as well as in the WMO/GAW Aerosol Measurement Procedures, Guidelines and Recommendations (report no 227).

See also http://www.wmo-gaw-wcc-aerosol-physics.org/recommen-dations.html

For the existing NFs, the guidelines should be in place.

3.4.1.2 Particle light scattering and backscattering coefficient

Measurement guidelines to operate integrating nephelometer for long-term atmospheric observations have been developed during EUSAAR, ACTRIS and within the GAW community. These have been published in the WMO/GAW Aerosol Measurement Procedures, Guidelines and Recommendations (report no 227).

See also http://www.wmo-gaw-wcc-aerosol-physics.org/recommen-dations.html

For the existing NFs, the guidelines should be in place.

3.4.1.3 Particle light absorption coefficient and equivalent black carbon concentration

Measurement guidelines to operate absorption photometers for long-term atmospheric observations have been developed during EUSAAR, ACTRIS and within the GAW community, These have been published in the WMO/GAW Aerosol Measurement Procedures, Guidelines and Recommendations, report no 227.

See also http://www.wmo-gaw-wcc-aerosol-physics.org/recommen-dations.html

For the existing NFs, the guidelines should be in place.

3.4.1.4 Mass concentration of particulate organic and elemental carbon

A European standard (EN 16909) for the measurement of OC and EC in ambient PM samples deposited on filters has been published (2017). It is mainly based and fully consistent with the SOP for the measurement of OC and EC developed under ACTRIS. The objectives of this SOP is that thermal-optical analysers are optimally operated, and above all that the necessary QA/QC operations are carried at the frequency needed to ensure data quality and traceability. The TC shall be responsible to check that the SOPs have been correctly followed before validating OC and EC data. While the SOP for off-line analyses is already in place, a SOP for semi-continuous instrument shall be developed, mainly focusing on the instrument calibration and participation in Round-Robin test. New SOPs shall be developed if new instrumentation types emerge.

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3.4.1.5 Particle number size distribution – optical and aerodynamic diameter

Measurement guidelines for optical and aerodynamic particle size spectrometers have not been developed for atmospheric observations. This is the task for the preparation phase of ACTRIS, working together with metrology institutes.

3.4.1.6 Particle number concentration

Measurement guideline for condensation particle counters are described in the standard FprCEN/TS 16976 developed in the working group CEN TC 264, WG 32, in which ACTRIS was actively was involved.

3.4.1.7 Mass concentration of particulate elements

Firstly SOPs shall be developed tailored to each analytical technique, then these SOPs shall be distributed to the NFs, and discussed and trained within the trainings at the TC. The successful implementation of the SOPs shall be controlled by continuous inter-laboratory comparisons. All SOPs (if not already available at the TC) shall be developed during the implementation phase and shall be fully available with the start of the operational phase. SOPs will address the sample treatment (filter material, sampling procedure, level of purity for solvents and extraction procedures when applicable, sample storage, etc.) and the use of proper calibration standards.

3.4.1.8 Mass concentration of particulate organic tracers

At a first stage SOPs shall be developed focusing on sample preparation, as this strongly affects the results of the analysis. In a second stage SOPs shall be provided recommending certain measurement techniques for each class of compounds to be analysed. These SOPs shall be distributed to the NFs and discussed and trained within the trainings at the TC. The successful implementation of the SOPs shall be controlled by continuous ILCs. If certain users are not able to follow the recommend measurement techniques (e.g. due to money issues) the TC will provide minimum requirements on alternative techniques (calibration, response factors, detection limits etc.).

All SOPs (if not already available at the TC) shall be developed during the implementation phase and shall be fully available with the start of the operational phase. For new classes of compounds or if fundamental new techniques emerge the TC will provide improved SOPs. Besides the recommendation of certain measurement techniques SOPs will address the following points:

- sample treatment: filter material, sampling proceeding, level of purity for solvents, extraction proceeding, derivatisation proceeding (if applicable), sample storage and maximum storage time
- authentic standard compounds: supplier or synthesis proceeding, level of purity, storage, stability

3.4.1.9 Cloud condensation nuclei number concentration

Measurement guidelines to cloud condensation nuclei counter for long-term atmospheric observations have been developed during ACTRIS. They are available at http://actris.nilu.no/Content/SOP. For the existing NFs, the guidelines should be in place.

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3.4.1.10 Mass concentration of non-refractory particulate organics and inorganics

Preliminary measurement guidelines have been defined within ACTRIS FP7 and ACTRIS2 H2020 projects. The TC unit shall be responsible for further updating related documents as well as new measurement guidelines for the ACSM calibration and operation. It shall also define rules for the transformation of raw data into level 1.5 validated data. All relevant procedures shall be openly shared and discussed amongst the user community, and will evolve over time based on the improving knowledge of the instrument operation. Likewise, the TC might develop and implement new measurement guidelines for every additional online aerosol chemical monitors being included into the field of the ACTRIS aerosol in situ TC (e.g. note that the TC unit will not be responsible for establishing procedures for the repair or heavy maintenance of the instrument (which is left to the manufacturer), but it can participate in the elaboration and/or the diffusion (e.g., through wiki pages, dedicated website, …) of relevant material (such as technical videos, e-learning tutorials, etc.).

3.4.1.11 Nanoparticle number concentration

The optimization and harmonization work of the number concentration measurements with the PSM relies on the work presented in Kangasluoma et al. 2016, which describes the inlet configurations. In the next years this is complemented by including a standardized method for performing a PSM cut-off calibration with one organic and one inorganic test aerosol, and a harmonized sample dilution that is a prerequisite in high number concentration environments, such as in China. Further harmonization for the field operation of the PSM shall be provided with regards to the particle composition and sample flow temperature and RH. The PSM data inversion is described in Lehtipalo et al. 2014. The knowledge is collected into a PSM SOP by 2021.

The responsibility of the TC is to develop and refine the abovementioned SOPs and distribute them within ACTRIS RI. The process is facilitated by SOP workshops organized at the TC for the NF operators.

3.4.1.12 Nanoparticle number size distribution

The procedures and measurements with the NAIS instrument was harmonized in ACTRIS. The corresponding document is published for the scientific audience in Manninen et al. 2016. This document describes the installation, sampling, operation and data analysis procedures for the NAIS. Within EUCAARI-project (Kulmala et al. 2010), the NAIS data protocols were developed enabling data delivery to EBAS. This shall be reinstated and put into operational phase by 2021 with near real-time data delivery.

The sub-0.01 µm size distribution measurements follow the general guidelines and best practices set for sub-micron aerosol number size distribution measurements (Wiedensohler et al. 2012) with the specific focus on minimizing nanoparticle losses by optimizing the sample lines and increasing sample flow rates. A new SOP for the sub-0.01 µm size distribution shall be elaborated during the following years and the use of high resolution Differential Mobility Analysers and higher sample flow rates for the Condensation Particle Counters are explored. The technical target for this activity is to improve the coherence of sub-0.01 µm size distribution measurements and bring this capacity into a wider use within ACTRIS. The next for the SOPs should be ready by 2025.

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The responsibility of the TC is to develop and refine the abovementioned SOPs and distribute them within ACTRIS RI. The process is facilitated by SOP workshops organized at the TC for the NF operators.

3.4.2 Definition of measurement quality-assurance criteria and procedures

3.4.2.1 Particle number size distribution – mobility diameter

The on-site quality assurance are described in detail in the publication of Wiedensohler et al. (2012) and at http://www.wmo-gaw-wcc-aerosol-physics.org/recommen-dations.html

Diagnostic data from the MPSS such as temperature, relative humidity and flow rates are the base for data flagging.

3.4.2.2 Particle light scattering and backscattering coefficient

Quality assurance procedures are related to on-site gas calibrations, which have to be done regularly as described at http://www.wmo-gaw-wcc-aerosol-physics.org/recommen-dations.html. Diagnostic data such as the relative humidity are the base for data flagging.

3.4.2.3 Particle light absorption coefficient and equivalent black carbon concentration

On-site quality assurance procedures have to be developed during the ATRIS preparation phase. Diagnostic data such as the relative humidity and flow rate are the base for data flagging.

3.4.2.4 Mass concentration of particulate organic and elemental carbon

The quality assurance criteria (bias and variability) defined for the measurement of OC and EC under ACTRIS and already included to the data files submitted to EBAS shall be determined by the specific TC Unit and communicated to beneficiaries. They shall be calculated from statistical analyses of the results of Round-Robin tests. The assigned values for OC and EC shall be determined form the robust average among the participant (ISO 13528). Additionally, synthetic reference samples shall be distributed to beneficiaries so that there measurements can be confronted to true values. The statistical outputs of the Round-Robin tests and the results of the analyses of the synthetic reference materials shall be used by the TC to investigate the reasons and the period for under-performance, if any. The data reported by the beneficiaries shall be flagged accordingly. The procedure for determining the data quality criteria shall be in place from the pre-operational phase. The TC shall adapt the thresholds for determining under-performance according to the evolution of analytical technologies.

3.4.2.5 Particle number size distribution – optical and aerodynamic diameter

Measurement quality assurance criteria and procedures for OPSS and APSS instruments currently only exist concerning particle sizing, using latex particles (Pfeifer at al., 2016). Criteria and calibration procedures for the size resolved particle number concentration are currently not existing, but are under development.

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3.4.2.6 Particle number concentration

On-site quality assurance procedures are described in the standard FprCEN/TS 16976 developed in the working group CEN TC 264, WG 32, in which ACTRIS was actively involved.

3.4.2.7 Mass concentration of particulate elements

The TC will provide protocols for each analytical technique that will address the key performance parameters such as external and internal calibration standards, number of blank measurements, number of repetitions, reproducibility, number of control samples. The developed protocols should be applied to each analytical technique. When all minimum parameters are fulfilled data will flagged as QA/QC controlled. If the data do not passed the control they shall be still available but without flagging. The protocols shall be developed during the implementation phase and shall be available in the operational phase. Additionally, synthetic reference samples shall be distributed to beneficiaries so that their measurements can be compared to true vales. The statistical outputs of the Round-Robin tests and the results of the analyses of the synthetic reference materials shall be used by the TC to investigate the reasons of under-performances, if any. The data reported by the beneficiaries shall be flagged accordingly. The TC shall adapt the thresholds for determining under-performance according to the evolution of analytical technologies.

3.4.2.8 Mass concentration of particulate organic tracers

The TC will provide protocols for each recommended technique that will address the following key performance parameters (in addition 3.3.1.1):

- external calibration: sequence design, concentration range, minimum number of dilution steps, minimum regression factor, number of blank measurements, storage and stability of standard dilutions
- measurement: column material for separation, number of repetitions, reproducibility, number of control samples
- mass calibration (if applicable): internal standard/calibrant composition

The developed protocol should be applied to each measurement and linked to created data set. Thus for each measurement the protocol is available. If all minimum parameters are fulfilled data can be flagged as QA/QC controlled. If the data do not passed the control they shall be still available but without flagging.

The protocols shall be developed during the implementation phase and are available in the operational phase. As this kind of protocols are not instrument specific they can be transfer to new emerging techniques. Nevertheless, for each emerging technique the TC will prove the applicability of the protocols and will provide updated recommendations (if necessary).

3.4.2.9 Cloud condensation nuclei number concentration

Quality assurance procedures have been developed during ACTRIS. They are available at http://actris.nilu.no/Content/SOP. For the existing NFs, the guidelines should be in place.

3.4.2.10 **Mass concentration of non-refractory particulate organics and inorganics**

Quality assurance for each instrument shall be based on a strict set of criteria for instrument setup at each observational site. Related quality assurance procedures notably include inspection of technical parameters (such as Air Beam value, mass spectrometer tunings, fittings for internal calibrations …), check of the ion balance, and PM mass and/or optical closure exercises (by comparison with collocated instruments). These criteria shall be defined and revised as part of the measurement guidelines. They will provide confidence to the NF and the TC, as well as ACTRIS as a whole, ensuring that quality requirements are fulfilled and/or less quality data are accurately flagged.

3.4.2.11 **Nanoparticle number concentration**

The procedures and criteria of the sub-0.01 µm total number concentration data are or shall be described in the developed SOPs (see 3.3.1). The technical target for the measurements is to provide harmonized observations in NRT data delivery. The NRT data stream shall be automatically flagged for preliminary quality checks.

The following instrument maintenance procedures are required with the PSM:

- Yearly cut-off and CPC concentration calibration
- Monthly PSM and CPC inlet flow rate measurements
- CPC pulse width monitoring
- Regular PSM zero measurement using particle free air
- Removing excess diethylene glycol from tubing as needed.

These procedures shall be elaborated in the SOPs for the PSM developed by the TC. In order to reach higher level data, automatic flagging shall be developed based on measured instrument operation parameters followed by manual data quality assurance by an expert, re-inversion if needed, flagging or removal of bad quality data.

The criteria and procedures for the PSM are intended to be in place 2019, co-incident with the development of the SOPs.

3.4.2.12 **Nanoparticle number size distribution**

The procedures and criteria of the sub-0.01 µm size distribution data are or shall be described in the developed SOPs (see 3.3.1). The technical target for the measurements is to provide harmonized observations in NRT data delivery. The NRT data stream shall be automatically flagged for preliminary quality checks.

The following instrument maintenance procedures are required with the NAIS:

- DMA column cleaning as needed,
- Ion and particle concentration and sizing calibration yearly,
- Inlet flow rate measurement monthly,
- Electrometer zero current monitoring.

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The NRT data stream shall be automatically flagged for preliminary quality checks. In order to reach higher level data, automatic flagging shall be developed based on measured instrument operation parameters followed by manual data quality assurance by an expert, re-inversion if needed, flagging or removal of bad quality data.

The UF-DMPS data quality assurance requires the same procedures as in ACTRIS documentation for the DMPS systems with the specific focus on sub-0.02 µm size distribution.

The criteria and procedures are intended to be in place 2021 (NAIS) and 2025 (UF-DMPS), co-incident with the development of the SOPs.

3.4.3 Development and provision of instrument-specific calibration

3.4.3.1 Particle number size distribution – mobility diameter

The calibration procedures of MPSS have been described in Wiedensohler et al. (2017) and are already applied during ACTRIS2. For the calibration at the calibration facility reference a MPSS, a CPC and a FCAE are needed. On-site intercomparisons include a MPSS and a CPC. Size calibrations are done with a certified PSL particle standard.

3.4.3.2 Particle light scattering and backscattering coefficient

For the calibration of integrating nephelometers, particle free air and CO2 is used. Calibration are also done at the calibration facility against a frequently calibrated reference integrating nephelometer

3.4.3.3 Particle light absorption coefficient and equivalent black carbon concentration

A reference set-up for absorption photometers was developed during ACTRIS2, see deliverable D34. This set-up includes a three extinction monitors for three different wavelengths and a multi-wavelengths integrating nephelometer. Laboratory-generated sulphate aerosol is used to calibrate the reference set-up. The absorption photometers are calibrated against the reference set-up and a reference absorption photometer using an absorbing aerosol.

There is no reference for the equivalent black carbon concentration mass concentration yet. This shall be a task for the preparation phase of ACTRIS.

3.4.3.4 Mass concentration of particulate organic and elemental carbon

The TC will provide remote access to its facilities for calibrating measurements of OC and EC in ambient PM samples deposited on filters. Round-Robin test shall be organised at least once a year from the beginning of the pre-operational phase, in order to cover all requests from beneficiaries. Synthetic certified materials shall be made available to beneficiaries at least from the beginning of the operational phase.

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3.4.3.5 Particle number size distribution – optical and aerodynamic diameter

The size calibration of optical and aerodynamic particle size spectrometers are done with certified PSL-particle standards. For the calibration of the size-resolved particle number concentration, a concept was developed in ACTRIS-2, see deliverable D96. The implementation shall be done during the preparation phase of ACTRIS.

3.4.3.6 Particle number concentration

The calibration of CPCs are done, using a calibrated FCAE, which is traceable to an SI-unit. The procedure is described in detail in Wiedensohler et al. (2017).

3.4.3.7 Mass concentration of particulate elements

The TC will provide remote access to its facilities for calibrating measurements of particulate elements and elements in ambient PM samples deposited on different kind of filters, according to the request of the beneficiaries. Round-Robin test shall be organised at least once a year from the beginning of the pre-operational phase. Synthetic certified standards shall be made available to beneficiaries at least from the beginning of the operational phase.

3.4.3.8 Mass concentration of particulate organic tracers

For each single instrument type, SOPs shall be developed that will also contain requirements about the internal and external calibration. Furthermore, the protocols defined in 3.3.2.1 are part of these SOPs. The SOPs shall be instrument specific as well as analyte specific. In general, for each single analysis the instrument has to be checked in terms of:

Mass calibration, response function, retention time of the standards, and instrument-specific performance indicator (flow rate, pressure etc.).

Furthermore, the TC unit will offer services in terms of inter-laboratory comparisons (ILCs) with subsequent workshops and Round-Robin tests with reference standards. For the ILC filter samples (from field and laboratory-generated) and reference standards shall be distributed. Each user should participate once per year in one ILC or Round-Robin test to evaluate the performance of the instrument. Besides this, internal and external users can be always in-touch with the TC unit operator for rapid assistance. Each kind of service shall be available from the beginning of the implementation phase and shall be further developed continuously.

3.4.3.9 Cloud condensation nuclei number concentration

The cloud condensation nuclei counter is calibrated with size-resolved ammonium sulphate particles, knowing the theoretical activation behaviour. This was described in detail by Rose et al. (2008) and is also given in the ACTRIS recommendation (http://actris.nilu.no /Content/SOP).

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3.4.3.10 Mass concentration of non-refractory particulate organics and inorganics

One of the main roles of the aerosol in situ measurement TC is to provide specific and advanced (*state-of-the-art*) calibration services to the users. This shall be done through dedicated calibration and intercomparison campaigns. These campaigns shall be performed regularly at the TC unit and involving ACSM reference instrument as well as a large set of co-located online instrument and particle samplers for the comprehensive measurements of aerosol physics and chemistry. A decisive advantage of achieving such calibration campaigns is also to gather an optimum number of users, increasing collaborations between groups as well as identifying the robustness of instrument operation from one system to the next. These intensive campaigns should also provide a unique opportunity for training in terms of instrument operation, and knowledge.

3.4.3.11 Nanoparticle number concentration

The TC will offer workshops for instrument calibrations and operation verification. At the beginning of the workshop, the initial status of the instruments is evaluated followed by required routine maintenance to increase the performance (e.g. cleaning, flow checks).

The PSM calibrations include 1) flow calibrations, 2) detection efficiency calibration with different test aerosols of variable chemical composition, 3) detection efficiency as a function of PSM operation parameters (internal flow rates, supersaturation) 4) CPC concentration calibration.

3.4.3.12 Nanoparticle number size distribution

The TC will offer workshops for instrument calibrations and operation verification. At the beginning of the workshop the initial status of the instruments is evaluated followed by required routine maintenance to increase the performance (e.g. cleaning, flow checks).

The NAIS calibration procedures are described in Manninen et al. 2016. These include: 1) flow calibration, 2) sizing calibration against high-resolution DMA, 3) concentration calibration against a reference electrometer and 4) side-by-side ambient sampling.

The UF-DMPS calibration include 1) flow calibrations, 2) sizing calibration against reference DMA (low resolution and high resolution), 3) loss measurements through the whole instrument, 4) detection efficiency measurements for the detector CPC with different test aerosols with variable chemical composition, 5) concentration calibration of the whole instrument and inversion code against a reference instrument.

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3.4.4 Development and provision of in-house check-up tools

3.4.4.1 Particle number size distribution – mobility diameter

The calibration procedure is described in Wiedensohler et al. (2017). For the size calibration, certified PSL particle size standards are used. To calibrate the condensation particle counter, a calibrated FCAE is employed, which is traced back to a SI unit.

3.4.4.2 Particle light scattering and backscattering coefficient

For the calibration of the integrating nephelometers, particle-free air and CO_2 is used, as described in the WNO-GAW report No 227.

3.4.4.3 Particle light absorption coefficient and equivalent black carbon concentration

The calibration procedure of absorption photometers was developed in ACTRIS. A calibrated reference multi-wavelengths integrating nephelometer and several reference extinction monitor are necessary.

3.4.4.4 Mass concentration of particulate organic and elemental carbon

In between the regular Round-Robin tests, the TC will offer the beneficiaries the possibility to get QC materials, including atmospheric PM deposited on large filters for repeatability and long term stability tests (from the pre-operational phase) and synthetic certified materials (from the beginning of the operational phase).

3.4.4.5 Particle number size distribution – optical and aerodynamic diameter

For the calibration of aerodynamic and optical particle size spectrometers, certified PSL particle size standards are used.

3.4.4.6 Particle number concentration

The calibration of condensation particle counter is based on a calibrated FCAE, which is traced back to a SI unit at a national metrology institute.

3.4.4.7 Mass concentration of particulate elements

The TC will offer the beneficiaries the possibility to get QC materials, such as atmospheric PM deposited on different kind of filters (from the pre-operational phase) and synthetic certified standard (from the beginning of the operational phase).

3.4.4.8 Mass concentration of particulate organic tracers

For each of the measurement technique a check-up tool shall be developed containing the QA/QC parameters defined in 3.3.2.1. This tool provides a quick overview how the data were created and if they meet the defined QA/QC standards. It shall be created as fast check-up protocol and can be made available to all users, in particular to the DC as a quick link for all uploaded data. This tool shall be developed within the implementation phase and has to be ready with the start of the operational phase.

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3.4.4.9 Cloud condensation nuclei number concentration

The calibration of cloud condensation particle counter is based on the well-known water take-up of ammonium sulphate.

3.4.4.10 Mass concentration of non-refractory particulate organics and inorganics

The TC unit will not provide any physical in-house check-up tools (such as standard reference material, which is not currently defined for the variables measured by the ACSM). Instead, it will provide NFs procedures and tools (software) for the data quality assurance based on validation of the operation parameters, raw data corrections and validation with co-located instruments, as explained above.

3.4.4.11 Nanoparticle number concentration

The development of tools required for on-site checking shall be developed by 2025. For the PSM an automatic sample handling system is endorsed (Kangasluoma et al. 2016, Ahonen et al. 2017). This will enable automatic zero measurements, ion and neutral separation, sample dilution in high concentrations and monitoring of the inlet conditions. This shall be put into place by 2018.

Additional tools to be provided to the NF capacity include e.g. an optimization of PSM supersaturation. These tools shall be procured by the NFs, but TC will help to operate them on a routine basis. This shall be put into place by 2020.

The laboratory set-ups for instrument checking and calibration (both hardware and software) shall be re-designed by 2025 to facilitate larger workshop with several instruments.

3.4.4.12 Nanoparticle number size distribution

The development of tools required for on-site checking shall be developed by 2025.

Additional tools to be provided to the NF capacity include e.g. a cluster ion source to verify the cluster ion measurements with the NAIS. These tools shall be procured by the NFs, but TC will help to operate them on a routine basis. This shall be put into place by 2020.

Although some of PSM and NAIS software will remain proprietary by the instrument manufacturer, the aim is to that the pre-processing of the NAIS, PSM and UF-DMPS data shall be done with open source software developed at TC. The final PSM and UF-DMPS inversion algorithms shall be open source.

The laboratory set-ups for instrument checking and calibration (both hardware and software) shall be re-designed by 2025 to facilitate larger workshop with several instruments.

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3.4.5 Development of data evaluation procedures and plausibility test

3.4.5.1 Particle number size distribution – mobility diameter

The data evaluation program of MPSS is described in Wiedensohler et al. (2012) and is worldwide harmonized. A reference condensation particle counter is used as an independent instrument to determine the total particle number concentration, which is compared to the integral over the particle number size distribution.

3.4.5.2 Particle light scattering and backscattering coefficient

Integrating nephelometer are traced back to SI-units. There are no further tools to perform plausibility tests.

3.4.5.3 Particle light absorption coefficient and equivalent black carbon concentration

The reference method of "particle light extinction minus scattering" is traced back to SI-units. Increasing uncertainties are related to the single scattering albedo. Otherwise, no additional plausibility test is needed.

3.4.5.4 Mass concentration of particulate organic and elemental carbon

The OC-EC unit shall apply ISO guides for the evaluation of the instruments' performance from Round-Robin tests and against certified reference materials. Instruments' performances shall be determined by comparison of the data they deliver with assigned values. This procedure implies a good knowledge of the statistical procedures for evaluating proficiency tests. Accreditation according to ISO 17043 would be an asset. It is probably not optimal that this procedure be transferred to the DC considering the specificity of the plausibility tests to be applied.

3.4.5.5 Particle number size distribution – optical and aerodynamic diameter

There is no common data plausibility test yet, since the reference for the particle number concentration of particles greater 3 µm is not developed yet. This is planned for the initialization phase of ACTRIS.

3.4.5.6 Particle number concentration

The calibration of condensation particle counters is described in Wiedensohler et al. (2017). No further development of a plausibility test is needed.

3.4.5.7 Mass concentration of particulate elements

Proficiency tests according to ISO guidelines for the evaluation of the performance of the analytical techniques and the associated experimental set-up from Round-Robin tests and against certified reference standards shall be applied.

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3.4.5.8 Mass concentration of particulate organic tracers

Data evaluation shall be ensured by

1) The QA/QC parameters defined in 3.3.2.1. These criteria shall be used to flag the data as QA/QC controlled.
2) The check-up tool defined in 3.3.4.1. The output of the tool shall be directly linked to the data uploaded to the DC.
3) Continuous ILCs to prove if all QA/QC standards were meet.

The check-up tool as well as the QA/QC standards shall be available to the NF and also to the DC. The usage of the tool and the accordance to the QA/QC standards shall be permanently controlled.

The data evaluation procedure will start with the implementation phase and shall be fully operational at the beginning of the operational phase.

3.4.5.9 Cloud condensation nuclei number concentration

The plausibility of the size-dependent Cloud condensation nuclei number concentration is based on the commonly used calibration procedure with ammonium sulphate as described in Rose et al. (2008). No further plausibility test is needed.

3.4.5.10 Mass concentration of non-refractory particulate organics and inorganics

Data evaluation algorithms to be applied by the user shall be developed under the activities of the TC unit. Checks based on co-located cross-instrumental (e.g., comparison of data provided by chemical monitors with outputs of mass concentration measurements/estimates) shall be proposed to ensure plausibility of the measurements.

Furthermore, the TC unit shall develop and apply tools based on cross-station checks to further ensure plausibility of the measurements at the whole RI level. This will include the development (by 2020) of a platform for data screening as well as regular review sessions - in collaboration with data providers - of level 1 datasets.

3.4.5.11 Nanoparticle number concentration

Data evaluation procedures and plausibility tests need to be developed for the PSM hand-in-hand with the measurement quality assurance criteria. The simplest plausibility test is to require that the total concentration of measured particles in the size range of the instrument in ambient air cannot be negative, equal zero or be larger than the total concentration over the full measurement range. More sophisticated tests will need to be instrument specific. These procedures and tests shall be developed in collaboration with TC for sub-micron size distribution measurements.

The main requirements for these procedures and tests are that they ensure that the data quality is sufficient that the data can pass from ACTRIS level 1 (automated inversion and flagging) to level 2 (quality assured data) and enable further analysis and data products (level 3).

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The initial tools for plausibility tests shall be put in place alongside the measurement quality assurance criteria and procedures (see 3.3.2) in 2019 (PSM) and be re-defined each time new mature and improved solutions are available.

3.4.5.12 Nanoparticle number size distribution

Data evaluation procedures and plausibility tests need to be developed for the NAIS and the UF-DMPS hand-in-hand with the measurement quality assurance criteria. The simplest plausibility test is to require that the total concentration of measured particles in the size range of the instrument in ambient air cannot be negative, equal zero or be larger than the total concentration over the full measurement range. More sophisticated tests will need to be instrument specific. These procedures and tests shall be developed in collaboration with TC for sub-micron size distribution measurements.

The main requirements for these procedures and tests are that they ensure that the data quality is sufficient that the data can pass from ACTRIS level 1 (automated inversion and flagging) to level 2 (quality assured data) and enable further analysis and data products (level 3).

The initial tools for plausibility tests shall be put in place alongside the measurement quality assurance criteria and procedures (see 3.3.2) in 2021 (NAIS) and 2025 (UF-DMPS) and be re-defined each time new mature and improved solutions are available.

3.4.6 Realization of observational site performance audits with reference samples or mobile systems

3.4.6.1 Particle number size distribution – mobility diameter

The reference MPSS has to be calibrate at the calibration facility before.

3.4.6.2 Particle light scattering and backscattering coefficient

On-site intercomparisons are not foreseen.

3.4.6.3 Particle light absorption coefficient and equivalent black carbon concentration

On-site intercomparisons are not foreseen.

3.4.6.4 Mass concentration of particulate organic and elemental carbon

On-site performances of OC and EC analysers are determined from the procedures described above. It is not envisaged that the Unit shall audit on-site the analysers showing under-performance to determine its causes.

3.4.6.5 Particle number size distribution – optical and aerodynamic diameter

On-site intercomparisons are not foreseen.

3.4.6.6 Particle number concentration

The reference CPC has to be calibrate at the calibration facility before.

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3.4.6.7 Mass concentration of particulate elements

On-site intercomparisons are not foreseen/applicable.

3.4.6.8 Mass concentration of particulate organic tracers

Observational site performance audits shall be done in terms of inter-laboratory comparisons (ILCs) with:

1) Samples collected from the field and from an aerosol chamber. These samples shall be collected under the same conditions and each participant will analyse an aliquot of a filter.

2) Reference standards. This standard will contain a defined mixture of organic aerosol constituents (mainly synthesized). The concentration shall be double-checked at the TC prior dispatch.

Both types of ILC (1 and 2) shall be conducted with the start of the implementation phase. Each observational site should participate (latest with the start of the operational phase) in one audit per year.

3.4.6.9 Cloud condensation nuclei number concentration

On-site intercomparisons are not foreseen.

3.4.6.10 Mass concentration of non-refractory particulate organics and inorganics

On-site intercomparisons are not foreseen.

3.4.6.11 Nanoparticle number concentration

The TC unit will have one reference PSM, which can be used for site performance audits on-site. During the site audit the reference instrument is put to sample next to the tested instrument nano-particle number concentrations shall be compared.

The PSMs shall be audited every year. The audition can be covered also in the calibration workshops taking place every year for the PSM.

3.4.6.12 Nanoparticle number size distribution

The TC will have one reference NAIS and UF-DMPS, which can be used for site performance audits on-site. During the site audit the reference instrument is put to sample next to the tested instrument, and 0.002 - 0.01, 0.002 - 0.04 or 0.001 – 0.0025 µm size resolved particle concentrations, respectively, shall be compared.

A mobile calibration system consisting of a high resolution DMA, particle source (wire generator and/or electrospray source) and a reference electrometer can be equally used in the site performance audits, and the system can be used in the field to audit each of the two instruments. With the mobile calibration system known concentration of size selected particles is guided to the tested instrument, and the response of the instrument is compared against the reference electrometer. The mobile calibration platform shall be available 2019.

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The UF-DMPS and NAIS systems shall be audited with either the reference instrument or the mobile calibration platform once every two years. The audition can be covered also in the calibration workshops taking place every second year for the NAIS and UF-DMPS.

3.4.7 Organization of regular exercises to assess the performances of the NFs, including instrument performance workshops

3.4.7.1 Particle number size distribution – mobility diameter

Frequent instrumental calibration workshops shall be organized by the TC (if necessary several per year).

3.4.7.2 Particle light scattering and backscattering coefficient

Frequent instrumental calibration workshops shall be organized by the TC (if necessary several per year).

3.4.7.3 Particle light absorption coefficient and equivalent black carbon concentration

Frequent instrumental calibration workshops shall be organized by the TC (if necessary several per year).

3.4.7.4 Mass concentration of particulate organic and elemental carbon

For off-line OC and EC analyses, NFs' performances would be determined from the procedures described above if beneficiaries apply regularly. No additional exercise would be suitable to such instruments.

The procedures described above should also apply to on-line OC-EC analysers. If persistent issues occur with the calibration and inter-comparison of on-line analysers during the pre-operational phase, side by side inter-instruments comparisons will have to be organized, at least annually, to cover the needs of the beneficiaries.

3.4.7.5 Particle number size distribution – optical and aerodynamic diameter

Frequent instrumental calibration workshops shall be organized by the TC (if necessary several per year).

3.4.7.6 Particle number concentration

Frequent instrumental calibration workshops shall be organized by the TC (if necessary several per year).

3.4.7.7 Mass concentration of particulate elements

Hands-on trainings for each analytical technique (i.e. PIXE, ED-XRP, ICP) shall be conducted typically once per year. Workshops shall be always conducted after each inter-laboratory comparison exercise, discussing the results, identifying threats and vulnerabilities, and solving open issues.

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3.4.7.8 Mass concentration of particulate organic tracers

Workshop shall be organised as scientific trainings and after the ILCs the results shall be discussed, vulnerabilities identified and open issues solved. Hands-on trainings shall be conducted continuously and with a special focus on 1-2 measurement techniques including also sample collection, preparation and quantification. ILCs workshops shall be always conducted after each ILC. Each kind of workshop will start with the implementation phase and shall be fully operational with the start of the operational phase.

3.4.7.9 Cloud condensation nuclei number concentration

Frequent instrumental calibration workshops shall be organized by the TC (if necessary several per year).

3.4.7.10 Mass concentration of non-refractory particulate organics and inorganics

Frequent instrumental calibration workshops shall be organized by the TC (if necessary several per year).

3.4.7.11 Nanoparticle number concentration

As indicated above, PSM systems should be calibrated every year. The TC will organize workshops for these activities. The technical target for the PSM is 15% in concentration.

3.4.7.12 Nanoparticle number size distribution

As indicated above, the NAIS and UF-DMPS calibration scheme should be completed once per two years. The TC will organize workshops for these activities.

In the NAIS system the technical target is 20% in concentration at 0.003 µm with a sizing accuracy of 15% at this size. The UF-DMPS system the technical target is 10% in concentration at 0.003 µm with 10 % sizing accuracy.

3.4.8 Contribution to documentation and traceability of level 0 to level 3 data products

3.4.8.1 Particle number size distribution – mobility diameter

The calibration reports of the TC are linked to the data of the DC. This is realized since 2017. Flagging of the data is a task of the data provider.

3.4.8.2 Particle light scattering and backscattering coefficient

The calibration reports of the TC are linked to the data of the DC. This is realized since 2017. Flagging of the data is a task of the data provider.

3.4.8.3 Particle light absorption coefficient and equivalent black carbon concentration

The calibration reports for the particle light scattering coefficient of the TC are linked to the data of the DC. This is realized since 2017. Flagging of the data is a task of the data provider.

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3.4.8.4 Mass concentration of particulate organic and elemental carbon

The calibration reports of the TC are linked to the data of the DC. This is realized since 2017. Flagging of the data is a task of the data provider.

The TC will make OC and EC data fully traceable when reported atmospheric data are linked to the measurements of certified reference materials. Such measurements, as well as the results of the Round-Robin tests described above, will allow the TC to calculate biases and variability, which can directly be used for correcting the data, and/or calculate (possibly asymmetric) uncertainties, flag and document the quality of the data.

For OC and EC, the TC should address level 2 data only, at the pre-operational stage. It should not be necessary to deal with level 0 and 1 at a later stage.

3.4.8.5 Particle number size distribution – optical and aerodynamic diameter

The calibration reports of the TC shall be linked to the data of the DC. Flagging of the data is a task of the data provider.

3.4.8.6 Particle number concentration

The calibration reports of the TC are linked to the data of the DC. This is realized since 2017. Flagging of the data is a task of the data provider.

3.4.8.7 Mass concentration of particulate elements

The calibration reports of the TC shall be linked to the data of the DC. Flagging of the data is a task of the data provider. For particulate elements and aerosol elements, the TC should address level 2 data only.

3.4.8.8 Mass concentration of particulate organic tracers

Each observational site participating in an audit will obtain a one-year certificate. If an observational site completely failed the ILC, a TC operator will visit the site or will invite the user to an additional training.

Besides this the data created by the NF shall be controlled by the check-up tool defined in 3.3.4.1 and flagged if the QA/QC standards were meet. The output of the check-up tool shall be directly linked to the data available in the database. With this, a full traceability of the data creation process can be guaranteed.

The calibration reports of the TC shall be provided to the data of the DC.

3.4.8.9 Cloud condensation nuclei number concentration

The calibration reports of the TC are linked to the data of the DC. This is realized since 2017. Flagging of the data is a task of the data provider.

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3.4.8.10 Mass concentration of non-refractory particulate organics and inorganics

After successful participation to an intercomparison/calibration exercise (and QC/QA requirement fulfilled) the data submitted by the concerned NF shall be certified for a period of two years. Calibration reports generated by the TC shall be available at the DC. Ongoing data verification shall be made by the data provider following the QC/QA flagging procedures outlined in section 3.3.3 and 3.3.5.

3.4.8.11 Nanoparticle number concentration

If the tested instruments do not agree with the reference instruments within the pre-set uncertainty range during the site audits or workshops, instrument specific maintenance procedures will take place. This is because of the verified concentration accuracy of the reference instruments.

3.4.8.12 Nanoparticle number size distribution

If the tested instruments do not agree with the reference instruments within the pre-set uncertainty range during the site audits or workshops, instrument specific maintenance procedures will take place. This is because of the verified sizing and concentration accuracy of the reference instruments. Similar procedure is in place with e.g. MPSS systems.

The site audit system shall be operational by 2025.

The NAIS data will include the following steps in order to be traceable and reproducible: level 0: logging of raw data (electrometer currents, operation voltages, flow rates), level 1: inversion of the raw data with documented and identifiable inversion algorithm (at the moment from the manufacturer) that takes into account inlet loss corrections, concentration correction (based on ion calibration in Wagner et al., 2016 and particle calibration in Autumn 2017), conversion to standard pressure and temperature and multiple charging. Automatic flagging based on operational parameters. Level 2: flagging by an expert user.

3.4.9 Contribution to CEN, ISO, or similar standardization activities

3.4.9.1 Particle number size distribution – mobility diameter

The TC contributes to respective ISO and CEN committees and a related EMPIR project for MPSS measurements.

3.4.9.2 Particle light scattering and backscattering coefficient

The TC intends to contribute to related ISO and CEN committees.

3.4.9.3 Particle light absorption coefficient and equivalent black carbon concentration

The TC intends to contribute to respective ISO and CEN committees and already contributes to related EMPIR projects for absorption photometer measurements.

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3.4.9.4 Mass concentration of particulate organic and elemental carbon

The H2020 project ACTRIS-2 and its ancestors have had an essential contribution to the development of the CEN standard EN 16909 for the measurement of OC and EC in PM2.5 deposited on filters. It is envisaged that the TC will participate actively in new working items in CEN TC 264 related to the measurements of atmospheric particulate carbonaceous species, including the applicability of EN16909 to the analysis of the PM10 fraction, and on automated measurements of OC and/or EC.

3.4.9.5 Particle number size distribution – optical and aerodynamic diameter

The TC intends to contribute to respective ISO and CEN committees in the future.

3.4.9.6 Particle number concentration

The TC contributed to the existing CEN standardization for condensation particle counters.

3.4.9.7 Mass concentration of particulate elements

Currently (2018) not.

3.4.9.8 Mass concentration of particulate organic tracers

The SOPs defined under 3.3.1 shall be developed following the GLP/GMP guidelines. The TC operator will have a GLC/GMP certificate.

3.4.9.9 Cloud condensation nuclei number concentration

Currently (2018) not.

3.4.9.10 Mass concentration of non-refractory particulate organics and inorganics

The TC unit outputs shall contribute to the works and outcomes of standardization activities, especially the ones within CEN/TC 264 Working groups 34 (water-soluble ions) and 35 (EC-OC).

The TC unit activities will also be presented to the EU association gathering National Reference Laboratories for air quality monitoring (AQUILA).

3.4.9.11 Nanoparticle number concentration

The work contributes to aerosol number concentration standardization (ISO 27891:2015, Aerosol particle number concentration - Calibration of condensation particle counters by extending the size range below 0.005 µm.

3.4.9.12 Nanoparticle number size distribution

Work is intended to contribute to aerosol number concentration standardization (ISO 27891:2015, Aerosol particle number concentration - Calibration of condensation particle counters) by extending the size range below 0.005 µm.

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3.5 Operation support for knowledge transfer and training

3.5.1 Training of operators and scientists

3.5.1.1 Particle number size distribution – mobility diameter

Training of operators and scientist is part of the frequent instrumental calibration workshops at the calibration facility. The training contains teaching of the technical operation procedures, quality assurances checks, data evaluation procedures as well as plausibility tests. The workshops are limited to maximum six participants that the training is effective.

3.5.1.2 Particle light scattering and backscattering coefficient

Training of operators and scientist is part of the frequent instrumental calibration workshops at the calibration facility. The training contains teaching of the technical operation procedures, quality assurances checks, data evaluation procedures as well as plausibility tests. The workshops are limited to maximum six participants that the training is effective.

3.5.1.3 Particle light absorption coefficient and equivalent black carbon concentration

Training of operators and scientist is part of the frequent instrumental calibration workshops at the calibration facility. The training contains teaching of the technical operation procedures, quality assurances checks, data evaluation procedures as well as plausibility tests. The workshops are limited to maximum six participants that the training is effective.

3.5.1.4 Mass concentration of particulate organic and elemental carbon

Since remote access would be the most cost effective way for the OC-EC unit to support beneficiaries, knowledge transfer and training is envisaged by means of a tutoring of those who ask for it (e.g. new comers), and those probably need it (as suggested by under-performance during the proficiency tests). A web-based forum would certainly be the best way to help beneficiaries operate their instruments and apply the required QA/QC tests at any time. Advice from the TC could be made available to the whole RI when they are of general interest, and could cover all the aspects of the analyses and QA/QC activities required under ACTRIS.

3.5.1.5 Particle number size distribution – optical and aerodynamic diameter

Training of operators and scientist is part of the frequent instrumental calibration workshops at the calibration facility. The training contains teaching of the technical operation procedures (if available), quality assurances checks, data evaluation procedures as well as plausibility tests. The workshops are limited to maximum six participants that the training is effective.

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3.5.1.6 Particle number concentration

Training of operators and scientist is part of the frequent instrumental calibration workshops at the calibration facility. The training contains teaching of the technical operation procedures, quality assurances checks, data evaluation procedures as well as plausibility tests. The workshops are limited to maximum six participants that the training is effective.

3.5.1.7 Mass concentration of particulate elements

Training of operators and scientists is part of the frequent hands-on training workshops at the calibration facility. The training contains teaching of the technical operation procedures, quality assurances checks, data evaluation procedures as well as plausibility tests. The workshops are limited to maximum six participants for the training to be effective.

3.5.1.8 Mass concentration of particulate organic tracers

The training course will address each step from sample collection to analysis of measurement results. Thus each participant will have hands-on experience during instrument- and target-dependent courses. It is planned to organize minimum one training course for each measurement technique per year. The number of participants will depend on the capacity of the TC and the level of experience of the participants. A second focus of the training shall be the instruction into the SOPs and QA/QC parameters defined under 3.3.1 and 3.3.2 as well as the usage of the check-up tool described under 3.3.4. The feedback of the training participants will also be used to improve the check-up tool.

Furthermore, the results of the ILC shall be distributed and discussed within the participant group. Vulnerabilities shall be identified and rectified.

3.5.1.9 Cloud condensation nuclei number concentration

Training of operators and scientist is part of the frequent instrumental calibration workshops at the calibration facility. The training contains teaching of the technical operation procedures, quality assurances checks, data evaluation procedures as well as plausibility tests. The workshops are limited to maximum six participants that the training is effective.

3.5.1.10 Mass concentration of non-refractory particulate organics and inorganics

Technical workshops and training sessions shall be organized once a year, along with intercomparison/calibration exercises. These workshops/trainings shall notably include tutorials for the application of measurement guidelines as well as check-up tools (evaluation procedures and plausibility tests) developed by the TC unit as defined above. Workshops will also be used to further define and/or revised these quality assurance procedures and standard operating procedures.

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3.5.1.11 **Nanoparticle number concentration**

The objective of the training activity is capacity building of ACTRIS RI in aerosol in-situ number concentration measurements in the size range below 0.01 µm. The knowledge transfer occurs during the workshops for PSM systems. These can be jointly organized e.g. in ACTRIS-wide summer / spring schools at the ACTRIS observational sites, such as Hyytiälä SMEAR II station in Finland. The workshops will start in 2018 and shall be organized annually. The workshops facilitate and speed up the process towards the development of the required SOPs.

3.5.1.12 **Nanoparticle number size distribution**

The objective of the training activity is capacity building of ACTRIS RI in aerosol in-situ number size distribution measurements in the size range below 0.01 µm. The knowledge transfer occurs during the workshops for NAIS and UF-DMPS systems. These can be jointly organized e.g. in ACTRIS-wide summer / spring schools at the ACTRIS observational sites, such as Hyytiälä SMEAR II station in Finland. The workshops will start in 2018 and shall be organized annually. The workshops facilitate and speed up the process towards the development of the required SOPs.

3.5.2 Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs

3.5.2.1 **Particle number size distribution – mobility diameter**

Consultancy for setting-up ne observational or exploratory platforms shall be provided by the TC on request. The existing relevant SOPs and measurement and sampling guidelines shall be provided and explained to the NF operators accordingly.

3.5.2.2 **Particle light scattering and backscattering coefficient**

Consultancy for setting-up ne observational or exploratory platforms shall be provided by the TC on request. The existing relevant SOPs and measurement and sampling guidelines shall be provided and explained to the NF operators accordingly.

3.5.2.3 **Particle light absorption coefficient and equivalent black carbon concentration**

Consultancy for setting-up ne observational or exploratory platforms shall be provided by the TC on request. The existing relevant SOPs and measurement and sampling guidelines shall be provided and explained to the NF operators accordingly.

3.5.2.4 **Mass concentration of particulate organic and elemental carbon**

Since a European standard for the measurement of OC and EC exists, which has been endorsed by ACTRIS, the consultancy offered to beneficiaries to start with OC-EC measurements shall be limited. The TC will not recommend any specific brands of OC-EC analysers. In contrast, the TC is expected to advise on the apparatus to be implemented for sampling atmospheric particulate matter for subsequent OC and EC analyses at the beginning of the implementation phase. This consultancy shall best be provided via a web based forum.

3.5.2.5 Particle number size distribution – optical and aerodynamic diameter

Consultancy for setting-up new observational or exploratory platforms shall be provided by the TC on request. Guidelines for appropriate sampling of larger aerosol particles already exist.

3.5.2.6 Particle number concentration

Consultancy for setting-up new observational or exploratory platforms shall be provided by the TC on request. The existing relevant SOPs and measurement guidelines shall be provided and explained to the NF operators accordingly.

3.5.2.7 Mass concentration of particulate elements

New observational and exploratory platforms shall be directly invited to attend training courses and inter-laboratory comparison exercises, in addition to have the possibility to visit the TC and get a brief instruction. The TC will provide consultancy to NFs planning to buy new instruments. This consultancy will include technical recommendations (minimum technical requirements to the instrument, demands of the instrument etc.) as well as instrument-dependent recommendations (number of operators, operating costs etc.). As the technology develops continuously, the consultancy support shall be developed and improved over the whole period of the project.

3.5.2.8 Mass concentration of particulate organic tracers

New observational and exploratory platforms

- shall be directly invited to participate into training courses and ILCs,
- can visit the TC and get a brief instruction.

The TC will provide consultancy if a NF plans to buy new instruments. This consultancy will include technical recommendations (minimum technical requirements to the instrument, demands of the instrument etc.) as well as instrument-dependent recommendations (number of operators, operating costs etc.). As the technology develops continuously, the consultancy support shall be developed and improved over the whole period of the project

3.5.2.9 Cloud condensation nuclei number concentration

Consultancy for setting-up new observational or exploratory platforms shall be provided by the TC on request. The existing relevant SOPs and measurement guidelines shall be provided and explained to the NF operators accordingly.

3.5.2.10 Mass concentration of non-refractory particulate organics and inorganics

The TC unit will offer assistance to NF that would like to implement new ACSM device. This shall be done by dissemination of existing SOPs and measurement guidelines, as well as direct exchange during teleconference and workshops, if necessary and on request.

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3.5.2.11 Nanoparticle number concentration

The measurement activities by the TC with PSM is by default a capacity building activity for the ACTRIS RI as this fills the observational gap between the trace gases and aerosol particles. A beneficial collaboration with exploratory platforms in relation to e.g. vertical profiling within the boundary layer with drones and aircrafts with the PSM instrumentation are foreseen. Additional vertical profiling in the surface layer is already on-going at few NFs (Hyytiälä, Järvselja). The analysis from these joint activities are facilitated in workshops, site visits and summer schools.

The activities with PSM connect to manufacturer organized workshops that facilitate harmonization of the observation methodology.

3.5.2.12 Nanoparticle number size distribution

The measurement activities by the TC with NAIS and UF-DMPS is by default a capacity building activity for the ACTRIS RI as this fills the observational gap between the trace gases and aerosol particles. A beneficial collaboration with exploratory platforms in relation to e.g. vertical profiling within the boundary layer with drones and aircrafts with the NAIS instrumentation are foreseen. Additional vertical profiling in the surface layer is already on-going at few NFs (Hyytiälä, Järvselja). The analysis from these joint activities are facilitated in workshops, site visits and summer schools.

3.6 Operation support for improvement of measurement methodologies

3.6.1 Testing of new measurement instruments and procedures

3.6.1.1 Particle number size distribution – mobility diameter

Operation support for improvements of measurement methodologies shall be provided on request and based on capacity.

3.6.1.2 Particle light scattering and backscattering coefficient

Operation support for improvements of measurement methodologies shall be provided on request and based on capacity.

3.6.1.3 Particle light absorption coefficient and equivalent black carbon concentration

Operation support for improvements of measurement methodologies shall be provided on request and based on capacity.

3.6.1.4 Mass concentration of particulate organic and elemental carbon

It is expected that the TC will test new measurement instruments for the determination of OC and EC deposited on filters, when substantial technological steps are made. Reproducibility tests making use of atmospheric samples shall be available from the beginning of the pre-operational phase. Proficiency tests based on the analysis of certified reference materials should be made possible by the beginning of the operational phase.

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The European standard EN16909:2017 is expected to be revised by the beginning of the pre-operational phase. Any revision of the analytical procedure should be tested against atmospheric samples for consistency with the procedure endorsed by the RI.

3.6.1.5 Particle number size distribution – optical and aerodynamic diameter

Operation support for improvements of measurement methodologies shall be provided on request and based on capacity.

3.6.1.6 Particle number concentration

Operation support for improvements of measurement methodologies shall be provided on request and based on capacity.

3.6.1.7 Mass concentration of particulate elements

The TC unit will offer benchmarking for novel instrumentation and procedures, by the beginning of the operational phase.

3.6.1.8 Mass concentration of particulate organic tracers

The TC will always follow the on-going development in scientific research and technical evolution. At the methodology side improvements are foreseen with regards to selective derivatisation procedures, enrichment processes and purification steps. Besides this, new methods shall be developed continuously for so-far unidentified classes of compounds. Special efforts shall be spend to develop environmental friendly methods by avoiding or at least reducing the amount of harmful chemicals and decrease the consumption of solvents of the instruments.

New and/or improved methods shall be made available continuously to the ACTRIS community.

On the other hand, the technical evolution will lead to instruments with higher mass resolutions and sensitivity, combined with an enhanced time resolution. This will lead to new requirements to the purity of the solvents, background corrections and data storage. The support with regards to the technical evolution is limited to the instruments available at the TC. Nevertheless, the TC will always work on recommendations and will have a link to manufacturers that can be used by the NF.

3.6.1.9 Cloud condensation nuclei number concentration

Operation support for improvements of measurement methodologies shall be provided on request and based on capacity.

3.6.1.10 Mass concentration of non-refractory particulate organics and inorganics

If new instruments are developed and interest is expressed by NFs, these instruments shall be tested at the TC unit as part of ongoing tests, notably based on comparison with reference instruments at the TC. Through collaboration with the manufacturer, different software analysis tools shall be developed, tested, and distributed to the ACTRIS community.

3.6.1.11 Nanoparticle number concentration

The TC unit will offer benchmarking for novel instrumentation for sub-0.01 µm aerosol measurements. The TC unit offers laboratory calibration services and intercomparison activities both in the field and in the laboratory. This activity shall be performed in collaboration with NFs. Several SMEs are already taking advantage of this opportunity.

3.6.1.12 Nanoparticle number size distribution

The TC unit will offer benchmarking for novel instrumentation for sub-0.01 µm aerosol measurements. The TC unit offers laboratory calibration services and intercomparison activities both in the field and in the laboratory. This activity shall be performed in collaboration with NFs. Several SMEs are already taking advantage of this opportunity.

3.6.2 Development of strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime

3.6.2.1 Particle number size distribution – mobility diameter

As there is a large variability among the MPSS instruments operated at ACTRIS NFs and moreover replacement parts are usually not very expensive, it is expected that the NFs will take care that the most common replacement parts for their instruments are at hand at the NFs.

3.6.2.2 Particle light scattering and backscattering coefficient

Replacement parts are usually not very expensive, hence it is expected that the NFs will take care that the most common replacement parts for their instruments are at hand at the NFs.

3.6.2.3 Particle light absorption coefficient and equivalent black carbon concentration

Replacement parts are usually not very expensive, hence it is expected that the NFs will take care that the most common replacement parts for their instruments are at hand at the NFs.

3.6.2.4 Mass concentration of particulate organic and elemental carbon

The TC will maintain / develop optimal relationships with the instruments' manufacturers and/or representatives in Europe. Based on information verified by both manufactures and the TC, "best practice" for optimising OC-EC analysers' lifetime shall be edited. It is expected that the OCEC unit will seek for an agreement with manufacturers / representatives to have the most "consumable" spare parts of the analysers available within acceptable delays in Europe. NB: this question mainly regards the on-line OC-EC analysers, since off-line instrument downtimes can be easily overcome by storing the filter samples for several months.

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3.6.2.5 Particle number size distribution – optical and aerodynamic diameter

As there is some variability between the OPSS instruments operated at ACTRIS NFs and moreover replacement parts are usually not very expensive, it is expected that the NFs will take care that the most common replacement parts for their instruments are at hand at the NFs.

3.6.2.6 Particle number concentration

As there is some variability between the CPCs operated at ACTRIS NFs and moreover replacement parts are usually not very expensive, it is expected that the NFs will take care that the most common replacement parts for their instruments are at hand at the NFs.

3.6.2.7 Mass concentration of particulate elements

The SOPs take into consideration the strategies to increase the duty cycle of the covered analytical techniques and provide guidance on the optimal operation procedures and maintenance. The TC expertise can be utilized the NF sites for trouble-shooting instrument problems.

3.6.2.8 Mass concentration of particulate organic tracers

Proper handling and careful maintenance can easily increase the lifetime of an instrument, both conducted by the user. The training courses will always include recommendation for cleaning procedures as well as basic instructions for the service. In urgent cases the support can be done remotely. Additionally, the TC can recommend special services offered by manufactures. The weighting between user-conducted service and manufacture-offered service might lead to a decrease of the operational costs of the NFs.

3.6.2.9 Cloud condensation nuclei number concentration

Replacement parts are usually not very expensive, hence it is expected that the NFs will take care that the most common replacement parts for their instruments are at hand at the NFs.

3.6.2.10 Mass concentration of non-refractory particulate organics and inorganics

By following the recommended operating procedures supplied to the ACTRIS community instrument operation, performance, and lifetime shall be optimised. Training courses run through the TC will provide assistance to new users on optimal instrument operation, as well as providing a place for the distribution of updated SOPs. This continuing work will lead to sets of corrections that can be applied to current and previous datasets.

3.6.2.11 Nanoparticle number concentration

The SOPs take into consideration the strategies to increase the duty cycle of the instruments and provide guidance on the optimal operation procedures and maintenance. When within the capacity of the TC, additional instrumentation can be loaned to cover observational gaps. The TC will negotiate with instrument manufacturers to have readily available crucial spare parts. The TC expertise can be utilized the NF sites for trouble-shooting instrument problems.

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3.6.2.12 Nanoparticle number size distribution

The SOPs take into consideration the strategies to increase the duty cycle of the instruments and provide guidance on the optimal operation procedures and maintenance. When within the capacity of the TC, additional instrumentation can be loaned to cover observational gaps. The TC will negotiate with instrument manufacturers to have readily available crucial spare parts. The TC expertise can be utilized the NF sites for trouble-shooting instrument problems.

3.6.3 Development of new technological products and methods

New measurement techniques, technological products and methods are developed by the TC in collaboration with the NFs. Depending on the situation, the TC may recommend to the ACTRIS RI Committee to decide on the implementation of such new techniques at the RI level. The TC has no obligation to develop the full set of operation support for such new techniques, unless they are embraced by ACTRIS and implemented as part of the NFs.

3.6.3.1 Particle number size distribution – mobility diameter

There exist already commercially available MPSS systems from several manufacturers. Hence the focus shall be to convince the manufacturers to follow with their instruments the guidelines set by the TC.

3.6.3.2 Particle light scattering and backscattering coefficient

There exist already commercially available nephelometers from at least two manufacturers. Hence the focus shall be to convince the manufacturers to follow with their instruments the guidelines set by the TC.

3.6.3.3 Particle light absorption coefficient and equivalent black carbon concentration

There exist already commercially available absorption photometers from several manufacturers. Hence the focus shall be to convince the manufacturers to follow with their instruments the guidelines set by the TC.

3.6.3.4 Mass concentration of particulate organic and elemental carbon

It is expected that the TC unit shall communicate the needs of the RI to the manufacturers to enhance the operability, the repeatability, the reproducibility, and the accuracy of the analyses. In the near future, analyser automation is foreseen. More sophisticated heating systems, enhanced control of the sample position in the analyser, additional instrument diagnosis parameters would be useful.

3.6.3.5 Particle number size distribution – optical and aerodynamic diameter

There exist already commercially available OPSS instruments from many manufacturers. For APSS instruments there is currently only one manufacturer. In both cases the focus shall be to convince the manufacturers to follow with their instruments the guidelines set by the TC.

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3.6.3.6 Particle number concentration

There exist already commercially available CPCs from many manufacturers. Hence the focus shall be to convince the manufacturers to follow with their instruments the guidelines and data quality criteria set by the TC. Close collaboration with CPC manufacturers exists concerning new CPC types and will continue in the future.

3.6.3.7 Mass concentration of particulate elements

The responsible TC unit shall communicate the needs of the RI to the manufacturers to enhance operability, sensibility and accuracy of the analytical techniques. TC may recommend the implementation of new technological products and developments (for instance, novel detectors) at the RI level.

3.6.3.8 Mass concentration of particulate organic tracers

Please see 3.5.1.

3.6.3.9 Cloud condensation nuclei number concentration

Currently, (2018), there is only one CCNC manufacturers, but their might be more in the near future. Focus shall be to advise the manufacturers and to convince them to follow with their instruments the guidelines set by the TC.

3.6.3.10 Mass concentration of non-refractory particulate organics and inorganics

Regular meetings with the user network, during either training schools or intercomparison workshops, will help determining the need for new tools and techniques by the ACTRIS community to develop new data products. In particular a better correction of sampling and/or measurement artefacts using harmonized tools is foreseen.

3.6.3.11 Nanoparticle number concentration

New measurement techniques, technological products and methods are developed by the TC unit in collaboration with the NFs. Depending on the situation, the TC may recommend to the ACTRIS RI Committee to decide on the implementation of such new techniques at the RI level. The TC has no obligation to develop the full set of operation support for such new techniques, unless they are embraced by ACTRIS and implemented as part of the NFs.

3.6.3.12 Nanoparticle number size distribution

New measurement techniques, technological products and methods are developed by the TC unit in collaboration with the NFs. Depending on the situation, the TC may recommend to the ACTRIS RI Committee to decide on the implementation of such new techniques at the RI level. The TC has no obligation to develop the full set of operation support for such new techniques, unless they are embraced by ACTRIS and implemented as part of the NFs.

Improvements in the sub-0.01 µm size distribution measurements are foreseen as suitable medium-to-high resolution DMAs start to be available. Higher flow rate CPCs improve the counting statistics

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particularly in the size distribution measurements, where single counts can transfer into high apparent number concentrations. These developments need to be considered, when mature enough for a wider application.

3.6.4 Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies

3.6.4.1 Particle number size distribution – mobility diameter

Tools for producing level 1 to 2 data already exist and shall be improved by the TC in the future.

3.6.4.2 Particle light scattering and backscattering coefficient

Tools for producing level 1 to 2 data already exist and shall be improved by the TC in the future.

3.6.4.3 Particle light absorption coefficient and equivalent black carbon concentration

Tools for producing level 1 to 2 data already exist and shall be improved by the TC in the future.

3.6.4.4 Mass concentration of particulate organic and elemental carbon

The determination of OC and EC does not involve the use of retrieval algorithms. It is expected that up-to-date tools to convert raw data to the level 2 data template are made available by the TC, at least from the pre-operational phase onwards.

3.6.4.5 Particle number size distribution – optical and aerodynamic diameter

Tools for producing level 1 to 2 data are currently (2018) under development and shall be improved by the TC in the future.

3.6.4.6 Particle number concentration

Tools for producing level 1 to 2 data shall be developed and improved by the TC in the future.

3.6.4.7 Mass concentration of particulate elements

The determination of particulate elements in PM samples does not involve the use of retrieval algorithms. It is expected that up-to-date tools to convert raw data to the level 2 data template are made available by the TC, at least from the pre-operational phase onwards.

3.6.4.8 Mass concentration of particulate organic tracers

The TC will cooperate with manufacturers in terms of software and method development. As a permanent user of different kind of instruments the TC can give well-founded feedback to beta-versions of software products.

3.6.4.9 Cloud condensation nuclei number concentration

Tools for producing level 1 to 2 data shall be developed and improved by the TC in the future.

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3.6.4.10 Mass concentration of non-refractory particulate organics and inorganics

The TC will participate in the development of software tools to be distributed to the community for data quality assurance prior to submission of level 1/1.5 data. Tools for the generation of new level 3 data products, such as the source apportionment of the organic aerosols, shall be also developed through collaborations with the instrument manufacturers and/or software providers.

3.6.4.11 Nanoparticle number concentration

Level 0: raw data- This is provided by the instruments. The TC facilitates data submission to ACTRIS DC in near-real-time.

Level 1: processed data –party provided by instruments (NAIS inversion software), partly developed during the process (automatic loss corrections, flagging, PSM and UF-DMPS inversion).

Level 2: final data – the algorithms and procedures for data quality assurance and plausibility tests need be developed (see 3.3.5)

Level 3: developed data products – algorithms for integrated size distribution using several instruments, condensation sink, and formation and growth rates are foreseen. A combined inversion of the aerosol number size distribution in the full ACTRIS measured size range (0.001 to 10 µm) could be one of the level 3 data products. These data products can be automated as soon as NRT data is available from the relevant ACTRIS parameters.

3.6.4.12 Nanoparticle number size distribution

Level 0: raw data- This is provided by the instruments. The TC facilitates data submission to ACTRIS DC in near-real-time.

Level 1: processed data –party provided by instruments (NAIS inversion software), partly developed during the process (automatic loss corrections, flagging, PSM and UF-DMPS inversion).

Level 2: final data – the algorithms and procedures for data quality assurance and plausibility tests need be developed (see 3.3.5)

Level 3: developed data products – algorithms for integrated size distribution using several instruments, condensation sink, and formation and growth rates are foreseen. A combined inversion of the aerosol number size distribution in the full ACTRIS measured size range (0.001 to 10 µm) could be one of the level 3 data products. These data products can be automated as soon as NRT data is available from the relevant ACTRIS parameters.

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4 Services provided to ACTRIS users

An ACTRIS user is a person, a team, or an institution using either ACTRIS data or any other ACTRIS service. ACTRIS users originate from academia, business, industry and public services, from ACTRIS member countries as well as from countries, which are not ACTRIS members, inside and outside Europe. The Centre for Aerosol In Situ Measurements will in particular serve atmospheric, climate, air quality, and aerosol research institutes, aerosol instrument manufacturers, environmental protection agencies, and industry companies.

Access to some ACTRIS services is open and free, most importantly the access to ACTRIS data, data products, and digital tools provided by the DC, which is the point of entry for free ACTRIS data services. Other access to ACTRIS services is considered competitive access based on capacity or excellence and will require a review process that is centrally managed by the HO/SAMU. SAMU is the single point of entry for user access to all TC services and to some specific services and data products provided by the DC. Access is regulated by both the ACTRIS access policy and the ACTRIS data policy, respectively.

4.1 Estimation of the need

Numbers in the following table are based on QA/QC expert estimates and give number of users (individuals) who currently (2018) benefit and might benefit in the future from ACTRIS services.

Type of ACTRIS user	Number of users to which ACTRIS can provide services		
	Now	by 2025	
		Min.	Max.
Academia	85	135	245
Business & Industry	40	62	155
Public services	80	95	185

4.2 Provision of measurement quality assurance and quality control procedures and tools

4.2.1 Particle number size distribution – mobility diameter

The same QA/QC tools as outlined in section 3.3.3 and 3.3.5 can be provided to ACTRIS users, such as the standard operating procedures and software tools.

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4.2.2 Particle light scattering and backscattering coefficient

The same QA/QC tools as outlined in section 3.3.3 and 3.3.5 can be provided to ACTRIS users, such as the standard operating procedures and software tools.

4.2.3 Particle light absorption coefficient and equivalent black carbon concentration

The same QA/QC tools as outlined in section 3.3.3 and 3.3.5 can be provided to ACTRIS users, such as the standard operating procedures and software tools.

4.2.4 Mass concentration of particulate organic and elemental carbon

Same as for operation support.

4.2.5 Particle number size distribution – optical and aerodynamic diameter

The same QA/QC tools as outlined in section 3.3.3 and 3.3.5 can be provided to ACTRIS users, such as the standard operating procedures and software tools.

4.2.6 Particle number concentration

The same QA/QC tools as outlined in section 3.3.3 and 3.3.5 can be provided to ACTRIS users, such as the standard operating procedures and software tools.

4.2.7 Mass concentration of particulate elements

The same QA/QC tools as outlined in section 3.3.3 and 3.3.5 can be provided to ACTRIS users, such as the standard operating procedures and software tools.

4.2.8 Mass concentration of particulate organic tracers

The SOPs (3.3.1), the check-up tool (3.3.4) and the QA/QC parameters (3.3.2) shall be made available to the ATCRIS users. The instruction into the procedures and tools shall be made by a clear documentation and during the training courses. If there is a special need, workshops or special sessions during conferences can be organized.

4.2.9 Cloud condensation nuclei number concentration

The same QA/QC tools as outlined in section 3.3.3 and 3.3.5 can be provided to ACTRIS users, such as the standard operating procedures and software tools.

4.2.10 Mass concentration of non-refractory particulate organics and inorganics

The same QA/QC tools as outlined in section 3.3.3 and 3.3.5 can be provided to ACTRIS users, such as the standard operating procedures and software tools.

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4.2.11 Nanoparticle number concentration

The TC should provide calibration services for PSM systems. The TC should organize audits and calibration workshops and develop SOPs in collaboration with the NFs. The data streams need to be developed and optimized. The data utilization need to be facilitated by network-wide data workshops.

4.2.12 Nanoparticle number size distribution

The TC should provide calibration services for NAIS and UF-DMPS systems. The TC should organize audits and calibration workshops and develop SOPs in collaboration with the NFs. The data streams need to be developed and optimized. The data utilization need to be facilitated by network-wide data workshops.

4.3 Instrument-specific calibration

4.3.1 Particle number size distribution – mobility diameter

The main role is to provide specific and advanced calibration services and specific hands-on training to NF and ACTRIS users.

4.3.2 Particle light scattering and backscattering coefficient

The main role is to provide specific and advanced calibration services and specific hands-on training to NF and ACTRIS users.

4.3.3 Particle light absorption coefficient and equivalent black carbon concentration

The main role is to provide specific and advanced calibration services and specific hands-on training to NF and ACTRIS users.

4.3.4 Mass concentration of particulate organic and elemental carbon

Same as for operation support.

4.3.5 Particle number size distribution – optical and aerodynamic diameter

The main role is to provide specific and advanced calibration services and specific hands-on training to NF and ACTRIS users.

4.3.6 Particle number concentration

The main role is to provide specific and advanced calibration services and specific hands-on training to NF and ACTRIS users.

4.3.7 Mass concentration of particulate elements

The main role is to provide specific and advanced calibration services and specific hands-on training to NF and ACTRIS users.

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4.3.8 Mass concentration of particulate organic tracers

Instrument dependent calibration proceedings are continuously trained during scientific trainings. These trainings are open to all users. Within these trainings special requests and critical issues can be addressed.

4.3.9 Cloud condensation nuclei number concentration

The main role is to provide specific and advanced calibration services and specific hands-on training to NF and ACTRIS users.

4.3.10 Mass concentration of non-refractory particulate organics and inorganics

The main role is to provide specific and advanced calibration services and specific hands-on training to NF and ACTRIS users.

Depending on the capacity, competition, and excellence, ACTRIS users can participate in organised instrument specific calibration and intercomparison campaigns. The advantages of participating in such calibration campaigns is to gather an optimum amount of users, increasing collaborations between groups as well as identifying the robustness of instrument operation from one system to the next. These intensive campaigns will provide a unique opportunity for the deployment of new instrument prototypes.

4.3.11 Nanoparticle number concentration

TC offers, limited by its resources, site audits and instrument specific workshops year for the PSMs, which are open to ACTRIS users. Workshop services are as in 3.3.3, and site audits as in 3.3.6.

4.3.12 Nanoparticle number size distribution

TC offers, limited by its resources, site audits and instrument specific workshops every two year for the NAIS and UF-DMPS, which are open to ACTRIS users. Workshop services are as in 3.3.3, and site audits as in 3.3.6.

4.4 Knowledge transfer and operator training

4.4.1 Particle number size distribution – mobility diameter

In addition to the services applied to ACTRIS users; training for new operators and scientists shall be provided on the recommended SOPs and the QA/QC tools developed for this specific measurements.

4.4.2 Particle light scattering and backscattering coefficient

In addition to the services applied to ACTRIS users; training for new operators and scientists shall be provided on the recommended SOPs and the QA/QC tools developed for this specific measurements.

4.4.3 Particle light absorption coefficient and equivalent black carbon concentration

In addition to the services applied to ACTRIS users; training for new operators and scientists shall be provided on the recommended SOPs and the QA/QC tools developed for this specific measurements.

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4.4.4 Mass concentration of particulate organic and elemental carbon

Same as for operation support.

4.4.5 Particle number size distribution – optical and aerodynamic diameter

In addition to the services applied to ACTRIS users; training for new operators and scientists shall be provided on the recommended SOPs and the QA/QC tools developed for this specific measurements.

4.4.6 Particle number concentration

In addition to the services applied to ACTRIS users; training for new operators and scientists shall be provided on the recommended SOPs and the QA/QC tools developed for this specific measurements.

4.4.7 Mass concentration of particulate elements

In addition to the services applied to ACTRIS users, training for new operators and scientists shall be provided on the recommended SOPs and the QA/QC tools developed for these specific measurements.

4.4.8 Mass concentration of particulate organic tracers

Knowledge transfer is a key focus of the scientific trainings. The training will cover each single step from sample collection until analysis of measurement results. The TC will spend special effort to offer each participant hands-on experience. With this the TC reaches the highest level of knowledge transfer that shall be afterwards controlled during the ILCs. If vulnerabilities were identified during the ILC, the problems were identified in a 1:1 discussion and if necessary an additional training can take place.

4.4.9 Cloud condensation nuclei number concentration

In addition to the services applied to ACTRIS users; training for new operators and scientists shall be provided on the recommended SOPs and the QA/QC tools developed for this specific measurements.

4.4.10 Mass concentration of non-refractory particulate organics and inorganics

In addition to the services applied to ACTRIS users; training for new operators and scientists shall be provided on the recommended SOPs and the QA/QC tools developed for these specific measurements.

4.4.11 Nanoparticle number concentration

The capacity building shall be organized in annual workshops that will provide operator training. The training sessions for the data analysis and data procedures occur during summer schools organized by the TC.

4.4.12 Nanoparticle number size distribution

The capacity building shall be organized in annual workshops that will provide operator training. The training sessions for the data analysis and data procedures occur during summer schools organized by the TC.

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4.5 Improvement of measurement and retrieval methodologies for aerosols, clouds, and reactive trace gases

4.5.1 Particle number size distribution - submicrometer

The TC will provide services of testing new prototypes, in close interactions with manufacturer. Requests for the development of specific software tools shall be considered on a case by case basis depending on the current interest and need within the community.

4.5.2 Particle light scattering and backscattering coefficient

The TC will provide services of testing new prototypes, in close interactions with manufacturer. Requests for the development of specific software tools shall be considered on a case by case basis depending on the current interest and need within the community.

4.5.3 Particle light absorption coefficient and equivalent black carbon concentration

The TC will provide services of testing new prototypes, in close interactions with manufacturer. Requests for the development of specific software tools shall be considered on a case by case basis depending on the current interest and need within the community.

4.5.4 Mass concentration of particulate organic and elemental carbon

Same as for operation support.

4.5.5 Particle number size distribution – optical and aerodynamic diameter

The TC will provide services of testing new prototypes, in close interactions with manufacturer. Requests for the development of specific software tools shall be considered on a case by case basis depending on the current interest and need within the community.

4.5.6 Particle number concentration

The TC will provide services of testing new prototypes, in close interactions with manufacturer. Requests for the development of specific software tools shall be considered on a case by case basis depending on the current interest and need within the community.

4.5.7 Mass concentration of particulate elements

The TC will provide services of testing new prototypes, in close interactions with manufacturer. Requests for the development of specific software tools shall be considered on a case by case basis depending on the current interest and need within the community.

4.5.8 Mass concentration of particulate organic tracers

Customized service of the TC shall be offered as direct support via telephone, email or remote access.

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4.5.9 Cloud condensation nuclei number concentration

The TC will provide services of testing new prototypes, in close interactions with manufacturer. Requests for the development of specific software tools shall be considered on a case by case basis depending on the current interest and need within the community.

4.5.10 Mass concentration of non-refractory particulate organics and inorganics

The TC will propose services for testing new prototypes, in close interactions with manufacturer. Requests for the development of specific software tools shall be considered on a case by case basis depending on the current interest and need within the community.

4.5.11 Nanoparticle number concentration

The TC should perform instrument development at the edge of the current knowledge to facilitate technology transfer from the scientific forefront to operational infrastructure. This will facilitate the TC to react to the needs arising from the user community.

4.5.12 Nanoparticle number size distribution

The TC should perform instrument development at the edge of the current knowledge to facilitate technology transfer from the scientific forefront to operational infrastructure. This will facilitate the TC to react to the needs arising from the user community.

5 Governance and management structure of the Centre for Aerosol In Situ Measurements

The Units of the Centre for Aerosol In Situ Measurements shall be organized according to the specific role of the CF, assuring that the CF complies with the requirements and obligations described in sections 6 and 8 of this document, and considering the general principles described in the *Baseline document for the concept of the Central Facilities*. The Centre for Aerosol In Situ Measurements shall be organized such that:

- It has a well-defined structure of Units,
- It has a well-defined decision-making process,
- It is coordinated by a CF Director and managed by a CF Management Board, which consists of the CF Director and the CF Unit Heads,
- It has clear and cost-efficient task sharing between the Units,
- It has a risk management strategy,
- It participates in the ACTRIS decision making by sending representative(s) to the ACTRIS legal entity bodies, e.g. to the RI committee.

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6 Requirements for the Centre for Aerosol In Situ Measurements

6.1 General requirements

In order to be labelled as the Centre for Aerosol In Situ Measurements, the candidate shall:

- Commit for long-term operation, at least 10 years starting with the next year after the implementation as a CF,
- Set-up an appropriate structure of Units, to ensure an adequate functionality of the CF, cost-effective operation, and scalability with respect to the user demands and advancement of the state-of-the art technology,
- Demonstrate the capacity (in terms of material and personnel resources), to ensure the provision of the needed services and operation support, as described in section 6.2
- Provide a feasible implementation and operation plan for the first five years, starting with the next year after the selection as CF,
- Commit to provide a minimum amount of user services, as described in section 4
- Commit to provide the mandatory operation support to the ACTRIS NFs, as described in section 3.

6.2 Technical requirements

6.2.1 Facilities

In view of the operation support and service provision, CAIS should have / put in place:

- Appropriate lab space, estimated to be in the order of 250 m^2 in total
- Appropriate office and storage room space, estimated to be in the order of 110 m^2 in total
- Appropriate instrumentation for aerosol particle generation, modification and characterisation, detailed for each variable in the following.

6.2.1.1 **Particle number size distribution – mobility diameter**

Three reference MPSS: two as reference instruments for the intercomparison workshops, and a third one that should be made available for on-site intercomparisons.

Three reference CPC: two as reference instruments for the intercomparison workshops, and a third one that should be made available for on-site intercomparisons.

Sufficient laboratory space to ensure that at least six instruments and users can participate during each intercomparison workshop. Additionally, a room for the external operators and scientists should be provided to evaluate their individual data.

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6.2.1.2 Multi-wavelength particle light scattering and backscattering coefficient

One multi-wavelengths reference Integrating nephelometer.

Sufficient laboratory space to ensure that at least six instruments and users can participate during each intercomparison workshop. Additionally, a room for the external operators and scientists should be provided to evaluate their individual data.

6.2.1.3 Multi-wavelength particle light absorption coefficient and equivalent black carbon concentration

One multi-wavelengths reference Integrating nephelometer, three single wavelengths reference extinction monitors with three different wavelengths, and two reference different reference absorption photometers.

Sufficient laboratory space to ensure that at least six instruments and users can participate during each intercomparison workshop. Additionally, a room for the external operators and scientists should be provided to evaluate their individual data.

6.2.1.4 Mass concentration of particulate organic and elemental carbon

For the OCEC unit, the minimum facilities required include:

- An aerosol collector able to sample aerosol particles on quartz fibre filters big enough to be split in aliquots suitable to fulfil beneficiaries' and users' demand in terms of number and size.
- An OCEC analyser with a repeatability sufficient to determine test filters' homogeneity with the precision required by the RI
- Gravimetric, dilution and deposition laboratory facilities for making artificial certified reference materials.

6.2.1.5 Particle number size distribution – optical and aerodynamic diameter

One reference APSS or OPSS as reference instruments for the intercomparison workshops, and one reference CPC.

Sufficient laboratory space to ensure that at least six instruments and users can participate during each intercomparison workshop. Additionally, a room for the external operators and scientists should be provided to evaluate their individual data.

6.2.1.6 Particle number concentration

One reference FCAE and one as reference CPC for the intercomparison workshops. Additionally, a generator for Nanoparticles is needed, preferably to produce silver particles.

Sufficient laboratory space to ensure that at least six instruments and users can participate during each intercomparison workshop. Additionally, a room for the external operators and scientists should be provided to evaluate their individual data.

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6.2.1.7 Mass concentration of particulate elements

For the mass concentration of particulate elements, the minimum facilities required include:

- One particle accelerator in the mega volt range, with a proton source and a dedicated beamline for PIXE measurements
- One ED-XRF spectrometer with secondary anodes or filters
- One ICP-MS instrument
- One ICP-AES instrument
- One aerosol resuspension chamber to produce synthetic aerosols reference standards
- Sufficient laboratory space to ensure that at least six users can participate during each intercomparison workshop and hands-on training
- A room for the external operators and scientists should be provided to evaluate their individual data.

6.2.1.8 Mass concentration of particulate organic tracers

Minimum technical requirements are one LC/MS system with high-resolution mass spectrometer and one with a time-of-flight mass spectrometer, one IC/PAD and one GC/MS with a normal inlet system and one with curie-point-pyrolysis. The technical equipment requires 2 laboratories. Additionally one laboratory is needed for sample preparation and one room for operators and users for data analysis and evaluation.

6.2.1.9 Cloud condensation nuclei number concentration

Needed instruments are one reference CCNC, one reference MPSS, and one reference CPC for the intercomparison workshops.

Needed is also sufficient laboratory space to ensure that at least six instruments and users can participate during each intercomparison workshop. Additionally, a room for the external operators and scientists should be provided to evaluate their individual data.

6.2.1.10 Mass concentration of non-refractory particulate organics and inorganics

One aerosol mass spectrometer is needed as reference measurements during the intercomparison workshops as well as for new devices and/or methodology testing purposes.

In order to perform calibrations, it is required to make use of nebulizers, DMA and CPC instruments, as well as a centrifugal particle mass analyser (CPMA). Furthermore, devices allowing for the generation of oxidised organic aerosols (e.g., using a Potential Aerosol Mass Oxidation Flow Reactor) is strongly recommended for examination of the accuracy of organics measurements.

Sufficient measurement techniques to provide satisfactory comparison with other techniques during intercomparison exercises, notably with total PM1, inorganic ions (online chromatography), organic carbon measurements (OCEC) are also needed.

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Laboratory space large enough to ensure that an adequate 15 instruments can participate during each intercomparison workshop. Additionally, a room for the external operators and scientists should be provided to evaluate their individual data.

6.2.1.11 Nanoparticle concentration

Technical requirements for test particle production are the following:

- Capability to reproducibly generate size-selected organic and inorganic sub-0.01 µm particles of all charging states (+, -, 0), of which composition can be verified.
- For CPC concentration calibration capability to size select 0.01 – 0.3 µm particles.
- For particle concentration reference capability to produce singly charged 0.1 µm particles of known concentration.

Instruments needed to fulfil these procedures include aerosol electrometer, tube furnace generator, atomizer, electrospray ionizing source, wire generator, DMA, high resolution DMA, PSM, NAIS, and UF-DMPS.

6.2.1.12 Nanoparticle number size distribution

Technical requirements for test particle production are following:

- Capability to reproducibly generate size-selected organic and/or inorganic sub-0.01 µm particles of all charging states (+, -, 0), of which composition can be verified.
- For particle size classification capability to size select charged sub-0.01 µm particles with minimum sizing resolution (Z/ΔZ) of 20 and aerosol flow rate of 10 slpm for PSM, UF-DMPS, and NAIS calibration.
- For CPC concentrations calibration capability to size select 0.01 – 0.3 µm particles.
- For particle concentration reference capability to produce singly charged 0.1 µm particles of known concentration.

Instruments needed to fulfil these procedures include aerosol electrometer, tube furnace, atomizer, electrospray ionizing source, wire generator, DMA, high resolution DMA, PSM, NAIS and UF-DMPS.

6.2.2 Human resources

In view of the needed operation support for the NFs and service provision for ACTRIS users the Centre for Aerosol In Situ Measurements should employ the following staff.

Scientific and technical staff			Management and administration staff		
Scientific expert	Qualified operator	Technician	Expert manager	Qualified officer	Administrative assistant
4.1	4.7	2.5	1.1	0.5	0.5

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The estimation of the needed human resource has been performed by QA/QC experts based on the proposed activities and assuming that the whole TC is fully operational. Numbers are expressed in FTE units.

6.2.3 Other requirements

6.2.3.1 Particle number size distribution – mobility diameter

License for handling radioactive sources is needed.

6.2.3.2 Multi-wavelength particle light scattering and backscattering coefficient

Provision for CO_2 gas must exist.

6.2.3.3 Multi-wavelength particle light absorption coefficient and equivalent black carbon concentration

None

6.2.3.4 Mass concentration of particulate organic and elemental carbon

The RPO responsible for the OCEC TC unit shall be at least accredited for OC-EC measurements (ISO 17025), and best for proficiency testing (ISO 17043).

6.2.3.5 Particle number size distribution – optical and aerodynamic diameter

None

6.2.3.6 Particle number concentration

Laser safety officer is needed. Provision for N_2 gas must exist.

6.2.3.7 Mass concentration of particulate elements

None

6.2.3.8 Mass concentration of particulate organic tracers

At least one of the TC operators should have a GLP/GMP (Good laboratory practice/Good manufacturing practice) certificate to ensure the highest level of QA/QC.

6.2.3.9 Cloud condensation nuclei number concentration

None

6.2.3.10 Mass concentration of non-refractory particulate organics and inorganics

License for handling radioactive sources is needed.

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6.2.3.11 Nanoparticle concentration

Provision for N_2 gas must exist.

6.2.3.12 Nanoparticle number size distribution

License for handling radioactive sources is needed.

7 Basic criteria for the selection of the Centre for Aerosol In Situ Measurements

The applications to host the Centre for Aerosol In Situ Measurements are evaluated against a set of criteria covering:

- The **level of commitment** for long-term operation
- The **capacity** to provide the operation support and the services described in sections 3 and 4
    - The availability of the necessary laboratories, instruments, equipment
    - The availability of human resources (no., expertise)
- The **efficiency** in providing the operation support and the services
    - The feasibility of the implementation plan (costs, resources, timeline)
    - The feasibility of the operation plan (methodology, costs per service)
- The level of maturity
    - Status of the development of the Units
    - No. of existing users
    - Adequacy of the decision-making
    - Risk management strategy

These criteria shall be detailed in the associated call documents.

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8 Obligations of the Centre for Aerosol In Situ Measurements

8.1 General obligations

The following general obligations shall apply to the Centre for Aerosol In Situ Measurements while operational:

- To organize its activities in a cost-efficient way, timely, and with high quality,
- To actively participate in the governance and sustainable development of ACTRIS,
- To provide services to users, according to the access procedures, availability of time, and material resources,
- To provide operation support to the NFs, according to the identified needs, agreed schedules, and procedures,
- To implement efficient user interaction activities by:
  - Organizing workshops, to interact with users,
  - Collecting user feed-backs,
  - Maintaining the CF and ACTRIS websites,
- To document its activities, accesses provided, key performance indicators, and finances, and provide this information to the HO,
- To contribute to minimize and assess the uncertainties related to data and data products, according to their role and in collaboration with each other.

8.2 Technical obligations

8.2.1 Technical obligations in relation with the ACTRIS National Facilities

Technical obligations of the Centre for Aerosol In Situ Measurements in relation with the ACTRIS NFs refer strictly to the measurement techniques described in this concept document and in *Technical concepts and requirements for ACTRIS Observational Platforms.* The operation of other techniques at the NFs does not imply a technical obligation for the Centre for Aerosol In Situ Measurements to provide operation support. New techniques / instrument types are only accepted as ACTRIS instruments after the approval of the RI Committee and after the development of the associated QA procedures by the CF.

8.2.1.1 Guidelines, quality assurance criteria and procedures

The Centre for Aerosol In Situ Measurements is responsible for the quality assurance procedures and guidelines of the ACTRIS measurements conducted at the NFs operating instruments for the physical or chemical in situ characterization of atmospheric aerosol particles as well as for particle sampling and subsequent laboratory analysis of these particles. For this, the TC should implement the following operation support for each of the measurement technique under its topics:

- Definition and establishment of standard operation procedures (as described in section 3.3.1)
- Definition of measurement quality-assurance criteria and procedures (as described in section 3.3.2)

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All the procedures, guidelines, quality assurance criteria, plausibility tests, etc. should be documented and accessible to all related NFs. Specific training sessions with the related NF operators should be organized to ensure a smooth and correct implementation of the above.

8.2.1.2 Tools, tests and consultancy for quality control of the measurements

It is duty of the Centre for Aerosol In Situ Measurements to assist the related NFs in the quality control of their measurements by providing the following operation support for each of the measurement techniques under its topics:

- Development and provision of instrument-specific calibration (as described in section 3.3.3)
- Development and provision of in-house check-up tools (as described in section 3.3.4)
- Development of data evaluation procedures and plausibility test (as described in section 3.3.5)
- Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs (as described in section 3.4.3.4.1.12)
- Testing of new measurement instruments and procedures (as described in section 3.5.1)

This operation support should be offered to the related NFs whenever there is a need, or a significant progress in the development of these tools, and accompanied by the appropriate training.

8.2.1.3 Assessment of performances, measurement flagging

The Centre for Aerosol In Situ Measurements is mandated to assist the DC and the related NFs in the quality control of the measurements and data, by:

- Realization of observational site performance audits with reference samples or mobile systems (as described in section 3.3.6)
- Organizing regular exercises to assess the performances of the NFs, including instrument performance workshops (as described in section 3.3.7)
- Contributing to documentation and traceability of level 0 to level 3 data products (as described in section 3.3.8)

The activities involving directly the NFs operating instruments for the physical or chemical in situ characterization of atmospheric aerosol particles as well as for particle sampling should be scheduled by the TC and provided regularly. The corresponding NFs should participate in these activities according to the plan proposed by the Centre for Aerosol In Situ Measurements and agreed together with the ACTRIS Scientific Advisory Board (SAB).

8.2.1.4 Transfer of knowledge and training

In addition to the training organized for the implementation of guidelines, procedures, and tools developed in support of the quality control of the measurements, the Centre for Aerosol In Situ Measurements should organize training sessions with the NFs operating instruments for the physical or chemical in situ characterization of atmospheric aerosol particles as well as for particle sampling and subsequent laboratory analysis of these particles as needed (see section 3.4.1).

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8.2.1.5 Improvement of measurement methodologies for Centre for Aerosol In Situ Measurements

Although it is not an obligation, the Centre for Aerosol In Situ Measurements should work to sustain a high level of performance and to stimulate the advancement of new techniques and methodologies in the in situ aerosol measurement field by:

- Development of strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime (as described in section 3.5.2)
- Development of new technological products and methods (as described in section 3.5.3)
- Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies (as described in section 3.5.4)
- Organizing regular events (at least once at 2 years) and other forums, in order to exchange knowledge with the NFs and other scientists
- Contributing to CEN, ISO, or similar standardization activities (as described in section 3.3.9)

8.2.2 Technical obligations in relation with the ACTRIS Data Centre

8.2.2.1 Data production and data products

The final in situ aerosol ACTRIS data products (ACTRIS data Level 1 and Level 2) consist of various aerosol particle properties together with the respective precision and accuracy, metadata and time dependent flags as specified by the DC and in the standard operating procedures.

For the online measurements, raw data (Level 0) at temperature and pressure conditions as provided by the instrument has to be stored together with the relevant standard and calibration measurements and all information and meta data, which is needed to calculate the higher-level data products. 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 DC 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**, **online or offline**.

For the **online 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 metadata and remarks needed in the further data production process. Level 0 data are to be submitted and archived at the DC 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, e.g. aerosol mass spectra. In this case, an alternative storage procedure has to be agreed between the Centre for Aerosol In Situ Measurements and the DC, 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

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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 DC unit, depending on variable. The distribution of work is included in the associated data production descriptions available from the DC. The quality control step between Levels 0 and 1 can be automatic (real-real time 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 **offline workflow**, the steps of sample medium pre-exposure treatment, exposure, preparation, sampling, and analysis are documented with standard operating procedures and protocols including metadata and remarks 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 Centre for Aerosol In Situ Measurements. From these protocols, the Level 2 data products are produced in the temporal resolution determined by the 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.

8.2.2.2 Data delivery and quality control

It is compulsory for the NF to produce at least Level 1 (online measurements) and Level 2 (online and offline measurements) data for archiving at the associated DC unit. Archiving of Level 0 data will depend on specific variables. 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 shall be discussed at the annual data quality meeting, 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 shall 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 DC in real-real-time (RRT), i.e., latest within 3 hours of measurement, for delivery of an RRT data product for operational services.

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8.2.3 Technical obligations in relation with the Centre for Cloud In Situ Measurements and the Centre for Reactive Trace Gases In Situ Measurements

Currently (2018), there are no technical obligations the Centre for Aerosol In Situ Measurements has to fulfil for other TCs. However, as the six scientific ACTRIS themes partly overlap, there is sometimes the need to agree among two TCs which of the two TCs is responsible for specific operation support or services. For the Centre for Aerosol In Situ Measurements this overlap exists with the Centre for Cloud In Situ Measurements concerning the cloud droplet or ice crystal activation properties of aerosol particles, as well as with the Centre for Reactive Trace Gases In Situ Measurements concerning the transition from gas molecule clusters to aerosol particles.

8.2.4 Technical obligations in relation with the ACTRIS users

The Centre for Aerosol In Situ Measurements should commit to provide a minimum amount of user services as described in section 4.

8.3 Evaluation of the activity of the Centre for Aerosol In Situ Measurements

Once established and operational, the Centre for Aerosol In Situ Measurements shall be evaluated for its performances, using the following Key Performance Indicators (KPIs):

No.	Criteria	Indicators	Score	Weight
1	Usefulness for ACTRIS NFs	No. of operation support units provided to ACTRIS NFs for quality assurance and quality control	1 … 10	50%
		No. of operation support units provided to ACTRIS NFs for knowledge transfer and training	1 … 10	
		No. of operation support units provided to ACTRIS NFs for Improvement of measurement and data processing methodologies	1 … 10	
		Average score of satisfaction received from NFs	1 … 10	
		Average of Usefulness for ACTRIS		
2	Usefulness for ACTRIS users	No. of service units provided to ACTRIS users for quality assurance and quality control	1 … 10	20%
		No. of service units provided to ACTRIS users for knowledge transfer and training	1 … 10	

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		No. of service units provided to ACTRIS users for improvement of measurement and data processing methodologies	1 ... 10	
		Average score of satisfaction received from ACTRIS users	1 ... 10	
		Average of Usefulness for external users		
3	Impact on science and technology	No. of new technological products, methods and algorithms developed/ improved	1 ... 10	15%
		No. of peer-review CF-related papers published	1 ... 10	
		No. of CF-related communications at scientific conferences/workshops	1 ... 10	
		No. of CF-related patents promoted	1 ... 10	
		Average of S&T Impact		
4	Integration into ACTRIS-RI	No. of participations to ACTRIS committees and boards	1 ... 10	15%
		No. of activities performed in collaboration with other TCs (joint SOPs, joint workshops, etc.)	1 ... 10	
		Average score of satisfaction received from ACTRIS DC for the contribution to documentation and traceability of data products	1 ... 10	
		Average score of satisfaction received from ACTRIS HO for the quality and readiness of the reports	1 ... 10	
		Average of Integration into ACTRIS-RI		
Total score				

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9 Glossary

ACTRIS data - are the ACTRIS variables resulting from measurements that fully comply with the standard operating procedures (SOP), measurement recommendations, and quality guidelines established within ACTRIS.

- **ACTRIS level 0 data:** Raw sensor output, either mV or physical units. Native resolution, metadata necessary for next level.
- **ACTRIS level 1 data:** Calibrated and quality assured data with minimum level of quality control.
- **ACTRIS level 2 data:** Approved and fully quality controlled ACTRIS data product or geophysical variable.
- **ACTRIS level 3 data:** Elaborated ACTRIS data products derived by post-processing of ACTRIS Level 0 -1 -2 data, and data from other sources. The data can be gridded or not.
- **ACTRIS syntheses product** (*Proper name to be defined later*)**:** Data product from e.g. research activities**,** not under direct ACTRIS responsibility, but ACTRIS offer repository and access.

ACTRIS Data Centre (DC) - the Central Facility responsible for ACTRIS data curation, preservation, and distribution of data, value-added products and tools**,** and hosting the ACTRIS data portal.

ACTRIS data originator - entity operating instruments at a National Facility or Topical Centre, resulting in ACTRIS data and delivering ACTRIS data to the Data Centre.

ACTRIS data provider - the Data Centre offering the ACTRIS data and value-added data products and tools to users.

ACTRIS digital tools and services - tailored codes and software for processing and visualization of ACTRIS data, production of ACTRIS data products, and for data analysis and research.

ACTRIS exploratory platform - National Facility (simulation chambers, laboratories, or mobile facilities) operating on campaign basis and delivering dedicated data to the Data Centre.

ACTRIS General Assembly (GA) - a council of ministry- and funding organization representatives of ACTRIS members after ACTRIS legal entity has been established, superior decision-making body of ACTRIS.

ACTRIS Head Office (HO) - a Central Facility coordinating and representing ACTRIS, and holding the statutory seat.

ACTRIS label - earmarks a data set or a measurement site as ACTRIS data or ACTRIS National Facility.

ACTRIS observational platform – ACTRIS National Facility performing long-term, regular observations and delivering standardized data to the Data Centre.

ACTRIS Topical Centres (TCs) – a Central Facility offering services and operation support for QA/QC of measurements and data (including training, calibration, QA/QC tools, and development of standard operation and evaluation procedures)

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ACTRIS variables - the measured atmospheric variables as described in the ACTRIS Data Management Plan[1].

Central Facility (CF) - a European level ACTRIS component that offers ACTRIS data or other ACTRIS services to users as well as operation support to ACTRIS National Facilities.

Central Facility Unit – part of a Central Facility located at, and operated by a research performing organization (RPO) or by ACTRIS ERIC.

CF Director – the person responsible for the coordination and representation of a Central Facility.

CF Unit Head – the person responsible for the coordination and representation of a Central Facility unit.

CF Management Board – consists of the CF Unit Heads and the CF Director; this board manages the Central Facility.

Data curation - the activity that stores, manages and ensures access to all persistent data sets produced within the infrastructure.

Data traceability - an unbroken chain of uniquely identified process steps leading from raw data to any kind of processed data, where identification of process steps follows the data.

In situ measurements - measured or sampled air and instrument are at the same location and in physical contact. In the context of ACTRIS, in situ measurements of aerosol, cloud, and reactive-trace-gas properties are performed at observational sites near the Earth surface, on mobile surface-based or airborne platforms, and in atmospheric simulation chambers and laboratories.

Interim ACTRIS Council - a council of ministry- and funding organization representatives of ACTRIS members before ACTRIS legal entity has been established (during the ACTRIS Preparation and Transition Phase), superior decision-making body of ACTRIS.

Measurement traceability - an unbroken chain of comparisons relating an instrument's measurements to a known standard, in the ideal case SI units.

National Facility (NF) - an observational or exploratory platform providing data and/or physical access to the platform within ACTRIS.

Quality assurance and control: Quality assurance is process oriented and focuses on defect prevention; quality control is product oriented and focuses on defect identification:

- **Quality Assurance (QA):** The process or set of processes used to ensure the quality of a product (e.g. data series, instrument, sample, measured value of a variable, etc.),
- **Quality Control (QC):** The process and activities of ensuring products and services meet the expectations.

Remote sensing - measured air and instrument are not at the same location and not in physical contact. In the context of ACTRIS, active and passive atmospheric remote-sensing techniques for the

[1] The ACTRIS data management plan and list of variables were approved by ACTRIS-2 scientific steering committee, October 2015. These documents are expected to be refined during ACTRIS-PPP (WP5).

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observation of aerosols, clouds, and trace gases are applied at observational sites and on mobile surface-based or airborne platforms.

RI committee – consists of up to two representatives from each Central Facility and [three] representatives from the National Facilities Assembly; the RI committee supports the (Interim) Director or Board of Directors in operating the RI.

Service and Access Management Unit (SAMU) - a part of ACTRIS Head Office facilitating the access to ACTRIS services.

User - a person, a team, or an institution making use of ACTRIS data or other ACTRIS services, including access to ACTRIS facilities.

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10 Reference documents

ACTRIS-PPP proposal

ACTRIS Data Management Plan, approved by ACTRIS-2 SSC 23 October 2015

ACTRIS Concept Documents

ISO 10012:2003: Measurement management systems — Requirements for measurement processes and measuring equipment

ISO 9000:2015: Quality management systems—Fundamentals and vocabulary

Baseline document for the Concepts of ACTRIS Central Facilities

Technical concepts and requirements for ACTRIS Observational Platforms

Technical concepts and requirements for ACTRIS Exploratory Platforms

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Annex: Provision of the operation support

Scheduled support

Mode	Type of support	Specific support	Frequency	Comments
In situ measurements	Instrument-specific calibration workshop at TC facility	Comparison with fixed reference instruments, intercomparison measurements, support for beneficiaries whose instrument under-performed	Once every 1-3 years, after major upgrades, or after replacement	TC distributes a schedule one year in advance and agrees with the NFs on potential adjustments of the schedule
	Site performance test with reference instruments operated at NFs	Round-Robin reference instrument, support for beneficiaries whose instrument under-performed		TC distributes a schedule one year in advance and agrees with the NFs on potential adjustments of the schedule
In situ sampling	Laboratory intercomparison at NFs	Round-Robin reference samples, support for beneficiaries whose instrument under-performed	Once every 1-2 years, after major upgrades, or after replacement	TC distributes a schedule one year in advance and agrees with the NFs on potential adjustments of the schedule
In situ measurements or In situ sampling	Training of operators and scientists	Training on particle measurement and sampling, exercises to access the performance of NFs, training on data evaluation	Once every 1-2 years	Mostly co-located with instrument calibration workshops, otherwise specific schools announced on the TC web page and with online registration

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Operation support on request

Mode	Type of support	Specific support	Comments
In situ measurements or sampling	Measurement guidelines	Definition and establishment of measurement guidelines and standard operation procedures	For new instruments and/or new ACTRIS variables, depending on capacity and time schedule, on request by the National Facilities Assembly and the RI Committee
	Quality-assurance criteria and procedures	Definition of measurement quality-assurance criteria and procedures	For new instruments and/or new ACTRIS variables, depending on capacity and time schedule, on request by the National Facilities Assembly and the RI Committee
	Instrument calibration	Development and provision of instrument-specific calibration	Unscheduled calibration, either at TC or at NF, depending on capacity and time schedule, on request by NFs via SAMU
	Measurement and data tools	Development and provision of in-house check-up tools	Depending on capacity and time schedule, on request by the NFs, the DC, the National Facilities Assembly, or the RI Committee
		Development of data evaluation procedures and plausibility tests	
	Site performance tests	Round-Robin test with either reference samples or reference instruments, analysis of samples collected by the NFs	Unscheduled site performance tests, e.g. after major site upgrades, depending on capacity and time schedule, on request by NFs via SAMU
	Training of operators and scientists	Training on particle measurement and sampling, exercises to access the performance of NFs, training on data evaluation	Unscheduled training, depending on capacity and time schedule, on request by NFs or RI Committee

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In situ measurements or sampling	New RI components	Consultancy for setting-up new observational or exploratory platforms and new instruments at NFs	Depending on capacity and time schedule, on request by NFs via SAMU
		Testing of new measurement instruments	
	Data production	Development of tools for producing level 1 to 3 data, including tools for producing NRT data	Depending on capacity and time schedule, on request by the DC, the National Facilities Assembly, or the RI Committee

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Section 4

Concept of the Centre for Aerosol Remote Sensing

ACTRIS PPP WP 4 task 4.1

22.2.2018

Public

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1 Purpose of the document

This document describes the relevance, mission, requirements and obligations of the ACTRIS Centre for Aerosol Remote Sensing.

2 Description and role of the Centre for Aerosol Remote Sensing

2.1 Framework

The Centre for Aerosol Remote Sensing (CARS) is one of the six ACTRIS Topical Centres organized around the main scientific themes of ACTRIS: aerosols, clouds, and reactive trace gases, each with a particular focus on either remote sensing or in situ measurement techniques.

The following documents are completing the current concept of the Centre for Aerosol Remote Sensing (CARS):

- **The ACTRIS framework** is described in the following documents:
  - ACTRIS ESFRI proposal
  - ACTRIS-PPP project
  - ACTRIS Stakeholders Handbook 2017
  - ACTRIS Science Case document
- **The general rules and principles for the ACTRIS Central Facilities** are described in the Baseline document for the Concepts of ACTRIS Central Facilities.
- **The measurements techniques operated by the ACTRIS National Facilities** for which the operation support should be offered, along with the specific requirements, are described in:
  - Technical concepts and requirements for ACTRIS Observational Platforms
  - Technical concepts and requirements for ACTRIS Exploratory Platforms

2.2 Scientific relevance

ACTRIS science case is described in *ACTRIS Stakeholder handbook* and *ACTRIS Science case document*.

In particular for the **Centre for Aerosol Remote Sensing (CARS)**, the focus is on measuring with high accuracy the optical properties of tropospheric and low stratospheric aerosols, and potentially derive their microphysical properties. CARS involves aerosols column and aerosol profiling measurement techniques as well as their synergetic uses at ground-based level.

Aerosol profile observations are covered in ACTRIS by automatic low-power lidars and high-power lidars. Due to the differences at the hardware level (e.g. laser power and sounding wavelengths), the data products which can be retrieved from these measurement techniques are essentially different.

- ***Automatic low-power lidars and ceilometers (ALC)*** are currently used to provide aerosol layering and attenuated backscatter at one wavelength (in IR), information which is used in combination with cloud radars and microwave radiometers to complete the cloud classification at the ACTRIS Cloud Remote Sensing National Facilities. In addition, these parameters could be used to study aerosol nucleation processes that are of great importance for visibility studies. The temporal coverage and low overlap of low power lidar instruments is a valuable add-on used to study the diurnal variation of aerosol layers and to trigger advanced measurements performed using high-power lidar instruments. Even single wavelength low-power lidars are able to detect high resolution dynamics of aerosol layers.

- ***Aerosol high-power aerosol lidars (AHL)*** are aerosol lidar which thanks to the higher power can provide besides the same quantities reported for the ALL, more quantitative information about the aerosol optical properties. In particular, AHL used to provide profile aerosol optical properties (aerosol backscatter coefficient, aerosol extinction coefficient and aerosol linear depolarization ratio) at one or more wavelengths, allowing subsequent calculation of several spectral parameters (Angstrom exponents, lidar ratios) of the lofted aerosol layers, and therefore aerosol typing.

It is estimated that, with the progress of the technology (especially lasers and detectors), these two measurement techniques will evolve in the future to a low-cost, low-maintenance, automatic multiwavelength aerosol profiler. For the moment, however, the procedures for QA/QC, as well as the algorithms for data processing are instrument-specific and should be treated separately by CARS.

Aerosol column observations are covered in ACTRIS by ***automatic sun/sky/lunar photometers (ASP)***. The state-of-the-art photometric measurement techniques and associated retrieval techniques provide aerosol properties both directly (e.g. daytime and night time spectral extinction AOD and daytime downward sky angular, spectral and polarized radiance) and indirectly (size distribution, refractive indexes, single scattering albedo, spherical fraction, scattering properties (Dubovik et al., 2000, 2014).

Synergies between aerosol profile and column observations are being greatly developed within ACTRIS-1/2 to provide higher-level aerosol variables such as daytime extinction, backscatter, absorption and mass concentration (total, fine, coarse) and columnar aerosols optical and microphysical properties.

2.3 Mission

The mission of the Centre for Aerosol Remote Sensing (CARS) is to offer operation support to ACTRIS National Facilities operating aerosol remote sensing instrumentation: high-power aerosol lidars, automatic low-power aerosol lidars, and automatic sun/sky/polarized/lunar photometer.

Additionally, the Centre for Aerosol Remote Sensing should offer specialized services for the above instruments and related ACTRIS variables, to ACTRIS users of various types: academia, business, industry, and public services.

3 Operation support provided to ACTRIS National Facilities

The main duty of the Centre for Aerosol Remote Sensing is to permit the operability of the NFs operating high-power aerosol lidars, automatic low-power aerosol lidars, and sun/sky/lunar photometers, and the compliance of their methodologies and products to the requirements of full traceability, high quality and full documentation.

The operation support provided by the Centre for Aerosol Remote Sensing consists of:

a) Procedures and tools for quality assurance and quality control of ACTRIS measurements and data
b) Transfer of knowledge and training to ACTRIS operators
c) Improvement of measurement methodologies

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The operation support should be offered to the National Facilities for the measurement techniques described in this concept document, also listed in the *Technical concepts and requirements for ACTRIS Observational Platforms*, and in the *Technical concepts and requirements for ACTRIS Exploratory Platforms.*

The Centre for Aerosol Remote Sensing is obliged to put in place and offer to NFs the specific operation support marked with * in this document. Other operation support described in this document is not mandatory for CARS, but recommended.

The operation support can be scheduled or on request:

- Participation at the scheduled activities is mandatory for the NFs. Measurements performed at NF not following the mandatory actions are not considered as ACTRIS-conform and do not yield ACTRIS data.
- NFs may request operation support which is not scheduled, depending on the identified need.

Specific operation support offered as scheduled or offered on request is detailed in *Annex: Provision of the operation support.* This annex will be updated each time is necessary (e.g. development of new testing or calibration methods and tools).

The Centre for Aerosol Remote Sensing should operate at the state-of-the-art, fostering the implementation of validated new techniques in ACTRIS. To sustain a high level of performance and to stimulate the advancement of new techniques and methodologies, the Centre for Aerosol Remote Sensing should also contribute to expert collaboration networks.

3.1 Measurement techniques covered by the Centre for Aerosol Remote Sensing, and related ACTRIS variables

Measurement techniques covered by the Centre for Aerosol Remote Sensing are described in detail in: *Technical concepts and requirements for ACTRIS Observational Platforms* and *Technical concepts and requirements for ACTRIS Exploratory Platforms.*

3.1.1 Aerosol high-power lidar (AHL)

At present, the minimum lidar requirement for effective aerosol profiling includes one elastic channel, one channel at the corresponding inelastic wavelength for aerosol extinction measurement and one channel to measure the aerosol depolarisation (1+1+1 configuration). The particular wavelength of these 3 channels can be in the visible or UV.

With this configuration, the **following ACTRIS variables** can be retrieved:

- Extensive aerosol optical properties (profiles): linear volume depolarization ratio, backscatter and extinction coefficients (single wavelength)
- Intensive aerosol layer optical properties (partial profiles): particle linear depolarization ratio, lidar ratio (single wavelength)
- Aerosol layer geometrical (height and thickness) and optical properties (extensive and intensive properties, mean-layer values, single wavelength)

A more **advanced setup** comprises three channels at elastic wavelengths, two channels at the corresponding inelastic wavelengths for aerosol extinction measurement, and two channels to measure the depolarisation at one wavelength (3+2+1 configuration). Such a multi-wavelength polarisation lidar system for night time and daytime measurements comprises a complex wavelength separation unit.

With this configuration, the **following ACTRIS variables** can be retrieved:

- Extensive aerosol optical properties (profiles): linear volume depolarization ratio, backscatter and extinction coefficients (multiple wavelengths)
- Intensive aerosol layer optical properties (partial profiles): particle linear depolarization ratio, lidar ratio, backscatter and extinction-related Angstrom exponent (multiple wavelengths)
- Aerosol layer geometrical (height and thickness) and optical properties (extensive and intensive properties, mean-layer values, multiple wavelengths)
- Aerosol type, aerosol microphysical properties (in particular cases and/or by synergy with photometer)

In future we expect 3+2+3 and even 3+3+3 setups, which will increase the complexity. Furthermore, it is highly desirable and expected that the detection range will be extended down to 200 m above ground level to include this part of the mixing layer which often contains most of the aerosol. This adds another order of magnitude to the dynamic range of the signals and much higher demands on the mechano-optical design of the lidar with more sources for larger systematic errors.

The collection, harmonisation, and development of standards and calibration techniques started in the framework of EARLINET and ACTRIS, e.g. the calculation of the Rayleigh scattering coefficients, the Rayleigh-fit, the trigger delay determination, the telecover tests, the dark signal subtraction, the specialised lidar pulse generator, and the polarisation calibration (Freudenthaler et al., 2017), mainly in the aim to avoid signal disturbance. **These should be considered as a starting base for the QA/QC program of the ACTRIS high-power aerosol lidars.**

This program should be further developed in order to: a) make these tests easier to be used on a regular basis by the ACTRIS NFs and users; b) establish new tools to quantify the signal disturbances; c) develop an error analysis of the final products which includes and combines systematic and random errors. Also, CARS should **consider future lidar developments** as, e.g., the High-Spectral-Resolution-Lidar (HSRL) technique and the circular depolarisation ratio.

3.1.2 Automatic low-power lidar / ceilometer (ALC)

Automatic low-power aerosol lidars and ceilometers are **elastic backscatter lidars, providing aerosol profiles** (attenuated backscatter) **at one wavelength** (in IR). These are mainly commercial systems, usually very robust, eye-safe, operated continuously and unattended, often at remote sites. Most of them are operated by national meteorological services and environmental agencies. Several low-power lidars are operated at ACTRIS NFs, mainly in combination with cloud radars and microwave radiometers to complete the cloud classification. Also, they are used as ancillary instruments to fill gaps in the operation time of high-power lidars or to provide basic knowledge about the vertical structure of the atmosphere at NFs for in-situ measurements of aerosols and trace gases.

The hardware issues are mainly the same as in case of high-power lidars, such as the incomplete overlap between laser and telescope, electronic background signals, saturation effects. Additionally, some of the low-power lidars operate at wavelengths which are influenced by water-vapour absorption.

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The calibration and quality assurance procedures which were developed for high-power lidars in ACTRIS and ACTRIS-2 cannot be directly applied to the low-power instruments. Calibration and quality assurance methods for low-power lidars have been recently developed by E-PROFILE community. **These should be considered as a starting base for the QA/QC program of the ACTRIS low-power aerosol lidars.**

In addition, a strong link with QA of AHL is required because both techniques are used to provide attenuated backscatter (intermediary product) for cloud processing.

3.1.3 Automatic sun/sky/polarized/lunar photometer (ASP)

The required instrument is a sun/sky/lunar photometer making two basic measurements, direct sun/moon and sky measurements, possibly including linear polarization, both within several programmed sequences or protocols. The direct measurements are currently made in nine spectral bands (340, 380, 440, 500, 670, 870, 940, 1020 and 1640) and will be likely performing with a higher spectral resolution in the future.

ACTRIS-I3 projects provides since 2011 a relevant support for (i) QC/QA activity, (ii) the consolidation of a dedicated European sun/sky/moon calibration centre based on French and Spanish complementary TC units, (iii) the integration with aerosol profiles and in situ communities through several ACTRIS Joint Research Activities, (iv) the development, implementation and operation, in the ACTRIS Data Centre, of an advanced processing system producing and delivering added-value information based on GRASP/GARRLIC high performances software (Lopatin et al., 2013; Dubovik et al., 2014). **This program should be considered as a starting base for the Centre for Aerosol Remote Sensing in close interaction with Data Centre.**

3.2 Estimation of the need

Measurement technique	**Number of instruments/groups[i] to which CARS is providing operational support**		
	Now (preparatory phase, by 2020)	**by 2025**	
		Min.	**Max.**
Aerosol high-power lidar (AHL)	25	30	70
Automatic low-power lidar / ceilometer (ALC)	15	20	25
Automatic sun/sky/polarized/lunar photometer (ASP)	25	30	70

These numbers refer strictly to the instruments operated by the potential ACTRIS NFs, considering the current ACTRIS partnership and the planned facilities, as described in the *ACTRIS Stakeholders Handbook 2017*.

[i] A group may be composed of several operators; it is assumed that one person will be trained for one instrument.

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3.3 Timeline for implementation of the mandatory operation support

Considering the ACTRIS roadmap, CARS should consider the following implementation plan for the mandatory operation support (including general tasks, scheduled and on request operation support, see *Annex: Provision of the operation support)*:

Operation support	Type	Preparation phase < 2020	Implementation phase 2020 - 2025	Operation phase > 2025
SOPs	General task	Basic SOPs for operation of the instruments (minimum requirements)	New SOPs for operation of advanced instruments (optimum setup)	Updates and new SOPs
QA criteria & procedures	General task	Basic procedures for controlling the quality of the measurements (minimum requirements)	New procedures for controlling the quality of the advanced measurements (optimum setup)	Updates and new procedures
	General task	Quality-assurance criteria for basic measurements (minimum requirements)	New quality-assurance criteria for advanced measurements (minimum requirements) (optimum setup)	Updates and new quality-assurance criteria
Instrument-specific calibration	On request	Direct comparison with fixed, state-of-the-art, reference instruments	Continue as support on request	Continue as support on request
	On request	Tests at CARS' laboratories or using remote methods (partially)	Tests at CARS' laboratories or using remote methods (new)	Continue as support on request
	On request		On-site expert inspection of the instruments	Continue as support on request
In-house check-up tools not applicable for ASP	General task		Tools for rapid assessment of critical behaviour of the instrument	Updates
	General task		Software for automatic submission of level 0 data	Updates
Data evaluation procedures and plausibility test not applicable for ASP	General task		Software for rapid assessment of the measurements' quality	Updates
Site performance audits with reference samples or mobile systems	Scheduled	Direct comparison with mobile reference system	Continue as scheduled activity	Continue as scheduled activity

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Operation support	Type	Preparation phase < 2020	Implementation phase 2020 - 2025	Operation phase > 2025
not applicable for ALC and ASP				
Instrument performance workshops not applicable for ASP	Scheduled	Annual assessment of the site performance through expert analysis of specific QA test results	Continue as scheduled activity	Continue as scheduled activity
Documentation and traceability	Scheduled		Codification of the results of the QA tests	Continue as scheduled activity
Training	Scheduled		Regular training sessions (at least twice per year) on pre-defined subjects	Continue as scheduled activity
	On request	Training during parallel activities (direct comparisons, audits, calibration)	Continue as support on request	Continue as support on request
	Scheduled	Documentation available on the CARS website: instrument setup, QC, QA protocols, operation and optimization of the instruments and data management	Continue as needed	Continue as needed
	Scheduled		Forums, webinars	Continue as needed
Consultancy	On request	Upgrading of the instruments, establishment of new observing stations, development of new exploratory platforms	Continue as support on request	Continue as support on request
	On request		Specific observation protocols	Continue as support on request
Testing of new instruments and procedures	On request		Testing of prototypes	Continue as support on request

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3.4 Operation support for quality assurance and quality control

3.4.1 Definition and establishment of standard operation procedures

The Centre for Aerosol Remote Sensing should develop, document, and distribute the SOPs to the corresponding ACTRIS NFs. Also, CARS should organize specific training sessions to help in the implementation of the SOPs. The actual implementation of the SOPs falls in the responsibility of the NFs.

All procedures should be developed and updated based on internal requirements and external user feedback, and should be applicable both to NFs and ACTRIS users.

3.4.1.1 Aerosol high-power lidar (AHL)

The standard operation procedures (SOP) should be designed to ensure the correct operation of high-power aerosol lidars operating at the ACTRIS National Facilities, as well as the defined schedule for the observation of aerosol optical properties in the Planetary Boundary Layer up to the lower stratosphere. The SOPs should cover both instrumental and data correction aspects since the two are interlinked, as follows:

- **Measurement set-up**: ordinary and extraordinary schedule, time resolution, spatial resolution
- **Maintenance**: recommended schedule for window cleaning, replacement of optical components, laser maintenance and replacements, dark measurement retrieval, overlap measurements, alignment check-ups.
- **General instrument operation procedures**: signal intensity and distortions, dark correction, daytime operation, lidar alignment
- **Typical procedures for specific lidar channels and product accuracy**: calibration of the depolarization channels, amplification and signal attenuation for the analogue channels, discrimination level for photon counting channels, correction of range dependency, signal distortions for the analogue channels, alignment of the output beam, assessment of lidar mechanical stability.

The SOPs should be based on the previous developments and lessons learnt during EARLINET, EARLINET-ASOS and ACTRIS technical projects (http://www.earlinet.org). The SOPs should foster:

- The observation of aerosol layers throughout the troposphere up to the lower stratosphere, weather permitting (in the absence of precipitation, fog and low clouds), with a resolution of at least 60 s in time and 100 m in height
- The optimal setting of the instruments to run the Single Calculus Chain (signal attenuation, signal linearity, SNR, minimum timeslot)

3.4.1.2 Automatic low-power lidar / ceilometer (ALC)

SOPs for automatic low-power aerosol lidars should provide information for the optimum operation and data analysis of these instruments, operating at NFs and/or ACTRIS users. They should cover the following aspects:

- **Measurement set-up**: optimum hardware setup (e.g. tilt angle), optimum firmware version and settings, time resolution, spatial resolution, frequency of data delivery, data submission protocols, generation of data in common format
- **Maintenance**: recommended schedule for window cleaning, laser replacements, dark measurements, overlap measurements.

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- **Retrieval and application of correction data**: measurements or statistical retrieval of dark measurements and corresponding correction, measurements or statistical retrieval of overlap correction function and its application, correction of water vapour absorption.

The SOPs should be based on:

- Previous developments and lessons learnt for high-power lidars during previous EARLINET, EARLINET-ASOS, ACTRIS projects, TOPROF and E-profile initiatives
- Statistical analysis of measurements with automatic low-power aerosol lidars in large operational networks
- Intercomparison campaigns (e.g. CeiLinEx2015, Interact) and long-term parallel measurements with a high-power lidar at a testbed site.

The goal of the SOPs is to enable NFs and non-expert operators of ALC networks to provide continuous observations of aerosol profiles throughout the troposphere with best achievable accuracy and known uncertainties.

3.4.1.3 Automatic sun/sky/polarized/lunar photometer (ASP)

The SOPs aim at ensuring nominal use of photometers, and should include:

- Full characterization of instrument (for new instrument)
- Remote monitoring of its status
- Quality Check (QC) during operation in the field
- Quality Assurance (QA).

SOPs should strictly be applied to monitor field and reference instruments QC and for calibration. The SOPs covered by CARS are:

- Level 0 data evaluation to detect failures
- Calibration check (at level 1) to evaluate pre- and post-field calibration to monitor instrument degradation
- Inspection of AOD data
- Cloud contamination check.

Calibration should be done regularly: AOD calibration (sun and moon) and radiometric calibration (sky and polarization), every 12 months (in average), for a field instrument and every 3 months, for the reference instrument. **CARS should also offer continuity service to prevent stop of observation during calibration phase.**

Most SOPs exist and are based on the long experience of worldwide sun/sky/moon photometer network (Smirnov et al., 2000, Holben et al., 2006). These should be updated and new SOPs have to be considered, e.g. adaptation to possible new instrument type in the future, during the implementation phase.

3.4.2 Definition of measurement quality-assurance criteria and procedures

3.4.2.1 Aerosol high-power lidar (AHL)

CARS should develop, document and distribute to the NFs:

- **Specific procedures for quality assurance:** zero-bin, dark measurements, Rayleigh-fit, telecover tests, Δ90-calibration for the depolarization - starting from the already available guidelines from EARLINET-ASOS and ACTRIS technical projects (Freudenthaler 2006-2016, https://www.meteo.physik.uni-muenchen.de/~stlidar/earlinet_asos/EARLINET-ASOS-NA3-QA.html).

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These procedures should be used by the NFs for controlling the quality of their measurements.

- **Quality-assurance criteria** to flag measurements (or parts of the measurements) that are not compliant with the requirements, e.g.: lidar signals with very low SNR, saturated signals, distorted signals, signals with a very limited dynamic range.

  Such criteria should be applied by CARS to: (a) assess the performances of the different instruments based on the QA tests performed and/or coordinated by the CARS (see section 3.4.6.1); (b) contribute to documentation and traceability of level 0 to level 3 data products (see section 3.4.8.1).

- **Mathematical methods to determine and combine the different errors** (starting e.g. from Bravo-Aranda et al, 2016 and Freudenthaler, 2016).
- **Methods for further improving the accuracy of the aerosol lidar measurements** addressing the further error sources affecting aerosol lidar measurements.

  These techniques will be developed and described in such a way that they can be generally applied in a homogenous way for different lidar systems.

3.4.2.2 Automatic low-power lidar / ceilometer (ALC)

CARS should develop, document and distribute to the NFs:

- **Specific procedures for quality assurance:** electronic background profile (dark measurements or statistical analysis of data); overlap correction (telecover tests, horizontal measurements, or statistical analysis of data); monitoring of temporal variability and trends of instrument specific calibration factors.

  Such criteria should be applied by CARS to: (a) assess the performances of the different instruments based on the QA tests performed and/or coordinated by the CARS (see section 3.4.6.2); (b) contribute to documentation and traceability of level 0 to level 3 data products (see section 3.4.8.2).

- **Additional methods for new automatic low-power aerosol lidars types** and new error sources which are not yet known

3.4.2.3 Automatic sun/sky/polarized/lunar photometer (ASP)

CARS should develop, document and distribute to the NFs:

- **Quality criteria and procedures**, as defined and in use for long time by AERONET-EU: instrument design, calibration (Holben et al., 2001; Smirnov et al., 2000, Li et al., 2010, 2013, 2016, 2017; Barreto et al., 2013, 2017), maintenance, training, database and network management and aerosol retrievals (Dubovik et al., 2011, 2014)

3.4.3 Development and provision of instrument-specific calibration

3.4.3.1 Aerosol high-power lidar (AHL)

The calibration of high-power lidars, as in case of all instruments for which a hard reference cannot be defined, consists of a combination of procedures to characterize the different parts, identify and correct for systematic biases, check and preserve the optimal setup and the correction factors. In this sense, the calibration of high-power aerosol lidars is closely linked to the implementation (at the corresponding ACTRIS NFs) of the standard operation and quality assurance procedures previously described.

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CARS should implement and provide to the NFs, **on request**, the following calibration support for AHLs:

- **Direct comparison** with fixed, state-of-the-art, reference instruments for identifying possible issues that may not be visible by following the QA program.
- **Laboratory tests** to assess key parameters used for retrieving major error sources of the instruments
- **On-site expert visits** to test and debug the instrument, including: test-pulse generator, polarisation calibration lamp setup, equipment to determine the state of the laser polarisation, laser wavelength meter.
- **Expert analysis** of the optical design, and of specific test measurements, to assess and reduce instrumental systematic errors: optical misalignments, design flaws, electronic induced errors, electronic synchronization, mechanical instability, aging effects (electronics and optics)

Calibration support should be provided by CARS after each major upgrade of the instrument, and/or at the duly justified request of the NFs.

3.4.3.2 Automatic low-power lidar / ceilometer (ALC)

As in case of high-power lidars, direct calibration of the instrument is closely linked to the implementation of the standard operation and quality assurance procedures previously described.

CARS should implement and provide to the NFs, **on regular basis**, the following calibration support for ALCs:

- **Statistical analysis** of network data **-** continuously, in near-real time (where applicable)

CARS should implement and provide to the NFs, **on request**, the following calibration support for ALCs:

- **Long-term parallel measurements with a reference instrument at a testbed site**, for characterization of effects and sources of uncertainty for characteristic sample instruments, new instrument types, or new firmware versions
- **Laboratory tests**: characterization of laser spectrum for the correction of water vapour absorption; detection of temperature dependencies, inspection of suspicious hardware components

Calibration support on request should be provided by CARS after each replacement of the instrument, and/or at the duly justified request of the NFs.

3.4.3.3 Automatic sun/sky/polarized/lunar photometer (ASP)

CARS should implement and provide to the NFs, **on regular basis**, the following calibration support for ASPs:

- **Direct comparison** with a reference instrument at specific outdoor calibration platforms, for day and night AOD calibration - yearly
- **Laboratory tests**: radiometric calibrations (sky radiance and polarization) - yearly
- **QC/QA monitoring during the operation in the field on a weekly basis**, to detect if instrument needs to be repaired and re-calibrated
- **Continuity Observation Service** during calibration phase using CARS temporary spare instrument or any similar organization to never stop observation.
- **Advanced Calibration Services** should be proposed to improve the calibration in the future (Li et al., 2010, 2013, 2016, 2017; Barreto et al., 2013, 2016, 2017).

More advanced calibration services should be proposed to improve the calibration in the future (Li et al., 2010, 2013, 2016, 2017; Barreto et al., 2013, 2016, 2017).

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3.4.4 Development and provision of in-house check-up tools

3.4.4.1 Aerosol high-power lidar (AHL)

Check-up and preservation of the high-power aerosol lidar calibration is under the responsibility of the NF. In order to facilitate the control of the quality of the measurements performed at the NFs, CARS should develop and distribute in-house check-up tools, as follows:

- **Software tools:**
  - For fast and dynamic assessment of the instrument alignment and signal linearity
  - For calculation of the depolarization correction factor, overlap function, real time data of range corrected signals, real time aerosol layering, etc.
  - For automatic submission of the measurements to the SCC
- **Convertors**
  - From the lidar native format to the QA tests format
  - From the lidar native format to the Single Calculus Chain (SCC) format

Preferably, these should be developed in an open source programming language (e.g. Python) and, if interaction with the operator is required, user-friendly interface should be embedded. If applicable, the tools should be distributed as pre-installed, upgradeable software toolbox in a plug-and-play hardware key.

3.4.4.2 Automatic low-power lidar / ceilometer (ALC)

Monitoring and preservation of instrument performance is in the responsibility of the NFs.

Most of the check-up tools for internal use are software tools, e.g. for monitoring of variability and trends in calibration factors or housekeeping data, calculation and monitoring of overlap functions. Those software tools should be open source and platform independent.

In order to facilitate the control of the quality of the measurements performed at the NFs, CARS should develop and distribute:

- **Recommendations** for commercial check-up tools (hardware provided by instrument manufacturer for dark measurements), or **'Open source' construction plans** for those tools
- **Software tools for monitoring of instrument performance**
- **Recommendations** of amount of house-keeping data

3.4.4.3 Automatic sun/sky/polarized/lunar photometer (ASP)

Not applicable.

Check-up of the ASPs is done centralized by CARS during the annual calibration. In some very rare case, for very remote and not easy to access NF, NF can be asked to perform simple internal check-up.

3.4.5 Development of data evaluation procedures and plausibility test

3.4.5.1 Aerosol high-power lidar (AHL)

High-power aerosol lidar (AHL) raw data acquired at NFs are mandatorily processed at the ACTRIS DC using the Single Calculus Chain (SCC).

For preventing collection of measurements of poor quality, CARS should develop and distribute to the NFs tools for on-site data evaluation procedures and plausibility tests, as follows:

- **Software tools** to continuously monitor: signal-to-noise ratio, maximum amplitude of the signals, beam pointing stability and mechanical stability

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- **Statistical tests** to check the long-term behaviour of electronic distortion (dark signal) and noise levels, to highlight electronic faults.

The data evaluation and plausibility tests are subject of regular updates during the implementation and operation phase. If proven useful, some of the plausibility tests will be transferred to the DC for implementation in the SCC.

3.4.5.2 Automatic low-power lidar / ceilometer (ALC)

For preventing collection of measurements of poor quality, CARS should develop and distribute to the NFs tools for on-site data evaluation procedures and plausibility tests, as follows:

- **Software tools:**
    - for the monitoring of housekeeping data
    - for the long-term analysis of variability and trends in calibration factors and detection range

Those data evaluation and monitoring tools should be provided to the NFs and external user as ‘open source’ platform independent software tools.

3.4.5.3 Automatic sun/sky/polarized/lunar photometer (ASP)

Not applicable.

Instrument performances during in the field operation should be monitored in near real time at CARS. Failures and calibration changes are detected, flagged and NF informed when necessary actions are requested to solve technical problem at instrument level.

3.4.6 Realization of observational site performance audits with reference samples or mobile systems

3.4.6.1 Aerosol high-power lidar (AHL)

CARS should provide (at the time of its full operation) mobile reference lidar systems for direct comparisons:

- **At least two mobile 3+2+3 reference lidar** working at the three elastic (355, 532, and 1064 nm) wavelengths with polarisation sensitivity, and at the two Raman wavelengths (387 and 607 nm) over a detection range from 200 m above ground level to 15 km

In case the technique for a third Raman wavelength evolves in the meantime, it should be included in the mobile instruments.

CARS should maintain, calibrate, and further develop such reference lidar systems as needed according to the advance of the knowledge, techniques, and improved accuracy needs (see Freudenthaler et al., 2016).

3.4.6.2 Automatic low-power lidar / ceilometer (ALC)

Not applicable.

In case of extremely strong accuracy requirements on instruments at specific NFs, those audits could be covered by the experts and reference system for high-power lidars.

3.4.6.3 Automatic sun/sky/polarized/lunar photometer (ASP)

Not applicable.

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Direct comparisons should only be done, each 3-months, between the reference instruments at the different CARS Units.

3.4.7 Organization of regular exercises to assess the performances of the NFs, including instrument performance workshops

3.4.7.1 Aerosol high-power lidar (AHL)

Periodically (at least once per year), CARS should organize exercises to assess the performances of the AHLs operating at the corresponding NFs, as follows:

- **Expert analysis of the quality assurance tests**: zero-bin, dark measurements, Rayleigh-fit, telecover tests, Δ90-calibration for the depolarization (Freudenthaler 2006-2016).

The QA tests performed and/or coordinated by the CARS should be codified and embedded into the SCC for the traceability and full documentation of the data quality.

3.4.7.2 Automatic low-power lidar / ceilometer (ALC)

Periodically (at least once per year), CARS should organize exercises to assess the performances of the ALCs operating at the corresponding NFs, as follows:

- **Expert analysis of the quality assurance tests**: dark measurements, overlap functions, signal artefacts, and variability and trends of calibration factors, or any other not yet known source of uncertainties.

3.4.7.3 Automatic sun/sky/polarized/lunar photometer (ASP)

Not applicable.

ASPs are fully automatic instruments. Their performances are regularly assessed during the annual calibration.

3.4.8 Contribution to documentation and traceability of level 0 to level 3 data products

3.4.8.1 Aerosol high-power lidar (AHL)

CARS should codify in a convenient way the results of the quality assurance program (see sections 3.4.3.1, 3.4.6.1, and 3.4.7.1) and transfer them to the ACTRIS Data Centre. The specific annotation should be agreed with the ACTRIS Data Centre, and should be complete, exhaustive and machine readable.

Additionally, CARS should make available to the ACTRIS Data Centre the full documentation on the standard operation procedures and on the measurement quality-assurance criteria and procedures.

3.4.8.2 Automatic low-power lidar / ceilometer (ALC)

CARS should codify in a convenient way the results of the quality assurance program (see sections 3.4.3.2, 3.4.6.2, and 3.4.7.2) and transfer them to the ACTRIS Data Centre. The specific annotation should be agreed with the ACTRIS Data Centre, and should be complete and exhaustive.

3.4.8.3 Automatic sun/sky/polarized/lunar photometer (ASP)

CARS should codify in a convenient way the results of the quality assurance program (see sections 3.4.3.3, 3.4.6.3, and 3.4.7.3) and transfer them to the ACTRIS Data Centre. The specific annotation should be agreed with the ACTRIS Data Centre, and should be complete and exhaustive.

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3.4.9 Contribution to CEN, ISO, or similar standardization activities

CARS should take the opportunity to send experts as part of the working groups in CEN, ISO or similar standardization activities whenever a related initiative is promoted. Depending on the maturity of the techniques covered by CARS and their potential transfer to the operational activities, CARS should propose to CEN, ISO (or similar) to start the standardization process.

3.5 Operation support for knowledge transfer and training

3.5.1 Training of operators and scientists

Training of operators and scientists at the ACTRIS NFs which fall under CARS guidance may be required for several cases:

- New operators that need to line up to the internal protocols and quality assurance criteria
- New operators that are inexperienced with data collection and data management
- Experienced operators and scientists facing a potential upgrade of their instrument
- Availability of new SOPs, QA procedures and tools, and/or data evaluation procedures and plausibility tests
- New types or firmware versions available for ALC and/or ASP

The training should be organized on various channels:

- Regular training sessions (at least once per year) on pre-defined subjects
- Training during campaigns for direct comparisons (at the NF or at CARS)
- Transfer of expertise during regular exercises to assess the performances of the NFs
- Transfer of expertise during the on-site expert visits to test and debug the instrument
- Documentation available on the CARS website: instrument setup, QC, QA protocols, operation and optimization of the instruments and data management
- Forums
- Regular WebEx sessions as follow-ups of the face-to-face training (quarterly)

In case of the face-to-face training, the number of participants should not exceed 40, with a ratio of trainers / trainees of min. 10%. The sessions may be organized in different CARS Units, depending on the subjects (required expertise and laboratories for hands-on).

CARS should prepare and distribute the training material to the participants, and collect feed-backs. A list of upcoming training sessions should be available on the CARS website and maintained updated.

Training support may be **scheduled** (for pre-defined subjects and needs) and **on request** (for specific needs of some NFs).

3.5.2 Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs

CARS should offer to the NFs, **on request**, consultancy regarding the state of the art of the remote sensing techniques, and/or the possibility to integrate the observations, in case of:

- Upgrading of the instruments
- Specific observation protocols
- Establishment of new observing stations
- Development of new exploratory platforms (laboratories and dedicated mobile instruments and facilities operating on campaign basis and following common standards)

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Consultancy may be provided during training sessions, workshops, meetings, site visits, direct comparison campaigns, or electronically via email or forums.

3.6 Operation support for improvement of measurement methodologies

3.6.1 Testing of new measurement instruments and procedures

CARS should apply all techniques and methods described under 3.4.3 for testing prototypes. CARS should develop further techniques and methods if those are needed for the testing, depending on the capacity of the Centre, available infrastructure and expertise, and costs. Such operation support should be made **on request**. The application should contain sufficient information to allow the Centre to assess the feasibility of providing this support, as well as an estimation of the added value for the scientific community in general and for ACTRIS in particular.

3.6.2 Development of strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime

CARS should develop, when possible, strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime. Such strategies may include:

- Temporary provision of spare parts
- Temporary provision of a spare instrument (mandatory for ASP)
- Negotiation of extended warranty and/or maintenance/service contracts with manufacturers
- Collective purchase of commonly used parts
- Specific operation schedule / protocols, etc.

3.6.3 Development of new technological products and methods

New measurement techniques, technological products and methods may be developed by the Centre in collaboration with the NFs. At the request of NFs, or by its own decision, CARS may investigate new technical solutions, experimental set-up and/or upgrades, new algorithms to retrieve new variables, new experimental configuration, approaches to increase accuracy, or integration of observations from different instruments.

Depending on the situation, the Centre may recommend to the RI Committee to decide on the implementation of such new techniques at the RI level. The Centre has no obligation to develop the full set of operation support for such new techniques, unless they are embraced by ACTRIS and implemented as part of the National Facilities.

3.6.4 Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies

3.6.4.1 Aerosol high-power lidar (AHL)

The Single Calculus Chain (SCC) is the centralized processing tool for AHLs, always improving according to new processing requirements and standards developed in the research community.

In view of the further implementation into the SCC, CARS should aim at:

- **developing optimized algorithms** for: extinction calculation (retrieval using vibrational and rotational Raman channels), cloud screening, smoothing, etc.

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- **developing new algorithms** for: high spectral resolution channels, water vapour mixing ratio, calculation of the intensive optical parameters (e.g. Angstrom parameter, Lidar Ratio, colour ratio), estimation of the aerosol type, calculation of the statistical climatological parameters, etc.
- **developing new techniques and procedures** for determination and, where possible, correction of instrumental uncertainties.

3.6.4.2 Automatic low-power lidar / ceilometer (ALC)

ALCs measurements are generally used for cloud studies, therefore development of new algorithms is generally covered by the cloud remote sensing component of ACTRIS. However, state-of-the-art instruments have a large potential to fill observational gaps in the network of high-power lidars with respect to aerosols.

In view of a potential use of aerosol information provided by the ALCs, CARS should aim at:

- **developing new algorithms** for calculation of: cloud base height, top height of atmospheric boundary layer, automatic detection of volcanic ash layers, etc.

3.6.4.3 Automatic sun/sky/polarized/lunar photometer (ASP)

CARS is in charge with the retrieval of Level 1-to-Level 2 stand-alone retrieval for ASPs. Level 3 data and higher based on GARRLIC/GRASP high performance retrieval software should be obtained at the ACTRIS Data Centre.

In view of future implementation of advanced retrievals, CARS should aim at:

- **developing uncertainty calculation** for Level 1-to-Level 2 data
- **developing updated/adjusted algorithms** for Level 1-to-Level 2 data for new instruments (wavelength, spectral resolution, angular and temporal samplings, etc.).
- **implementing existing algorithm exploiting** synergy of ASP with single ALC or multi-wavelength AHLs
- **developing new algorithms** for Level 3 data and higher, based on GRASP/GARRLIC to exploit new synergy of ASP, ALCs, AHLs with in situ and satellite

4 Services provided to ACTRIS users

The operation support offered by the Centre for Aerosol Remote Sensing should also reply to the need of ACTRIS users in the assessment of the aerosol remote sensing instruments and products. A large number of users is expected by research community which are not part of ACTRIS, both in Europe and worldwide. The services offered to ACTRIS users and in particular to the private sector will be an innovation driver for the aerosol remote sensing community as a whole, with a potential positive feedback for ACTRIS.

The Service and Access Management Unit (SAMU) should be considered as the single point of entry for user access to all CARS services. The access is regulated by both the ACTRIS access policy and the ACTRIS data policy, and will not be detailed in this document.

4.1 Estimation of the need

CARS expects various types of users: individual academic and private users, national and worldwide networks (AERONET, E-PROFILE, GAW, ICOS, UK and Chinese MET-Offices, SONET, EARLINET, MPLNET, LALINET, etc.), private sector (mostly SMEs), etc. Users are mostly located in Europe, South America, Africa and Asia. Most of them are expected to be regular users requesting calibration, maintenance and access to aerosol variables through the processing of field instrument data. Some users, leading other networks,

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can request regularly the calibration of reference instrument, which is particularly relevant to develop traceability at international level.

An estimation of the number of users who could benefit from the services of CARS is presented below.

Type of ACTRIS user	Measurement technique	Number of users to which ACTRIS is providing services		
		Now (in the preparatory phase, by 2020)	by 2025	
			Min.	Max.
Academia	**Total**	92	92	145
	Aerosol high-power lidar	7	7	15
	Automatic low-power lidar / ceilometer	30	30	60
	Automatic sun/sky/lunar photometer	55	55	70
Business & industry	**Total**	10	10	20
	Aerosol high-power lidar	1	1	2
	Automatic low-power lidar / ceilometer	15[2]	15[iv]	27[iv]
	Automatic sun/sky/lunar photometer	2	2	5
Public services	**Total**	31	31	50
	Aerosol high-power lidar	10	10	15
	Automatic low-power lidar / ceilometer	10[3]	10[v]	20[v]
	Automatic sun/sky/lunar photometer	11	11	15

These numbers refer strictly to users (institutional), excluding ACTRIS NFs. The numbers should be revised at a later stage, according to the estimations in *User requirements* document.

4.2 Provision of measurement quality assurance and quality control procedures and tools

All procedures and tools which are provided as operational support to ACTRIS NFs should also be offered to ACTRIS users - as far as the capacities of the Centre allows. It is not foreseen to develop customized tools (other than those developed in support of the ACTRIS NFs) for the ACTRIS users.

4.3 Instrument-specific calibration

All of the calibration methods developed at CARS should be offered as services to ACTRIS users. No custom methods should be developed for the ACTRIS users.

4.4 Knowledge transfer and operator training

Out of the knowledge transfer and training activities foreseen as operational support to NFs, the following should be also offered to ACTRIS users, on request:

- Consultancy for instrument set-up - for new users or users not familiarized with the new instruments
- Training regarding the retrieved aerosol variables - for new users or users not familiarized with the new variables

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[2] Commercial operators of ALC networks (e.g. heli rescue)

[3] National organizations which operate networks of up to 100 ALCs

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- Training for the implementation of SOPs (maintenance, general instrument operation procedures, retrieval and application of correction data) – for new users or users not familiarized with the new SOPs
- Transfer of knowledge regarding new measurement techniques, technological solutions, retrieval algorithms – for all kind of users

The dissemination of knowledge should be organized by CARS for the ACTRIS users through the following channels:

- Publication of related documents (e.g. SOPs, training material) through the ACTRIS portal
- Publication of general achievements (e.g. methodologies) in scientific papers
- Technical and scientific expert and user meetings
- On request access to CARS for specific training

4.5 Improvement of measurement and retrieval methodologies for aerosols, clouds, and reactive trace gases

CARS should actively be in contact with instrument manufacturers in order to assess the applicability of their related products for the scientific purposes of the NFs, discuss latest developments and needs, necessary and possible improvements and standards, and develop solutions for new measurement methods.

Interaction of the Centre with the instrument manufacturers may take place during conferences and exhibits, dedicated workshops and meetings, as well as part of joint projects.

Both for measurement and retrievals, the user must provide sufficient information to assess the feasibility of providing this support, as well as an estimation of the added value for the scientific community in general, and for ACTRIS in particular with respect to the minimum requirements.

5 Governance and management structure of the Centre for Aerosol Remote Sensing

The Units of the Centre for Aerosol Remote Sensing shall be organized according to the specific role of the CF, assuring that the CF complies with the requirements and obligations described in sections 6 and 8 of this document, and considering the general principles described in the *Baseline document for the concept of the Central Facilities*. The Centre for Aerosol Remote Sensing shall be organized such that:

- It has a well-defined structure of Units,
- It has a well-defined decision-making process,
- It is coordinated by a CF Director and managed by a CF Management Board, which consists of the CF Director and the CF Unit Heads,
- It has clear and cost-efficient task sharing between the Units,
- It has a risk management strategy,
- It participates in the ACTRIS decision making by sending representative(s) to the ACTRIS legal entity bodies, e.g. to the RI committee.

6 Requirements for the Centre for Aerosol Remote Sensing

6.1 General requirements

In order to be labelled as the Centre for Aerosol Remote Sensing, the candidate shall:

- Commit for long-term operation, at least 10 years starting with the next year after the implementation as a CF,
- Set-up an appropriate structure of Units, to ensure an adequate functionality of the CF, cost-effective operation, and scalability with respect to the user demands and advancement of the state-of-the art technology,
- Demonstrate the capacity (in terms of material and personnel resources), to ensure the provision of the needed services and operation support, as described in section 6.2
- Provide a feasible implementation and operation plan for the first five years, starting with the next year after the selection as CF,
- Commit to provide a minimum amount of user services, as described in section 4
- Commit to provide the mandatory operation support to the ACTRIS NFs, as described in section 3.

6.2 Technical requirements

6.2.1 Facilities

In view of the operation support and service provision CARS should have / put in place:

	Spaces	Instrumentation	IT infrastructure
AHL	• Indoor laboratories: at least 50 m² air temperature stabilized lidar operation lab with access to sky (roof window) for two lidar systems; at least 30 m² air temperature stabilized optical lab with at least 10 m² clean room cabin ISO 6; at least 20 m² electronic lab; All with water supply, electrical power line filter and electrical grounding. • Outdoor space to simultaneously operate at least 3 lidar systems, power supply and internet connection;	• At least 1 lidar (3 beta + 2 alpha + 3 delta), dynamic range 200 m to 20 km; complemented by ancillary instrumentation (meteorology) • At least 3 mobile lidars (3 beta + 2 alpha + 3 delta), dynamic range 200 m to 15 km • Optical laboratory for characterization of lidar blocks (optics and electronics, lasers)	• Computers • Internet connection • Storage capability for QA annotation in machine readable format • Software (general lidar data analysis software (elastic inversion, Raman inversion, linear and circular depolarisation ratio) adaptable to all possible raw data formats, but especially SCC format. • Teleconference tools
ALC	• Outdoor laboratories with enough capacity (electrical power, space) to simultaneously operate further 5-10 other low power lidars during campaigns and permission to operate the	• Reference lidar(s) which o covers the wavelength range of the low-power lidars, o with depolarization option	• Computer infrastructure for statistical error retrievals o Sufficient internet bandwidth and data storage and

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	reference lidar(s) and test instruments (eye safety issues) and additional (reference and ancillary) instrumentation • Offices (at least for 2 people) • Meeting room for training purposes (at least for 10 people)	o is fully certified as ACTRIS high-power lidar o covers an altitude range between lower ABL and tropopause o operated continuously • Ancillary measurements o Sun/moon photometer which covers the wavelength range of the low-power lidars. o Water vapour profile measurements • At least 1 (better two) of the most commonly used types of low-power lidars	processing capacities.
ASP	• Outdoor laboratories: platforms (4) for transferring sun-calibration and performing functional tests: o one at high-altitude (with easy access) o 2 at medium-altitude o all with clean atmospheric situation and good weather conditions o geographically distributed in N and S Europe • Indoor laboratories (3) for characterization, maintenance and repair, calibration in radiance and polarization and control of sensitivity to temperature • Offices / meeting rooms (at least for 10 people)	• Reference sun/sky/moon photometers to enable calibration transfer, by 3 lines, of about 10 x (robot + data logger) each, to receive field instruments to be calibrated in AOD (absolute error < 0.01) and tested • At least one calibrated integrating spheres for sky radiance calibration (relative error < 3%) • Specific linear polarizing system to calibrate polarization (absolute error < 0.005) • Thermal chambers to measure temperature sensitivity • Solar simulator to adjust solar tracking system • Mobile reference photometer for internal and external radiance traceability between calibration • Spectrometers to control filter transmission	• Dedicated data storage and computing capacities

		• A dedicated set of reference mobile sun/sky/moon photometers to be involved in field campaign or inter-comparison exercises • Sky-imager and lidar as complementary instruments	

6.2.1 Human resources

In view of the operation support and service provision CARS should have / employ:

	Scientific & technical staff			Management & administration staff		
	Scientific expert	**Qualified operator**	**Technician**	**Expert manager**	**Qualified officer**	**Administrative assistant**
AHL	5	3	2	0.75	0.75	
ALC	1	2	0.5	0.25	0.25	
ASP	2	4	2.5	0.75	0.25	

The estimation of the needed human resource has been performed on the basis of the proposed activities and of the ACTRIS-2 and national efforts (reference year =2016). Numbers are expressed in FTE units.

The scientific and technical staff should have the necessary expertise to operate the facilities, instruments and IT infrastructure of CARS at the state of the art, and to develop and provide the operation support and services described above. As a minimum they should have:

- expert scientists: >5 years of experience in related field
- engineer/qualified operator/engineer: >3 years of experience
- technician: > 1 year of experience
- expert manager, qualified officer, and administrative assistance: at least 3 years of experience in the administrative area.

6.2.2 Other requirements

The improvement of the retrieval algorithms for the ASPs, ALCs, AHLs synergies by CARS, requires in addition from other CFs, the following:

- o Easy access to cloud-free QC SCC level 1 data
- o Water vapour profiles as ancillary data to analyse atmospheric situation.
- o Back-trajectories associated to each retrieval

7 Basic criteria for the selection of the Centre for Aerosol Remote Sensing

The applications to host the Centre for Aerosol Remote Sensing are evaluated against a set of criteria covering:

- The **level of commitment** for long-term operation
- The **capacity** to provide the operational support and the services described in sections 3 and 4
    - The availability of the necessary laboratories, instruments, equipment
    - The availability of human resources (no., expertise)
- The **efficiency** in providing the operational support and the services
    - The feasibility of the implementation plan (costs, resources, timeline)
    - The feasibility of the operation plan (methodology, costs per service)
- The **level of maturity**
    - Status of the development of the Units
    - No. of existing users
    - Adequacy of the decision-making
    - Risk management strategy

These criteria will be detailed in the associated call documents.

8 Obligations of the Centre for Aerosol Remote Sensing

8.1 General obligations

The following general obligations shall apply to the Centre for Aerosol Remote Sensing while operational:

- To organize its activities in a cost-efficient way, timely, and with high quality,
- To actively participate in the governance and sustainable development of ACTRIS,
- To provide services to users, according to the access procedures, availability of time, and material resources,
- To provide operation support to the NFs, according to the identified needs, agreed schedules, and procedures,
- To implement efficient user interaction activities by:
    - Organizing workshops, to interact with users,
    - Collecting user feed-backs,
    - Maintaining the CF and ACTRIS websites,
- To document its activities, accesses provided, key performance indicators, and finances, and provide this information to the HO,
- To contribute to minimize and assess the uncertainties related to data and data products, according to their role and in collaboration with each other.

8.2 Technical obligations

8.2.1 Technical obligations in relation with the ACTRIS National Facilities

Technical obligations of the Centre for Aerosol Remote Sensing in relation with the ACTRIS National Facilities refer strictly to the measurement techniques described in this concept document and in *Technical concepts and requirements for ACTRIS Observational Platforms.* The operation of other techniques at the NFs does not imply a technical obligation for the Centre for Aerosol Remote Sensing to provide operation support. New techniques / instrument types are only accepted as ACTRIS instruments

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after the approval of the RI Committee and after the development of the associated QA procedures by the CF.

ACTRIS NFs are responsible for controlling the quality of their measurements by:

a) Applying the SOPs and QA procedures, and using in a proper manner the in-house check-up tools developed by CARS
b) Participating to all scheduled QA activities described in *Annex: Provision of the operation support - Scheduled support*
c) Notifying CARS, and requesting access to specialized services described in *Annex: Provision of the operation support - Operation support on request*, whenever the instrument is not performing well or a major upgrade has been made

CARS, on the other hand, is responsible to provide the mandatory operation support to all corresponding NFs, and maintain a continuous collaboration with the operators and scientists at the NFs, in order to facilitate the control of the measurements quality.

8.2.1.1 Guidelines, quality assurance criteria and procedures

The Centre for Aerosol Remote Sensing is responsible for the quality assurance procedures and guidelines of the ACTRIS measurements conducted at the NFs (high and low power aerosol lidars, sun/sky/lunar photometers). For this, CARS should implement the following operation support for each of the measurement technique under its topics:

- Definition and establishment of standard operation procedures (as described in section 3.4.1)
- Definition of measurement quality-assurance criteria and procedures (as described in section 3.4.2)

All the procedures, guidelines, quality assurance criteria, plausibility tests, etc. should be documented and accessible to all related NFs. Specific training sessions with the related NF operators should be organized to ensure a smooth and correct implementation of the above.

8.2.1.2 Tools, tests and consultancy for quality control of the measurements

It is duty of the Centre for Aerosol Remote Sensing to assist the related NFs in the quality control of their measurements by providing the following operation support for each of the measurement techniques under its topics:

- Development and provision of instrument-specific calibration (as described in section 3.4.3)
- Development and provision of in-house check-up tools (as described in section 3.4.4)
- Development of data evaluation procedures and plausibility test (as described in section 3.4.5)
- Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs (as described in sections 3.5.2)
- Testing of new measurement instruments and procedures (as described in sections 3.6.1)

This operation support should be offered to the related NFs whenever there is a need, or a significant progress in the development of these tools, and accompanied by the appropriate training.

8.2.1.3 Assessment of performances, measurement flagging

The Centre for Aerosol Remote Sensing is mandated to assist the Data Centre and the related NFs in the quality control of the measurements and data, by:

- Realization of observational site performance audits with reference samples or mobile systems (as described in section 3.4.6)

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- Organizing regular exercises to assess the performances of the NFs, including instrument performance workshops (as described in section 3.4.7)
- Contributing to documentation and traceability of level 0 to level 3 data products (as described in section 3.4.8)

The activities involving directly the NFs operating high and low power lidars, sun/sky/lunar photometers should be scheduled by CARS and provided regularly. The corresponding NFs should participate in these activities according to the plan proposed by the Centre for Aerosol Remote Sensing and agreed together with the ACTRIS Scientific Advisory Board (SAB).

8.2.1.4 Transfer of knowledge and training

In addition to the training organized for the implementation of guidelines, procedures, and tools developed in support of the quality control of the measurements, the Centre for Aerosol Remote Sensing should organize training sessions with the NFs operating high and low power lidars, sun/sky/lunar photometers as needed (see sections 3.5.1).

8.2.1.5 Improvement of measurement methodologies for aerosol remote sensing

Although it is not an obligation, the Centre for Aerosol Remote Sensing should work to sustain a high level of performance and to stimulate the advancement of new techniques and methodologies in the aerosol remote sensing field by:

- Development of strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime (as described in sections 3.6.1)
- Development of new technological products and methods (as described in sections 3.6.3)
- Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies (as described in section 3.6.4)
- Organizing regular events (at least once at 2 years) and other forums, in order to exchange knowledge with the NFs and other scientists
- Contributing to CEN, ISO, or similar standardization activities (as described in section 3.4.9)

8.2.2 Technical obligations in relation with the ACTRIS Data Centre

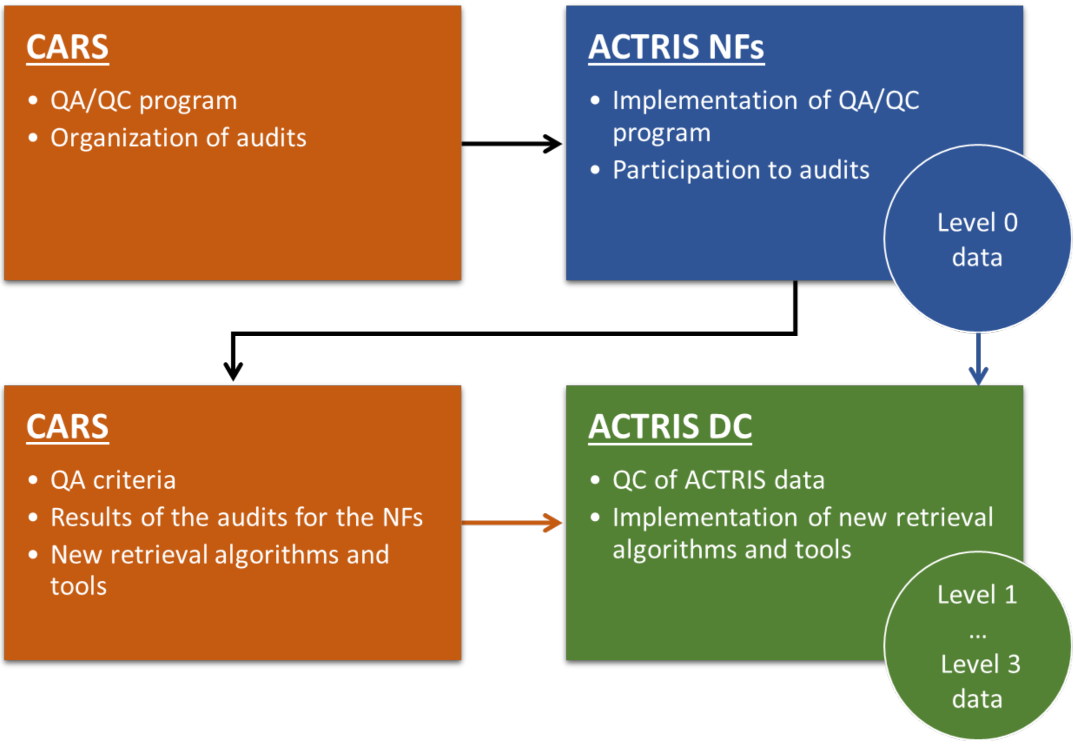
The following general share of responsibilities between the Centre for Aerosol Remote Sensing and the ACTRIS Data Centre applies:

Responsibilities at CARS	Responsibilities at ACTRIS DC
The Centre for Aerosol Remote Sensing is responsible for **developing and facilitating the implementation of the QA/QC procedures and tools at the ACTRIS NFs** operating high- and low-power aerosol lidars and automatic sun/sky/polarized/lunar photometers, in order to allow the respective NFs to keep control on the quality of their measurements (level 0 data)	ACTRIS Data Centre is responsible for the **QC of the ACTRIS data** produced from the respective measurements (level 1 to level 3 data), which are made available through the ACTRIS data portal
The Centre for Aerosol Remote Sensing is responsible for **auditing the ACTRIS NFs** operating high- and low-power aerosol lidars	ACTRIS Data Centre is responsible for the **traceability and full documentation of the data quality** of the ACTRIS data produced by

and automatic sun/sky/polarized/lunar photometers, **documenting the quality of the measurements**, and providing all results to the ACTRIS Data Centre, in order to allow the traceability of the ACTRIS data which are made available through the ACTRIS data portal	high- and low-power aerosol lidars and automatic sun/sky/polarized/lunar photometers, which are made available through the ACTRIS data portal. Results of quality assurance procedures applied by the Centre for Aerosol Remote Sensing will be traced into the data products.
The Centre for Aerosol Remote Sensing is responsible for **developing and testing new retrieval algorithms or tools** for producing level 1 to 3 data, including the exploitation of instrument synergies	ACTRIS Data Centre is responsible for **implementing the approved retrieval algorithms or tools** into the ACTRIS Data Centre operation

The workflow between the ACTRIS NFs, the Centre for Aerosol Remote Sensing and the ACTRIS Data Centre is described in the diagrams below, for each component:

8.2.2.1 Aerosol high-power lidar (AHL)



Note: Processing of the high-power aerosol lidar data is done at the ACTRIS DC. Aerosol remote sensing NFs should transfer level 0 data directly to the DC. CARS should transfer the results of QA procedures in machine readable format to the ACTRIS DC.

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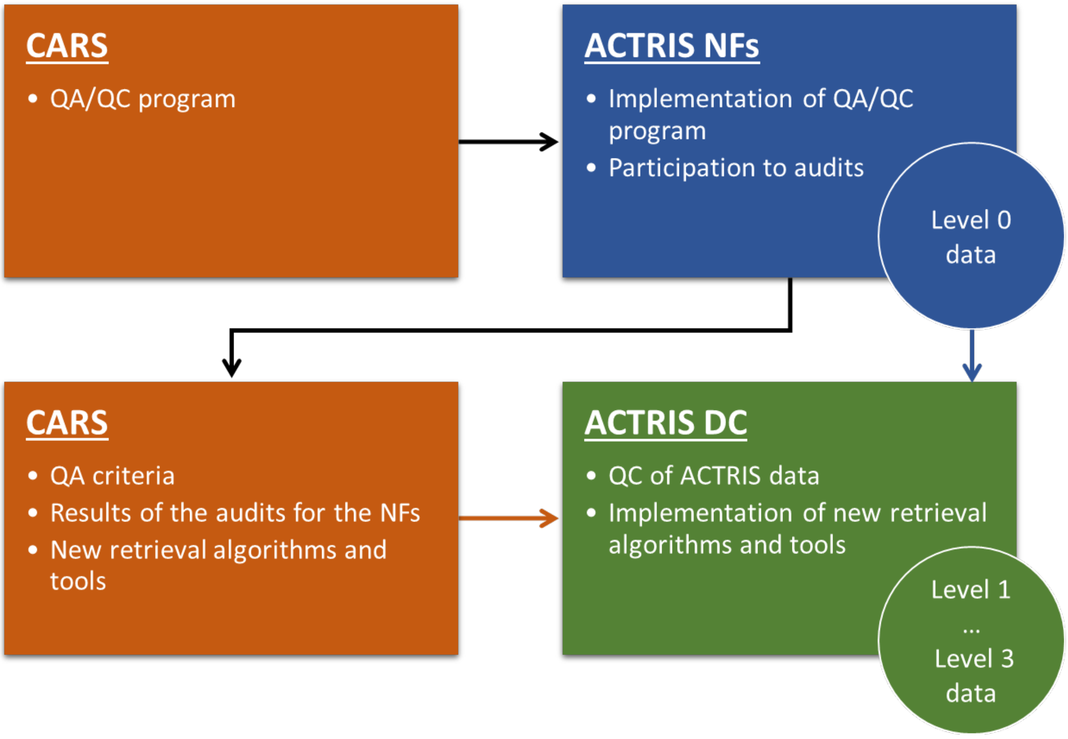
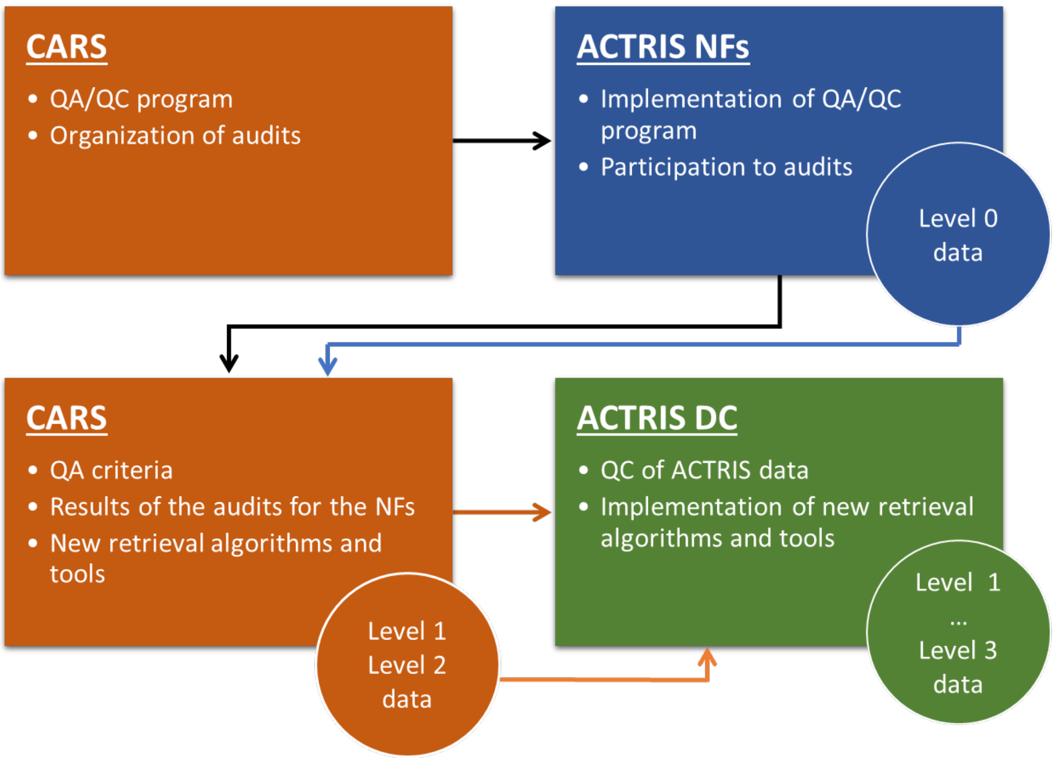


Note: Aerosol data products retrieved from ALCs which are collocated with cloud radars and microwave radiometers will be used as inputs in the processing chain for cloud remote sensing. This data will be passed to the DC for further calculation of the related ACTRIS variables. Aerosol data products retrieved from the automatic low-power lidars which are not accompanied by cloud radar and microwave radiometer will be processed and managed at CARS until a specialized Unit will be put in place at the DC.

8.2.2.2 Automatic sun/sky/polarized/lunar photometer (ASP)



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Note: Level 0 data will be received, stored and archived at CARS. Level 1 and current Level 2 are produced at CARS, and corresponding data flow sent to DC. Higher levels production and products will be performed and stored, and archived at ACTRIS DC both for single instrument processing and synergetic processing and products.

Note: For synergy between photometer and lidar, easy access to cloud-free QC SCC level 1 is requested. Link to, at least, ground-based co-located in situ (ground and in altitude) scattering and absorption coefficients has to be considered too.

8.2.3 Technical obligations in relation with the Centre for Cloud Remote Sensing

There is a close link to the Centre for Cloud Remote Sensing because low-power lidars belong to the minimum required instrumentation of NFs for cloud remote sensing. All quality assurance activities concerning cloud products from ALCs are covered by the TC for cloud remote sensing, but should be strongly supported by CARS. An intensive communication between CARS and the Centre for Cloud Remote Sensing is mandatory to ensure that all recommended SOPs and methods do not reduce the quality of cloud products from automatic low-power lidars at NFs for cloud remote sensing (CLOUDNET sites).

As a feed-back, information from the cloud remote sensing NFs should be used for improving cloud detection in the retrieval algorithm of ASP and AHL (a posteriori).

8.2.4 Technical obligations in relation with the ACTRIS users

The Centre for Aerosol Remote Sensing should commit to provide a minimum amount of user services as described in section 4. The provision of services will be made on case-by case situation.

As an important contribution of the Centre for Aerosols Remote Sensing to worldwide networks like AERONET is foreseen that the service, currently free in ACTRIS-2 will remain free for academic and public users, at least.

8.3 Evaluation of the activity of the Centre for Aerosol Remote Sensing

Once established and operational, the Centre for Aerosol Remote Sensing will be annually evaluated for its performances, against the following KPIs:

Criteria	Indicator	Planned value	Achieved value	Percentage of achievement[4]	Weight
	GENERAL SCORE				
Usefulness for	**CRITERIA TOTAL SCORE**				**40%**
	No. of operation support units provided to ACTRIS NFs for quality assurance and quality control				
	No. of operation support units provided to ACTRIS NFs for knowledge transfer and training				

[4] With regard to the planned and approved values

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	No. of operation support units provided to ACTRIS NFs for Improvement of measurement and data processing methodologies				
	Average score of satisfaction received from NFs *Including utility, fairness and timeliness of the activities for operation support*				
Usefulness for ACTRIS users	**CRITERIA TOTAL SCORE**				**20%**
	No. of service units provided to ACTRIS users for quality assurance and quality control				
	No. of service units provided to ACTRIS users for knowledge transfer and training				
	No. of service units provided to ACTRIS users for improvement of measurement and data processing methodologies				
	Average score of satisfaction received from ACTRIS users *Including utility, fairness and timeliness of the services performed*				
Impact on science &	**CRITERIA TOTAL SCORE**				**20%**
	No. of new technological products, methods and algorithms developed / improved				
	No. of peer-review CF-related papers published				
	No. of CF-related communications at scientific conferences/workshops				
	No. of CF-related patents promoted				
Integration into ACTRIS	**CRITERIA TOTAL SCORE**				**20%**
	No. of participations to ACTRIS committees and boards				
	No. of activities performed in collaboration with other TCs (joint SOPs, joint workshops, etc.)				
	Average score of satisfaction received from ACTRIS DC for the contribution to documentation and traceability of data products				
	Average score of satisfaction received from ACTRIS HO for the quality and readiness of the reports				

List of acronyms

ABL – Aerosol Boundary Layer

AHL – High-power Aerosol Lidar

ALC – Automatic Low-power aerosol Lidar

ASP – Automatic Sun/sky/lunar Photometer

CARS – Centre for Aerosol Remote Sensing

CF – Central Facility

HoI - Handbook of Instruments

NF – National Facility

NRT – Near Real Time

QA – Quality Assurance

QC – Quality Control

SCC – Single Calculus Chain

SOP – Standard Operation Procedure

TC – Topical Centre

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Glossary

ACTRIS data - are the ACTRIS variables resulting from measurements that fully comply with the standard operating procedures (SOP), measurement recommendations, and quality guidelines established within ACTRIS.

- **ACTRIS level 0 data:** Raw sensor output, either mV or physical units. Native resolution, metadata necessary for next level.
- **ACTRIS level 1 data:** Calibrated and quality assured data with minimum level of quality control.
- **ACTRIS level 2 data:** Approved and fully quality controlled ACTRIS data product or geophysical variable.
- **ACTRIS level 3 data:** Elaborated ACTRIS data products derived by post-processing of ACTRIS Level 0 - 1 -2 data, and data from other sources. The data can be gridded or not.
- **ACTRIS syntheses product** (*Proper name to be defined later*)**:** Data product from e.g. research activities**,** not under direct ACTRIS responsibility, but ACTRIS offer repository and access.

ACTRIS Data Centre (DC) - the Central Facility responsible for ACTRIS data curation, preservation, and distribution of data, value-added products and tools**,** and hosting the ACTRIS data portal.

ACTRIS data originator - entity operating instruments at a National Facility or Topical Centre, resulting in ACTRIS data and delivering ACTRIS data to the Data Centre.

ACTRIS data provider - the Data Centre offering the ACTRIS data and value-added data products and tools to users.

ACTRIS digital tools and services - tailored codes and software for processing and visualization of ACTRIS data, production of ACTRIS data products, and for data analysis and research.

ACTRIS exploratory platform - National Facility (simulation chambers, laboratories, or mobile facilities) operating on campaign basis and delivering dedicated data to the Data Centre.

ACTRIS General Assembly (GA) - a council of ministry- and funding organization representatives of ACTRIS members after ACTRIS legal entity has been established, superior decision-making body of ACTRIS.

ACTRIS Head Office (HO) - a Central Facility coordinating and representing ACTRIS, and holding the statutory seat.

ACTRIS label - earmarks a data set or a measurement site as ACTRIS data or ACTRIS National Facility.

ACTRIS observational platform – ACTRIS National Facility performing long-term, regular observations and delivering standardized data to the Data Centre.

ACTRIS Topical Centres (TCs) – a Central Facility offering services and operation support for QA/QC of measurements and data (including training, calibration, QA/QC tools, and development of standard operation and evaluation procedures)

ACTRIS variables - the measured atmospheric variables as described in the ACTRIS Data Management Plan[5].

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[5]The ACTRIS data management plan and list of variables were approved by ACTRIS-2 scientific steering committee, October 2015. These documents are expected to be refined during ACTRIS-PPP (WP5).

Central Facility (CF) - a European level ACTRIS component that offers ACTRIS data or other ACTRIS services to users as well as operation support to ACTRIS National Facilities.

Central Facility Unit – part of a Central Facility located at, and operated by a research performing organization (RPO) or by ACTRIS ERIC.

CF Director – the person responsible for the coordination and representation of a Central Facility.

CF Unit Head – the person responsible for the coordination and representation of a Central Facility unit.

CF Management Board – consists of the CF Unit Heads and the CF Director; this board manages the Central Facility.

Data curation - the activity that stores, manages and ensures access to all persistent data sets produced within the infrastructure.

Data traceability - an unbroken chain of uniquely identified process steps leading from raw data to any kind of processed data, where identification of process steps follows the data.

In situ measurements - measured or sampled air and instrument are at the same location and in physical contact. In the context of ACTRIS, in situ measurements of aerosol, cloud, and reactive-trace-gas properties are performed at observational sites near the Earth surface, on mobile surface-based or airborne platforms, and in atmospheric simulation chambers and laboratories.

Interim ACTRIS Council - a council of ministry- and funding organization representatives of ACTRIS members before ACTRIS legal entity has been established (during the ACTRIS Preparation and Transition Phase), superior decision-making body of ACTRIS.

Measurement traceability - an unbroken chain of comparisons relating an instrument's measurements to a known standard, in the ideal case SI units.

National Facility (NF) - an observational or exploratory platform providing data and/or physical access to the platform within ACTRIS.

Quality assurance and control: Quality assurance is process oriented and focuses on defect prevention; quality control is product oriented and focuses on defect identification:

- o **Quality Assurance (QA):** The process or set of processes used to ensure the quality of a product (e.g. data series, instrument, sample, measured value of a variable, etc.),
- o **Quality Control (QC):** The process and activities of ensuring products and services meet the expectations.

Remote sensing - measured air and instrument are not at the same location and not in physical contact. In the context of ACTRIS, active and passive atmospheric remote-sensing techniques for the observation of aerosols, clouds, and trace gases are applied at observational sites and on mobile surface-based or airborne platforms.

RI committee – consists of up to two representatives from each Central Facility and [three] representatives from the National Facilities Assembly; the RI committee supports the (Interim) Director or Board of Directors in operating the RI.

Service and Access Management Unit (SAMU) - a part of ACTRIS Head Office facilitating the access to ACTRIS services.

User - a person, a team, or an institution making use of ACTRIS data or other ACTRIS services, including access to ACTRIS facilities.

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Reference documents

ACTRIS-ESFRI proposal

ACTRIS-PPP proposal

ACTRIS Stakeholders Handbook 2017

ACTRIS Science Case document

ACTRIS Data Management Plan, approved by ACTRIS-2 SSC 23 October 2015

Baseline document for the Concepts of ACTRIS Central Facilities

Technical concepts and requirements for ACTRIS Observational Platforms

Technical concepts and requirements for ACTRIS Exploratory Platforms

ISO 10012:2003: Measurement management systems — Requirements for measurement processes and measuring equipment

ISO 9000:2015: Quality management systems—Fundamentals and vocabulary

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Annex: Provision of the operation support

Scheduled support

Some of the activities performed by CARS as operation support will be scheduled and, therefore, mandatory for the aerosol remote sensing NFs to participate. The schedule will be announced on the CARS and ACTRIS websites, and communicated with the PIs. A web tool should be developed as part of the CARS website to allow easy and fast registration to the scheduled activities.

Technique	Type of support	Specific support	Frequency	Comments
Aerosol high-power lidar (AHL)	Provision of instrument-specific calibration	Comparison with fixed reference at calibration site	Once each 5 years and after each major upgrade	If the lidar system can be moved to the fixed reference
	Site performance audits with reference samples or mobile systems	Direct comparison with a mobile reference lidar	Once each 5 years and after each major upgrade	If the lidar system cannot be moved to the fixed reference
	Organization of regular exercises to assess the performances of the NFs, including instrument performance workshops	Expert analysis of the quality assurance tests	Once per year	And each time is necessary (instrument low performance)
	Contribution to documentation and traceability of level 0 to level 3 data products	Reports to ACTRIS DC	Once per year	Linked to the expert analysis of the quality assurance tests
	Training of operators and scientists	Regular training sessions on pre-defined subjects (implementation of SOPs, implementation of the in-house check-up tools, implementation of the data evaluation procedures and plausibility tests, etc.)	Twice per year	
		Regular WebEx sessions	Quarterly	

Technique	Type of support	Specific support	Frequency	Comments
Automatic low-power lidar / ceilometer (ALC)	Organization of regular exercises to assess the performances of the NFs, including instrument	Expert analysis of the quality assurance tests	Once per year	And each time is necessary (instrument low performance)

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Technique	Type of support	Specific support	Frequency	Comments
	performance workshops			
	Training of operators and scientists	Regular training sessions on pre-defined subjects	Once per year	

Technique	Type of support	Specific support	Frequency	Comments
Automatic sun/sky/polarized/lunar photometer (ASP)	Provision of instrument-specific calibration	Calibration of reference instrument at high altitude site o Radiance and polarization calibration o Temperature sensitivity o Spare Instrument during calibration phase	Once per year	If instrument upgrade
	Site performance audits with reference samples or mobile systems	Mobile instrument to transfer sky radiance between units	Each 3 months	
	Contribution to documentation and traceability of level 0 to level 2 data products		Once per year	
	Training of operators and scientists	Regular training sessions on pre-defined subjects	Twice per year	

Operation support on request

Aerosol remote sensing NFs may face difficulties in their operation, and CARS should put in place appropriate support. This support should be offered on request. Requests for support should be addressed by the NFs to CARS, through direct communication between the PIs and the CARS Management Board (preferable by email). CARS should put in place a suitable framework for exchanging relevant information and documentation with the PIs, to prepare the operation support. CARS Management Board is responsible to prioritize and decide about the actual support to be offered (timeline, responsible Unit, specific conditions).

Technique	Type of support	Specific support	Comments
Aerosol high-power lidar (AHL)	Provision of instrument-specific calibration	Comparison with fixed reference at calibration site	During campaigns
		Laboratory tests	
		On-site expert visits for debugging	
		Expert analysis of the optical design	
	Development and provision of in-house check-up tools	Software tools for fast and dynamic assessment of the instrument alignment and signal linearity	Embedded into a hardware key or as a stand-alone software (open source)
		Software for conversion of the QA tests into the data format for expert analysis	Embedded into a hardware key or as a stand-alone software (open source)
		Software tools for calculation of the depolarization correction factor, overlap function, etc.	Embedded into a hardware key or as a stand-alone software (open source)
		Software tools for data evaluation and plausibility tests	Embedded into a hardware key or as a stand-alone software (open source)
		Software for real-time conversion of the raw signals to the SCC format, and submission of the measurements to the SCC	Embedded into a hardware key or as a stand-alone software (open source)
	Development of data evaluation procedures and plausibility tests	Not specific at this stage	Depending on the progress of the Single Calculus Chain
	Realization of observational site performance audits with reference samples or mobile systems	Direct comparison with a mobile reference lidar	
	Training of operators and scientists	Not specific at this stage	Depending on the specific needs

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Technique	Type of support	Specific support	Comments
	Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs	Consultancy regarding the instrument technical specifications	
		Consultancy regarding the set-up of the instrument on site	
		Other, not specific at this stage	
	Testing of new measurement instruments and procedures	Not specific at this stage	Depending on the progress of the technology
	Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies	Not specific at this stage	Depending on the progress of the Single Calculus Chain

Technique	Type of support	Specific support	Comments
Automatic low-power lidar / ceilometer (ALC)	Provision of instrument-specific calibration	Direct inter-comparison with a reference instrument.	
	Development and provision of in-house check-up tools	Monitoring of variability and trends in calibration factors and detection range	
		Calculation and monitoring of overlap functions	
		Monitoring of housekeeping data	
	Development of data evaluation procedures and plausibility test	Dark measurements, overlap functions, signal artefacts	
		Variability and trends of calibration factors	
	Training of operators and scientists	Not specific at this stage	Depending on the specific needs
	Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs	Consultancy regarding the instrument technical specifications	
		Consultancy regarding the set-up of the instrument on site	
	Testing of new measurement instruments and procedures	Comparison with reference lidar	
		Comparison with previous hardware or firmware versions	

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Technique	Type of support	Specific support	Comments
		Testing the applicability and adopting of self-test tools	

Technique	Type of support	Specific support	Comments
Automatic sun/sky/polarized/lunar photometer (ASP)	Provision of instrument-specific calibration	AOD, sky radiance and polarisation, temperature calibration Provide spare instrument during calibration	
	Realization of observational site performance audits with reference samples or mobile systems	Direct comparison with a reference system	
	Training of operators and scientists	Organization of training sessions at the TC or remote	
	Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs	Expert visit and discussions	
		Discussion with manufacturers	
	Testing of new measurement instruments and procedures	Direct comparison with a reference system	
		Characterization of parts / / prototypes in the testing laboratory	

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Section 5

Concept of the Centre for Cloud In Situ Measurements (CIS)

ACTRIS PPP WP 4 task 4.1

22.2.2018

Public

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1 Purpose of the document

This document describes the relevance, mission, requirements and obligations of the ACTRIS Centre for Cloud In Situ Measurements.

2 Description and role of the Centre for Cloud In Situ Measurements

2.1 Framework

ACTRIS is the European platform for fostering the use of research data and data analysis tools in the fields of atmospheric aerosols, clouds, and reactive trace gases. ACTRIS Central Facilities (CFs) represent the key operative entities of this Research Infrastructure (RI) and have a fundamental role as they provide operation support to the National Facilities (NFs), i.e. the observational and exploratory platforms, as well as services to the users according to the ACTRIS access policy. CFs are operated at the European level and are part of the governance and decision-making structure of the RI. Each CF may have several operational Units that can be located in the same or different locations, and are operated by research performing organizations (RPOs) or by ACTRIS ERIC.

The Centre for **C**loud **I**n **S**itu Measurements (CIS) is one of the six ACTRIS Topical Centres (TCs) organized around the main scientific themes of ACTRIS: aerosols, clouds, and reactive trace gases, each with a particular focus on either remote sensing or in situ measurement techniques. CIS is serving the need for cloud related weather and climate research and cloud in situ observations, as already reflected in the aerosol-cloud activities of ACTRIS-2 (WP3) and EUROCHAMP-2020 (10 and 11). The need for developing and using standardized instrument operation, data analysis, and calibration procedures is also recognized by the EUROCHAMP-2020 work package 8, which offers transnational access to four calibration facilities, with one focusing on cloud related parameters.

The future ACTRIS focus on cloud processes and cloud observations is also outlined in the description of the technical concepts for the ACTRIS observational platforms and exploratory platforms. It is foreseen that more resources are made available within the ACTRIS RI to achieve a higher coverage and higher level of the services in cooperation with the NFs to provide the highest quality level of the data. In addition, with the introduction of several units, the load of the services will be shared by several institutions in Europe which are well recognized for their high expertise in the measurement of cloud related parameters and quality management.

The cloud formation, properties and impacts depend on aerosol particles acting as cloud condensation nuclei (CCN) and ice nucleating particles (INPs). Clouds also markedly contribute to the removal of aerosol particles from the atmosphere by precipitation and scavenging processes, and they process and modify aerosols by a variety of microphysical and chemical processes. Therefore, clouds are closely linked to aerosol and reactive trace gas processes, and the activities of the Centre for Cloud in situ Measurements will closely be linked to and coordinated with the Centre for Aerosol In Situ Measurements and the Centre for Reactive Trace Gases In Situ Measurements.

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2.2 Scientific relevance

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 on climate, hydrology, air quality, and ecosystems. Clouds directly influence the radiative fluxes through the atmosphere, influence the global circulation systems by latent heat effects, and are the source of precipitation in its various forms and intensities. Currently, there are large uncertainties for the cloud representation in weather and climate models and the understanding of aerosol-cloud microphysical and chemical processes is low. Furthermore, the formation, life cycles and impacts of clouds may change in a changing environment and climate through numerous processes and feedbacks. Therefore, it is of central importance to further explore cloud processes and monitor their properties and impacts over longer time periods. This will be conducted in ACTRIS National Facilities including both laboratory cloud simulation chambers (exploratory platforms) and field observatories (observational platforms).

Cloud observations in ACTRIS and preceding networks have so far focused 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. Aerosol-cloud interactions are also on the scope of previous and ongoing EUROCHAMP projects in order to extend capabilities for the operation of and the access to European atmospheric simulation chambers for exploratory work on important aerosol and cloud related processes.

Cloud in 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 by 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 standardization 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.

2.3 Mission

The key-mission of CIS should be to offer operational support to ACTRIS NFs operating instrumentation for continuous long-term measurements of cloud occurrence, cloud water content, and cloud droplet effective diameter at observational platforms, or for episodic measurements of e.g. droplet and ice crystal size distributions, chemical cloud water composition, and ice nucleating particles during dedicated laboratory and field campaigns. While the main activities should focus on the ACTRIS community, specialized services should be offered to users from academia, business, industry, and public services depending on the respective resources.

The aim of CIS will be to develop and adapt its procedures and performance to future needs continuously responding to new research and development projects, with a focus on the operation of existing

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instruments and methods, and the development and implementation of improved and new methods in cooperation with NFs and other TCs within their capacity and depending on their available resources.

3 Operation support provided to ACTRIS National Facilities

The operation support to NFs which should be provided by the CIS include: a) procedures and tools for quality assurance and quality control of measurements and data, b) transfer of knowledge and training to operators, and c) improvements of measurement methodologies. The operation support should focus on ACTRIS variables and measurement techniques described in this concept document, also listed in the *Technical Concepts and Requirements for ACTRIS Observational and Exploratory Platforms*.

The CIS activities should include

1. establish adequate procedures and methodologies for the measurement of cloud parameters and microphysical processes at NFs;
2. perform quality assurance and quality control of the measurements and data in close cooperation with NFs and the DC;
3. ensure a high performance of NFs by conducting station audits and training sessions;
4. perform regular instrument calibration either at TC units (stationary calibration activities) or onsite by using mobile reference instruments and methods (round robin activities);
5. organise instrument and method intercomparison campaigns at both observational and exploratory platforms;
6. organise regular science, instrument and data analysis workshops;
7. promote technological development and knowledge transfer to NFs and users.

The operation support can be scheduled or on request. Participation at the scheduled activities is mandatory for the NFs. Measurements not following the mandatory actions are not considered as ACTRIS-conform and do not yield ACTRIS data. In addition, NFs may request operation support which is not scheduled, depending on the identified need. Specific operation support offered as scheduled or offered on request is detailed in *Annex: Provision of the operation support.* This annex will be updated routinely as necessary (e.g. following input from development of new testing or calibration methods and tools).

3.1 Measurement techniques covered by the Centre for Cloud In Situ Measurements, and related ACTRIS variables

The ACTRIS variables covered by Cloud In Situ observational and exploratory platforms should include the following variables: (1) cloud occurrence, (2) liquid water content and droplet effective diameter, (3) cloud droplet number concentration and size distribution, (4) ice particle number concentration and size distribution, (5) ice nucleating particle (INP) number concentration and temperature spectra, (6) cloud droplet and ice residuals number concentration and chemical composition, (7) total and interstitial aerosol number concentration and size distribution, and (8) bulk cloud water chemical composition.

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3.1.1 Cloud Occurrence

During cloud formation, CCN activate to cloud droplets, leading to the presence of significant amount of liquid water in a given air volume. The occurrence of clouds can therefore be defined and calculated as a level 3 data product from a threshold value of liquid water content, as e.g. be measured with open path integrating cloud probes like the Particle Volume Monitor (PVM) or the Present Weather Detector (PWD). In addition to that, sites may be equipped with standard fog visibility sensors (e.g.SWS-100 or VPF-710) which may be used for data quality control of cloud microphysical instrument data products. The visibility data can also be used for the provision of level 1 cloud frequency of occurrence data and also precipitation rate and type to a first approximation.

3.1.2 Total Liquid Water Content and droplet effective diameter

A number of instruments are available to measure the Liquid Water Content (LWC), commonly expressed as the amount of liquid water per cubic metre 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-120) 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, that 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 report 3.1.2). Calibration procedures should be performed on site once a month, and instruments should be sent to the calibration centre every few years at least.

The cloud droplet effective diameter is a single variable that gives an indication on the average size of a given cloud droplet population. It is commonly 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, the effective diameter is derived. These two filters guarantee a linear relationship between scattering intensity and LWC or PSA for droplets diameter from 3 to 50 µm (Gerber et al., 1994). Calibration for instrument droplet diameter is the same as that mentioned above for LWC. Recommended standard operating procedures (SOP) for cloud droplet distribution measurements have been supplied in ACTRIS 2 (Deliverable report 3.1.2). Calibration procedures should be performed on site once a month, and instruments should be sent to the calibration centre every few years at least.

3.1.3 Cloud Droplet Number Concentration and Size Distribution

The number size distribution of cloud droplets depends on many factors like the cloud condensation nuclei (CCN) concentration, the CCN chemical composition and the peak water supersaturation. The mean cloud droplet diameters are typically 5-15 µm, the whole size distribution typically spreads from about 1 to 100 µm. Clouds typically contain a few hundred droplets per cubic centimetre, varying from a few tens to a

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few thousands per cubic centimetre. The number size distribution of cloud droplets can be measured optically taking advance of forward scattering of light from liquid droplets. There are several so-called cloud droplet probes available, most of them are designed to be installed into aircrafts (e.g. Lance et al. 2010). Such cloud probes need special inlet arrangements to get droplets through the measurement area when applied for 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 or spinning pinholes.

3.1.4 Ice Particle Number Concentration and Size Distribution

These variables are important for those platforms where mixed-phase or ice clouds occur naturally, or can be investigated in simulation chambers and other laboratory experiments. They are usually measured with cloud-ice probes like the photodiode imaging spectrometers (2DS, 2DS-GS), the cloud/precipitation imaging probes (CIP-15, CIP-15, PIP), the cloud aerosol precipitation spectrometers (CAPS), the high volume precipitation spectrometer (HVPS), the CCD imaging probes (e.g. CPI, µCPI, µCOPP), the 2D spatial scattering imaging probes like the small ice detectors and phase particle discriminators (SID, PPD-2), the holographic Spectrometers (e.g. HaloHolo, Holimo), or the depolarisation particle spectrometers like the cloud aerosol spectrometer with polarisation (CAS-POL) or the 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 1µm 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 some of the above mentioned instruments. Ice cloud parameters include ice crystal number size distribution 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. the total ice particle concentration, the ice water content (IWC), or the ice particle size distribution as accurate mixed-phase and ice cloud products. 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 (Section 3.1.3), 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.

To deliver data assurance, a calibration and chamber simulation database for each instrument should be shared and maintained via a community data portal. This will be used for monitoring instrument performance and to pre-empt any potential instrument failure prior to field operation.

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3.1.5 Ice Nucleating Particle Number Concentration and Temperature Spectra

Ice Nucleating Particles (INPs) can currently only episodically be measured with aerosol sampling based methods and offline 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 CIS has to provide guidance for such new developments and develop calibration protocols and procedures.

3.1.6 Droplet and Ice Residuals Number Concentration and Chemical 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; Twohey 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-of 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 offline physical and chemical analysis, e.g. with electron microscopy (Worringen et al., 2015), or directly be analysed with proper instruments like condensation particle counters 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.

3.1.7 Total and Interstitial Aerosol 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 (D50) and (with assumption or knowledge of the particle hygroscopicity) the maximum supersaturation (Smax) 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 (cloud condensation nuclei, 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. 2002a) at

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different research field stations (Jungfraujoch, Pallas, Puy-de-Dome). 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).

The second component is the aerosol particle size distribution measurement device. In order to derive the D50 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 is frequently intercompared, calibrated and technically standardized (Wiedensohler et al., 2012) and the respective standards and SOPs are defined by the aerosol in-situ TC and will need to be followed. Both inlets and SMPS systems can be operated in an autonomous way, so that their deployment are proposed as a minimum requirement at each future cloud station. Standards and SOPs regarding the inlets and the aerosol instruments connected to them will be developed and supported by the TC for Aerosol In Situ Measurements.

3.1.8 Bulk Cloud Water Chemical Composition

The chemical composition of cloud water is most often determined from bulk cloud water collectors, which 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 harmonise and standardise both the collection and the chemical analysis will be reinforced within the ACTRIS pre-operational phase to define standards and SOPs for the determination of cloud water chemical composition.

3.2 Estimation of the need

In Europe, more than 10 observational sites are currently operating instruments for physical or chemical cloud characterisation on a continuous or episodic way. In addition, 4 ACTRIS exploratory platforms perform cloud experiments and extend their cloud simulation capabilities as part of EUROCHAMP-2020. For INP measurements, about 15 groups in Europe develop and use offline techniques based on aerosol sampling, and more than 10 in situ sampling instruments are used or currently developed for field

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observations. About 5 teams have started to develop or already fly cloud in situ instrumentation on unmanned aerial vehicles (UAVs) for remotely piloted activities around or even inside clouds with both in situ measurements of cloud relevant variables and sampling of aerosols for offline INP analysis. This sector has a high potential for future research and monitoring tasks and the need for operational support, QA/QC issues and technological developments will largely grow during the next years.

With cloud in-situ measurements being a new ACTRIS activity, the number of sites and groups operating in this area is expected to significantly grow over time with continued efforts of CIS and NFs to provide measurement guidelines and operational support. The following table gives an estimates on the number of ACTRIS NFs operating cloud in situ instruments. It is based on number of existing platforms and their activities as well as information about potential ACTRIS activities listed in the first version of the Stakeholder Handbook 2017:

Measurement technique	**Number of ACTRIS National Facilities to which CIS should provide operational support**		
	Now (preparatory phase, by 2020)	**by 2025**	
		Min.	**Max.**
Integrating cloud probes	10	12	15
Cloud droplet probes	10	12	15
Cloud ice probes	5	5	10
Ice nucleating particle instruments	5	10	15
Droplet and ice selective PCVI	3	3	5
Total and interstitial aerosol inlets	10	12	15
Bulk cloud water chemical analysis	5	5	10

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3.3 Timeline for implementation of the mandatory operation support

Considering the ACTRIS roadmap, CIS should consider the following implementation plan for the mandatory operation support (including general tasks, scheduled and on request operation support, see *Annex: Provision of the operation support)*:

Operation support	Type	Preparation phase	Implementation phase	Operation phase
		< 2020	2020 - 2025	> 2025
SOPs	General task	Basic SOPs for operation of the instruments (minimum requirements)	New SOPs for operation of advanced instruments (optimum setup)	Updates and new SOPs
QA criteria & procedures	General task	Basic procedures for controlling the quality of the measurements (minimum requirements)	New procedures for controlling the quality of the advanced measurements (optimum setup)	Updates and new procedures
	General task	Quality-assurance criteria for basic measurements (minimum requirements)	New quality-assurance criteria for advanced measurements (minimum requirements) (optimum setup)	Updates and new quality-assurance criteria
Instrument-specific calibration	On request	Direct comparison with fixed, state-of-the-art reference instruments	Continue as support on request	Continue as support on request
	On request	Tests and direct comparison with mobile reference instruments and methods	Tests at CIS laboratories or using mobile instruments	Continue as support on request
	On request		On-site expert inspection of the instruments	Continue as support on request
In-house check-up tools	General task		Tools for rapid assessment of critical behaviour of the instrument	Updates
	General task		Software for automatic submission of level 0 data	Updates

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Operation support	Type	Preparation phase	Implementation phase	Operation phase
		< 2020	2020 - 2025	> 2025
Data evaluation procedures and plausibility test	General task		Software for rapid assessment of the measurements' quality	Updates
Site performance audits with reference samples or mobile systems	Scheduled	Direct comparison with mobile reference instruments	Continue as scheduled activity	Continue as scheduled activity
Instrument performance workshops	Scheduled	Annual assessment of the site performance through expert analysis of specific QA test results	Continue as scheduled activity	Continue as scheduled activity
Documentation and traceability	Scheduled		Codification of the results of the QA tests	Continue as scheduled activity
Training	Scheduled		Regular training sessions on pre-defined subjects	Continue as scheduled activity
	On request	Training during parallel activities (direct comparisons, audits, calibration)	Continue as support on request	Continue as support on request
	Scheduled	Documentation available on the CIS website: instrument setup, QC, QA protocols, operation and optimization of the instruments and data management	Continue as needed	Continue as needed
	Scheduled		Forums, webinars	Continue as needed
Consultancy	On request	Upgrading of the instruments, establishment of new observing stations, development of new exploratory platforms	Continue as support on request	Continue as support on request
	On request		Specific observation protocols	Continue as support on request

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Operation support	Type	Preparation phase	Implementation phase	Operation phase
		< 2020	2020 - 2025	> 2025
Testing of new instruments and procedures	On request		Testing of prototypes	Continue as support on request

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3.4 Operation support for quality assurance and quality control

3.4.1 Definition and establishment of Measurement Guidelines (MG)

The observation of cloud in situ parameters on a continuous basis is still new to most observational sites. Therefore, it will be one of the first tasks of the respective units of CIS to define respective procedures and protocols and support the observational platforms to implement continuous observations.

So far, cloud in situ activities have mostly been performed on a campaign-like basis. In order to improve and test instruments, and to achieve high international standards of respective research, intercomparison campaigns for cloud probes, INP instruments, and water vapour instruments have been conducted both at field sites and in the laboratory. Such instrument and method oriented campaigns will also be an important activity of CIS and will regularly be organized for instruments that can be shipped to the respective platform and operated together with the other participating instruments. The participation in these activities is mandatory for all instruments operated at ACTRIS observational and exploratory platforms.

The objective should be to compile state-of-the-art measurement guidelines (MG) for each instrument operated either continuously or episodically at cloud in situ platforms. This will be achieved in close collaboration among the NF instruments experts with the CIS as competence centre coordinating the relevant expert knowledge transfer and having a leading role in writing and reviewing state-of-the-art MGs. The MGs should include a description of the measurement techniques and procedures as well as all fields of QA and QC of measurements, calibrations, data evaluation and data delivery. These MGs define how ACTRIS measurements of the corresponding variables should be performed in order to achieve the ACTIRS label. The CIS will decide in consultancy with the ACTRIS assemblies of NFs and the Research Infrastructure Committee about revisions and the development of new MGs.

3.4.2 Definition of measurement quality-assurance criteria and procedures

Measurement quality-assurance criteria and procedures should be included in the corresponding MGs and Standard Operation Procedures (SOPs). The QA processes are assumed to be similar for the different variables and techniques.

Briefly, the QA processes should combine:

- Implementing and following the MGs for measurements, data processing, data delivery and documentation.
- Participating instrument calibration and inter-comparison activities proposed by CIS.
- Using transfer standards for on-site calibration as developed and coordinated by CIS.
- Establishing plausibility plots and evaluations.
- Contributing to data quality workshops and to station performance audits.
- Participating in training activities.

3.4.3 Development and provision of instrument-specific calibration

- Instrument-specific calibration should be achieved by CIS in one of the following ways:
- calibration to laboratory standards and reference instruments in respective units of CIS,
- on site comparison and calibration to travelling reference instruments, and
- round-robin or side-by-side intercomparison activities.

3.4.4 Development of data evaluation procedures and plausibility test

A number of evaluations procedures and plausibility tests have already been developed and tested in activities related to ACTRIS and EUROCHAMP projects. Data evaluation procedures and plausibility tests should be further developed for all of the mentioned measurement techniques hand-in-hand with the measurement quality assurance criteria in order to enable stations to perform mature plausibility checks and develop a good understanding of the quality of the data. This should be an ongoing activity of the CIS.

Common data analysis tools for calibration to laboratory standards, comparison to travelling reference instruments, and the participation in round-robin and side-by-side intercomparisons will be maintained and improved to take into account new knowledge. Training in use of these tools should be provided.

3.4.5 Realization of platform audits

Site performance audits with reference samples (for INP and optical instruments) or mobile systems should be provided by the CIS. A period between station visits of 1 year should be envisioned and should be supplemented by calibration checks, round robin exercises, target-gas checks and intercomparison experiments. New stations and stations encountering problems with data quality and data flow should get more frequent audits upon necessity.

The performance audits check the conformity of a station to the QA requirements as specified in this document and the corresponding MGs. The reference for conformity of a station should evolve as the QA system evolves. During the audit at a station the following parts should be evaluated:

- The sampling and instrument set-up.
- The calibration systems.
- The QA/QC procedures implemented.
- The training and instructions sessions.
- The data delivery.
- The results from intercomparison exercises.
- The uncertainty evaluation.
- The logbooks (instrument, measurements, station).
- The scientific use of the data.
- The overall equipment of the station.

3.4.6 Organization of instrument performance and operator training workshops

Yearly QA/QC workshops checking the plausibility and quality of the NF data should be performed. The objective is the conformity with the DQOs as defined in the MGs. That should include assessments of the year-to-year consistency of the reported data, within network station-to-station consistency, for both observational and exploratory platforms. Instrument performance and training workshops are envisioned on a regular bases aiming at a 2-year period.

3.4.7 Contribution to documentation and traceability of level 0 to level 3 data products

The CIS should define together with the DC the data submission templates for the NFs according to the data flow documents developed between the DC and the CIS. This should include reporting the measurement uncertainty evaluated according the MGs in order assess the quality level of the data and to track any change in data quality. These documents, the MGs, and the data submission procedures

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regulate the appropriate documentation of the data. All the references on the used calibration procedures and materials should be reported as meta-data together with each data submission. In addition, bias and repeatability/reproducibility of targeted cloud in situ measurements and in round robin measurements, as well as results of intercomparisons should be made available in the data base.

3.5 Operation support for knowledge transfer and training

3.5.1 Training of operators and scientists

For improving and maintaining high data quality in the ACTRIS cloud in situ network it is essential to train on a regular basis operators and scientists of the NFs. In training workshops with thematic training courses, the necessary expertise should be shared with the corresponding station staff. The annual concept of the training schedule should be developed together with the NFs. Objectives of the training should cover all aspects of the MGs, QA/QC procedures and data management. Beside the specific training centres, the data QC workshops, the audits, and the side-by-side intercomparisons should be used for training. Besides teaching of technical aspects of the instruments, the training should also provide knowledge about basics of cloud microphysics and sampling issues in clouds, so that the trainees will be able to identify suspicious data features and sampling artefacts.

3.5.2 Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs

The CIS should identify gaps in the measurement network in Europe. Thus, CIS should provide the respective consultancy to the corresponding decision bodies in ACTRIS. Furthermore, the CIS should consult new stations in setting up their monitoring infrastructure and quality management system. Consultancy is provided via the MGs, direct communication, reference station visits, and visits of the new to build stations. Consultancy will be available from the beginning of the implementation phase.

3.6 Operation support for improvement of measurement methodologies

3.6.1 Testing of new measurement instruments and procedures

The CIS should track new developments in measuring and analysing cloud variables and ice nucleating particles and should be involved in testing and developing new instrumentation for assessing the ACTRIS cloud in situ variables. Specifically, the suitability of new instruments for long-term monitoring within ACTRIS and the conformity with DQOs should be tested and characterized. Recommendations of the suitability of new measurement technologies for achieving high data quality in the ACTRSI-RI should be provided. For this activity, specific joint-projects should be envisaged considering further the maturity of the new technologies. During the topical NFs assemblies, initiatives or requirements towards new instrumentation can be discussed and decided. The presently intended new techniques include the continuous and highly time-resolved measurement of INP concentrations as a function of temperature.

3.6.2 Development of strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime

The CIS should contribute to develop optimised methods and procedures in order to reduce breakdown and maintenance times to ensure maximum possible operation time of the continuously operated instruments.

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3.6.3 Development of new technological products and methods

The CIS should be involved in the development of new measurement techniques, technological products and methods by the NFs. Depending on the situation, the CIS may recommend to the ACTRIS RI Committee to decide on the implementation of such new techniques at the RI level. The Centre has no obligation to develop the full set of operation support for such new techniques, unless they are embraced by ACTRIS and implemented as part of the NFs.

3.6.4 Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies

The CIS should contribute to developments of optimised procedures for level 1 and 2 products with automated quality test tools.

4 Services provided to ACTRIS users

An ACTRIS user is a person, a team, or an institution using either ACTRIS data or any other ACTRIS service. ACTRIS users originate from academia, business, industry and public services, from ACTRIS member countries as well as from countries, which are not ACTRIS members, inside and outside Europe. All user employing or developing instruments for measuring the ACTRIS variables in reactive trace gases may benefit from the QA/QC capabilities developed and available for service by the CIS.

Access to some ACTRIS services is open and free, most importantly the access to ACTRIS data, data products, and digital tools provided by the DC, which is the point of entry for free ACTRIS data services. Other access to ACTRIS services is considered competitive, based on the CIS capacity, and will require a review process that is centrally managed by the HO/SAMU. SAMU is the single point of entry for user access to all TC services and to some specific services and data products provided by the DC. Access is regulated by both the ACTRIS access policy and the ACTRIS data policy, respectively.

Within the CIS, service provided to ACTRIS users is only provided in a restricted manner considering the limited resources of the TC, the service fee covered by the user, and the priority to ACTRIS NFs support. The units of CIS will decide about provision of services to users. CIS should agree on these issues with SAMU.

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4.1 Estimation of the need

The CIS is able to schedule some of its potential capabilities for service to ACTRIS users. Table 4-1 summarises the current availability estimates.

Table 4-1: The CIS service estimation for potential ACTRIS users

Type of ACTRIS user	Number of users to which ACTRIS is providing services		
	Now	by 2025	
		Min.	Max.
Academia	80	80	150
Business / Industry	5	5	10
Public Services	0	5	10

4.2 Provision of measurement quality assurance and quality control procedures and tools

The CIS should offer all documents and data-plausibility control procedures to users. Furthermore, depending on resources, CIS should offer participation in round-robin, side-by-side intercomparison and yearly data quality control workshops. In individual cases and on short-term, also calibration of laboratory standards and the provision of calibration or reference materials may be offered to users. However, on long-term, such stations should become part of the ACTRIS RI.

4.3 Instrument-specific calibration

The CIS can offer, depending on resources, calibration of laboratory standards, comparison to travelling reference instruments, and the participation in round-robin and side-by-side intercomparisons which should be used to check the calibration and performance of the instruments including ambient samples under realistic measurement conditions. Besides this, instruments for ice nucleating particles can be calibrated by on-site reference aerosols.

4.4 Knowledge transfer and operator training

As outlined in 3.4.1, also knowledge transfer and training for users can be offered by CIS in restricted extent, mainly depending on resources, with priority for ACTRIS NFs support.

4.5 Improvement of measurement and retrieval methodologies for aerosols, clouds, and reactive trace gases

The CIS can contribute to developments relevant for specific requirements arising from the aerosol-cloud-reactive trace gases interaction, i.e. when processes at the boundaries of respective atmospheric states require the observation of new variables.

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5 Governance and management structure of the Centre for Cloud In Situ Measurements

The CIS shall be organized in different units according to the specific role of each unit in addressing the ACTRIS variables, assuring that CIS complies with the requirements and obligations described in sections 6 and 8 of this document, and considering the general principles described in the *Baseline document for the concept of the Central Facilities*. The Centre for Cloud In Situ Measurements shall be organized such that:

- It has a well-defined structure of Units,
- It has a well-defined decision-making process,
- It is coordinated by a CF Director and managed by a CF Management Board, which consists of the CF Director and the CF Unit Heads,
- It has clear and cost-efficient task sharing between the Units,
- It has a risk management strategy,
- It participates in the ACTRIS decision making by sending representative(s) to the ACTRIS legal entity bodies, e.g. to the RI committee.

6 Requirements for the Centre for Cloud In Situ Measurements

6.1 General requirements

In order to be labelled as the Centre for Cloud In Situ Measurements, the candidate shall:

- Commit for long-term operation, at least 10 years starting with the next year after the implementation as a TC,
- Set-up an appropriate structure of Units, to ensure an adequate functionality of the CF, cost-effective operation, and scalability with respect to the user demands and advancement of the state-of-the-art technology,
- Demonstrate the capacity (in terms of material and personnel resources), to ensure the provision of the needed services and operation support, as described in section 6.2
- Provide a feasible implementation and operation plan for the first five years, starting with the next year after the selection as CF,
- Commit to provide a minimum amount of user services, as described in section 4
- Commit to provide the mandatory operation support to the ACTRIS NFs, as described in section 3.

6.2 Technical requirements

6.2.1 Facilities

The CIS should share the tasks between different units. All units should be established in well recognized institutes with long-term experience in the field of aerosol-cloud exploratory studies or continuous long-term monitoring of aerosol-cloud processes and cloud variables in the atmosphere. The various units should contribute with their specific and complementary competences to achieve a share of the multiple tasks. Sharing the tasks is necessary because no unit itself has all the needed resources. The number of

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units should be reasonably balanced between available resources, competence and capacity, and enhanced coordinative and administrative work.

All units shall be able to provide calibration, QA/QC, and training services as outlined above. Otherwise, the intended services shall be complimentary, with the coordinating unit having capacity and know-how in the majority of services proposed.

The basic facilities required at the different CIS units are

- cloud simulation chambers for the calibration and intercomparison of cloud droplet and ice probes at well controlled cloud formation conditions (all probes sampling from the same cloud parcel),
- sufficient indoor (for exploratory platform) or outdoor (for observational platform) space for mounting a large number instruments during instrument intercomparison activities,
- training facilities with reference measurement systems the unit is in charge of,
- set-ups for travelling reference instruments or reference aerosol systems.
- offices for participants in calibration and intercomparison activities.
- Meeting rooms to host training and knowledge transfer workshops.

With respect to mobile reference instruments and materials, transport in the EU should easily be feasible. The location of different units in different European countries would shorten transport and travel distance to the NFs and to coordinated activities and assemblies.

6.2.2 Human resources

Regarding the operation support and service provision for the cloud in situ measurements techniques as outlined in section 3, the CIS may be structured in 3 to 4 units located at laboratory and observational platforms, which may need the following human resources:

	Scientific & technical staff			**Management & administration staff**		
	Scientific expert	**Qualified operator**	**Technician**	**Expert manager**	**Qualified officer**	**Administrative assistant**
All	1	3	3	0.4	0.4	

The needed human resources were estimated on the basis of the proposed activities. Numbers are expressed in FTE units.

The scientific and technical staff should have the necessary expertise to operate the facilities, instruments and IT infrastructure of CIS, and to develop and provide the operation support and services described above. As a minimum they should have:

- expert scientists: >5 years of experience in related field
- engineer/qualified operator/engineer: >3 years of experience
- technician: > 1 year of experience
- expert manager, qualified officer, and administrative assistance: at least 3 years of experience in the administrative area.

6.2.3 Other requirements

Not applicable

7 Basic criteria for the selection of the Centre for Cloud In Situ Measurements

The applications to host the Centre for Cloud In Situ Measurements are evaluated against a set of criteria covering:

- The **level of commitment** for long-term operation
- The **capacity** to provide the operational support and the services described in sections 3 and 4
  - The availability of the necessary laboratories, instruments, equipment
  - The availability of human resources (no., expertise)
- The **efficiency** in providing the operational support and the services
  - The feasibility of the implementation plan (costs, resources, timeline)
  - The feasibility of the operation plan (methodology, costs per service)
- The **level of maturity**
  - Status of the development of the Units
  - No. of existing users
  - Adequacy of the decision-making
  - Risk management strategy

These criteria will be detailed in the associated call documents.

8 Obligations of the Centre for Cloud In Situ Measurements

8.1 General obligations

The following general obligations shall apply to the Centre for Cloud In Situ Measurements while operational:

- To organize its activities in a cost-efficient way, timely, and with high quality,
- To actively participate in the governance and sustainable development of ACTRIS,
- To provide services to users, according to the access procedures, availability of time, and material resources,
- To provide operation support to the NFs, according to the identified needs, agreed schedules, and procedures,
- To implement efficient user interaction activities by:
- Organizing workshops, to interact with users,
- Collecting user feed-backs,
- Maintaining the CF and ACTRIS websites,
- To document its activities, accesses provided, key performance indicators, and finances, and provide this information to the HO,
- To contribute to minimize and assess the uncertainties related to data and data products, according to their role and in collaboration with each other,
- To remain at the forefront of the technology for Cloud In Situ measurements.

8.2 Technical obligations

8.2.1 Technical obligations in relation with the ACTRIS National Facilities

Technical obligations of the Centre for Cloud In Situ Measurements in relation with the ACTRIS National Facilities refer strictly to the measurement techniques described in this concept document and in *Technical concepts and requirements for ACTRIS Observational Platforms and Exploratory Platforms.* The operation of other techniques at the NFs does not imply a technical obligation for the Centre for Cloud In Situ Measurements to provide operation support. New techniques / instrument types are only accepted as ACTRIS instruments after the approval of the RI Committee and after the development of the associated QA procedures by the CF.

ACTRIS NFs are responsible for controlling the quality of their measurements by:

- Applying the SOPs and QA procedures, and using in a proper manner the in-house check-up tools developed by CIS
- Participating to all scheduled QA activities described in *Annex: Provision of the operation support - Scheduled support*
- Notifying CIS, and requesting access to specialized services described in *Annex: Provision of the operation support - Operation support on request*, whenever the instrument is not performing well or a major upgrade has been made

CIS, on the other hand, is responsible to provide the mandatory operation support to all corresponding NFs, and maintain a continuous collaboration with the operators and scientists at the NFs, in order to facilitate the control of the measurements quality.

8.2.1.1 **Guidelines, quality assurance criteria and procedures**

The Centre for Cloud In Situ Measurements is responsible for the quality assurance procedures and guidelines of the ACTRIS measurements conducted at the NFs with measurement techniques as described in Section 3.1. For this, CIS should implement the following operation support for each of the measurement techniques under its topics:

- Definition and establishment of standard operation procedures;
- Definition of measurement quality-assurance criteria and procedures.

All the procedures, guidelines, quality assurance criteria, plausibility tests, etc. should be documented and accessible to all related NFs. Specific training sessions with the related NF operators should be organized to ensure a smooth and correct implementation of the above.

8.2.1.2 **Tools, tests and consultancy for quality control of the measurements**

It is duty of the Centre for Cloud In Situ Measurements to assist the related NFs in the quality control of their measurements by providing the operation support listed in the previous sections, specifically:

- Development and provision of instrument-specific calibration;
- Development and provision of in-house check-up tools;
- Development of data evaluation procedures and plausibility test;
- Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs;
- Testing of new measurement instruments and procedures.

This operation support should be offered to the related NFs whenever there is a need, or a significant progress in the development of these tools, and accompanied by the appropriate training given that sufficient resources are available at the CIS.

8.2.1.3 **Assessment of performances, measurement flagging**

The Centre for Cloud In Situ Measurements is mandated to assist the Data Centre and the related NFs in the quality control of the measurements and data, by:

- Realization of observational site performance audits with reference samples or mobile systems;
- Organizing regular exercises to assess the performances of the NFs, including instrument performance workshops;
- Contributing to documentation and traceability of level 0 to level 3 data products.

The activities involving directly the NFs operating instruments for measuring cloud variables and INPs covered by the TC should be scheduled by the TC and provided regularly. The corresponding NFs should participate in these activities according to the plan proposed by the Centre for Cloud In Situ Measurements and agreed on with the ACTRIS Scientific Advisory Board (SAB).

8.2.1.4 **Transfer of knowledge and training**

In addition to the training organized for the implementation of guidelines, procedures, and tools developed in support of QA/QC of the measurements and data, the Centre for Cloud In Situ Measurements should organize training sessions with the NFs as needed.

8.2.1.5 **Improvement of measurement methodologies for the Centre for Cloud In Situ Measurements**

Although it is not an obligation, the Centre for Cloud In Situ Measurements should work to sustain a high level of performance and to stimulate the advancement of new techniques and methodologies for measuring cloud variables and INPs in the atmosphere by:

- Development of strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime;
- Development of new technological products and methods;
- Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies;
- Organizing regular events (at least once every 2 years) and other forums, in order to exchange knowledge with the NFs and other scientists;
- Contributing to CEN, ISO, or similar standardization activities.

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8.2.2 Technical obligations in relation with the ACTRIS Data Centre

The following general share of responsibilities between the Centre for Aerosol Remote Sensing and the ACTRIS Data Centre applies:

Responsibilities at CIS	Responsibilities at ACTRIS DC
The Centre for Aerosol Remote Sensing is responsible for **developing and facilitating the implementation of the QA/QC procedures and tools at the ACTRIS NFs** operating cloud in situ instruments, INP instruments and offline chemical analytics, in order to allow the respective NFs to keep control on the quality of their measurements (level 0 data)	ACTRIS Data Centre is responsible for the **QC of the ACTRIS data** produced from the respective measurements (level 1 to level 3 data), which are made available through the ACTRIS data portal
The Centre for Aerosol Remote Sensing is responsible for **auditing the ACTRIS NFs** operating cloud in situ instruments, INP instruments and offline chemical analytics, **documenting the quality of the measurements**, and providing all results to the ACTRIS Data Centre, in order to allow the traceability of the ACTRIS data which are made available through the ACTRIS data portal	ACTRIS Data Centre is responsible for the **traceability and full documentation of the data quality** of the ACTRIS data produced cloud in situ instruments, INP instruments and offline chemical analytics, which are made available through the ACTRIS data portal. Results of quality assurance procedures applied by the Centre for Cloud In Situ Measurements will be traced into the data products.
The Centre for Aerosol Remote Sensing is responsible for **developing and testing new retrieval algorithms or tools** for producing level 1 to 3 data, including the exploitation of instrument synergies	ACTRIS Data Centre is responsible for **implementing the approved retrieval algorithms or tools** into the ACTRIS Data Centre operation

The workflow between the ACTRIS NFs, the Centre for Cloud In Situ Measurements and the ACTRIS Data Centre is as follows:

- CIS develops and provides QA/QC procedures
- ACTRIS NF implements and applies QA/QC procedures and participates in audits
- ACTRIS NF delivers level 0 data to the DC for archiving and to CIS for quality control and approval
- The NF creates level 1 and level 2 data according to procedures implemented and approved by CIS and send these data to the data centre for archiving
- For variables with automatic quality control the DC will process the level 0 data.

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8.2.3 Technical obligations in relation with the Centre for Aerosol In Situ Measurements

Service for inlets as well as instruments operated at ACTRIS NFs will be serviced by the Centre for Aerosol In Situ Measurements. Aerosol instruments needed at CIS units for measuring and controlling aerosols during INP instrument calibrations have to be serviced and calibrated at the Centre for Aerosol In Situ Measurements. An intensive communication between CIS and the Centre for Aerosol In Situ Measurements is mandatory to ensure high quality of the total and interstitial aerosol data measured at observational platforms.

8.2.4 Technical obligations in relation with the ACTRIS users

The Centre for Cloud In Situ Measurements should commit to provide a minimum amount of user services as described in section 4. The provision of services will be made on case-by case situation.

8.3 Evaluation of the activity of Centre for Cloud In Situ Measurements

Once established and operational, the Centre for Cloud In Situ Measurements will be annually evaluated for its performance, against the following Key Performance indicators (KPIs). The KPI and the corresponding scores are listed in Table 8-1.

Table 8-1: Key Performance indicators for the yearly evaluation of the CIS activities

Criteria	Indicator	Planned value	Achieved value	Percentage of achievement[1]	Weight
	GENERAL SCORE				
Usefulness for ACTRIS NFs	**CRITERIA TOTAL SCORE**				**50%**
	No. of operation support units provided to ACTRIS NFs for quality assurance and quality control				
	No. of operation support units provided to ACTRIS NFs for knowledge transfer and training				
	No. of operation support units provided to ACTRIS NFs for Improvement of measurement and data processing methodologies				
	Average score of satisfaction received from NFs *Including utility, fairness and timeliness of the activities for operation support*				
Usefulness for ACTRIS users	**CRITERIA TOTAL SCORE**				**20%**
	No. of service units provided to ACTRIS users for quality assurance and quality control				
	No. of service units provided to ACTRIS users for knowledge transfer and training				
	No. of service units provided to ACTRIS users for improvement of measurement and data processing methodologies				

[1] With regard to the planned and approved values

	Average score of satisfaction received from ACTRIS users *Including utility, fairness and timeliness of the services performed*				
Impact on science & technology	**CRITERIA TOTAL SCORE**				**20%**
	No. of new technological products, methods and algorithms developed / improved				
	No. of peer-review CF-related papers published				
	No. of CF-related communications at scientific conferences/workshops				
	No. of CF-related patents promoted				
Integration into ACTRIS	**CRITERIA TOTAL SCORE**				**10%**
	No. of participations to ACTRIS committees and boards				
	No. of activities performed in collaboration with other TCs (joint SOPs, joint workshops, etc.)				
	Average score of satisfaction received from ACTRIS DC for the contribution to documentation and traceability of data products				
	Average score of satisfaction received from ACTRIS HO for the quality and readiness of the reports				

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Glossary

***In situ* measurements** - measured or sampled air and instrument are at the same location and in physical contact. In the context of ACTRIS, *in situ* measurements of aerosol, cloud, and reactive-trace-gas properties are performed at observational sites near the Earth surface, on mobile surface-based or airborne platforms, and in simulation chambers and laboratories.

Remote sensing - measured air and instrument are not at the same location and not in physical contact. In the context of ACTRIS, passive (radiometer) and active atmospheric remote-sensing techniques[2] (lidar, radar) for the observation of aerosols, clouds, and trace gases are applied at observational sites or on mobile surface-based and airborne platforms.

ACTRIS data - are the ACTRIS variables resulting from measurements that fully comply with the standard operating procedures (SOP), measurement recommendations, and quality guidelines established within ACTRIS.

- **ACTRIS level 0 data:** Raw sensor output, either mV or physical units. Native resolution, metadata necessary for next level.
- **ACTRIS level 1 data:** Calibrated and quality assured data with minimum level of quality control.
- **ACTRIS level 2 data:** Approved and fully quality controlled ACTRIS data product or geophysical variable.
- **ACTRIS level 3 data:** Elaborated ACTRIS data products derived by post-processing of ACTRIS Level 0 - 1 -2 data, and data from other sources. The data can be gridded or not.
- **ACTRIS syntheses product** (*Proper name to be defined later*)**:** Data product from e.g. research activities**,** not under direct ACTRIS responsibility, but ACTRIS offer repository and access.

ACTRIS Data Centre (DC) - the Central Facility responsible for ACTRIS data curation, preservation, and distribution of data, value-added products and tools**,** and hosting the ACTRIS data portal.

ACTRIS data originator - entity operating instruments at a National Facility or Topical Centre, resulting in ACTRIS data and delivering ACTRIS data to the Data Centre.

ACTRIS data provider - the Data Centre offering the ACTRIS data and value-added data products and tools to users.

ACTRIS digital tools and services - tailored codes and software for processing and visualization of ACTRIS data, production of ACTRIS data products, and for data analysis and research.

ACTRIS exploratory platform - National Facility (simulation chambers, laboratories, or mobile facilities) operating on campaign basis and delivering dedicated data to the Data Centre.

ACTRIS General Assembly (GA) - a council of ministry- and funding organization representatives of ACTRIS members after ACTRIS legal entity has been established, superior decision-making body of ACTRIS.

ACTRIS Head Office (HO) - a Central Facility coordinating and representing ACTRIS, and holding the statutory seat.

ACTRIS label - earmarks a data set or a measurement site as ACTRIS data or ACTRIS National Facility.

ACTRIS observational platform – ACTRIS National Facility performing long-term, regular observations and delivering standardized data to the Data Centre.

[2] *In contrast to remote sensing of the Earth's surface (terrestrial and oceanic remote sensing), which is typically done from satellite or aircraft, atmospheric remote sensing is performed from satellite-borne and airborne as well as from surface-based platforms. In ACTRIS, mainly surface-based remote observations are carried out.*

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ACTRIS Topical Centres (TCs) – a Central Facility offering services and operation support for QA/QC of measurements and data (including training, calibration, QA/QC tools, and development of standard operation and evaluation procedures)

ACTRIS variables - the measured atmospheric variables as described in the ACTRIS Data Management Plan[3].

Central Facility (CF) - a European level ACTRIS component that offers ACTRIS data or other ACTRIS services to users as well as operation support to ACTRIS National Facilities.

Central Facility Unit – part of a Central Facility located at, and operated by a research performing organization (RPO) or by ACTRIS ERIC.

CF Director – the person responsible for the coordination and representation of a Central Facility.

CF Unit Head – the person responsible for the coordination and representation of a Central Facility unit.

CF Management Board – consists of the CF Unit Heads and the CF Director; this board manages the Central Facility.

Data curation - the activity that stores, manages and ensures access to all persistent data sets produced within the infrastructure.

Data traceability - an unbroken chain of uniquely identified process steps leading from raw data to any kind of processed data, where identification of process steps follows the data.

Interim ACTRIS Council - a council of ministry- and funding organization representatives of ACTRIS members before ACTRIS legal entity has been established (during the ACTRIS Preparation and Transition Phase), superior decision-making body of ACTRIS.

Measurement traceability - an unbroken chain of comparisons relating an instrument's measurements to a known standard, in the ideal case SI units.

National Facility (NF) - an observational or exploratory platform providing data and/or physical access to the platform within ACTRIS.

Quality assurance and control: Quality assurance is process oriented and focuses on defect prevention; quality control is product oriented and focuses on defect identification:

- **Quality Assurance (QA):** The process or set of processes used to ensure the quality of a product (e.g. data series, instrument, sample, measured value of a variable, etc.),
- **Quality Control (QC):** The process and activities of ensuring products and services meet the expectations.

RI committee – consists of up to two representatives from each Central Facility and [three] representatives from the National Facilities Assembly; the RI committee supports the (Interim) Director or Board of Directors in operating the RI.

Service and Access Management Unit (SAMU) - a part of ACTRIS Head Office facilitating the access to ACTRIS services.

User - a person, a team, or an institution making use of ACTRIS data or other ACTRIS services, including access to ACTRIS facilities.

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[3] The ACTRIS data management plan and list of variables were approved by ACTRIS-2 scientific steering committee, October 2015. These documents are expected to be refined during ACTRIS-PPP (WP5).

Reference documents

ACTRIS (2011-2017): Measurement Guidelines and Standard Operation Procedures available at: http://actris.nilu.no/Content/SOP).

ACTRIS-PPP proposal

ACTRIS Stakeholders Handbook 2017

ACTRIS Science Case document

ACTRIS Data Management Plan, approved by ACTRIS-2 SSC 23 October 2015

Baseline document for the Concepts of ACTRIS Central Facilities

Technical concepts and requirements for ACTRIS Exploratory Platforms

Technical concepts and requirements for ACTRIS Observational Platforms

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Annex: Provision of the operation support

Scheduled support

CIS will arrange so-called scheduled support which will be mandatory for the cloud in situ NFs to participate. The schedule will be announced on the CIS and ACTRIS websites, and communicated with the PIs of CIS measurement techniques operated at the NF. A web tool should be developed as part of the CIS website to allow easy and fast registration to the scheduled activities. This support should be managed by the lead unit of the CIS.

QA/QC activities like round robin or intercomparison experiments which are open to all users, should be announced on the CIS web-page at least 3 months before the event, with number of potential participants and conditions for contribution. Applications should be selected by the CIS units in one of the regular teleconferences of the CIS. Results of these activities should be made openly available on the CIS webpage.

Scheduled support	Measurement technique	Frequency
Direct calibration to fixed (at TC unit) or mobile (provided by TC unit) reference instrument or transfer standards (round robin)	Integrating cloud probes Cloud droplet probes Cloud ice probes INP instruments Cloud water chemical analysis	Every few years (may be instrument specific)
Instrument/method intercomparison campaigns at observational or exploratory platforms	Integrating cloud probes Cloud droplet probes Cloud ice probes INP instruments Cloud water chemical analysis	Every few years (may be instrument specific)
Expert visit and audits to NFs to check QA/QC procedures and measurement guidelines, implement software tools, test design, performance and operation of inlets and sampling systems.	all	Once per year
Training sessions or workshops for operators and scientist	All, both established/standardized and new instruments	Once per year at respective unit
Workshop on scientific aspects, instruments, methods, software, data systems, new developments.	All instruments, software, data systems, new developments, …	Once per year, open to users

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Operation support on request

Cloud in situ NFs may face difficulties in the implementation or operation of instruments, and CIS should put in place appropriate support. This support should be offered on request. Requests for support should be addressed by the NFs to CIS, through direct communication between the PIs and the CIS Management Board. CIS should put in place a suitable framework for exchanging relevant information and documentation with the PIs, to prepare the operation support. CIS Management Board is responsible to prioritize and decide about the actual support to be offered (timeline, responsible unit, and specific conditions).

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Section 6

Concept of the Centre for Cloud Remote Sensing (CCRES)

ACTRIS PPP WP 4 Task 4.1

21.2.2018

Public

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1 Purpose of the document

This document describes the relevance, mission, requirements and obligations of the ACTRIS Centre for Cloud Remote Sensing.

2 Description and role of the Centre for Cloud Remote Sensing

2.1 Framework

ACTRIS is the European platform for fostering the use of research data and data analysis tools in the field of atmospheric aerosols, clouds, and reactive trace gases. ACTRIS CFs represent the key operative entities of this Research Infrastructure (RI) and have a fundamental role as they provide services to the users according to the ACTRIS access policy as well as operation support to the National Facilities (NFs). CFs are operated at the European level and are part of the governance and decision-making structure of the RI. Each CF may have several operational Units that can be located in the same or different locations, and are operated by research performing organizations (RPOs) or by ACTRIS ERIC. The CFs link the NFs, i.e. the observational and exploratory platforms, which are operated at the national level and produce the majority of the ACTRIS measurement data.

The Centre for Cloud Remote Sensing is one of the six ACTRIS Topical Centres organized around the main scientific themes of ACTRIS: aerosols, clouds, and reactive trace gases, each with a particular focus on either remote sensing or in situ measurement techniques.

2.2 Scientific relevance

Cloud processes are important fields of scientific research because of their role in meteorology, climate change at the global scale, and climate variability at the regional scale. Additionally, clouds and cloud-related weather conditions can have significant impact on human activities (e.g. water resources, transport, renewable energies).

Clouds as a major component of meteorology and climate, cannot be studied independently from boundary layer processes, atmospheric dynamics, including radiative, microphysical, thermodynamical, dynamical and turbulent processes. Hence cloud studies require knowledge of essential variables such as cloud geometrical boundaries, cloud water content, cloud droplet effective radius, in-cloud dynamics such as droplet velocity, but also temperature, humidity, wind profiles, and the surface energy budget.

Scientific research questions and societal applications linked to cloud and boundary-layer processes are numerous. Detailed and high-quality observations of cloud properties, atmospheric thermodynamic and dynamic variables are essential for the following applications:

- Studies of cloud microphysical, radiative, dynamic and thermodynamic processes, including cloud-aerosol interactions
- Cal/Val activities to support satellite-based global-scale observations

- Numerical weather prediction, severe weather (model verification, data assimilation, development of new parametrizations)
- Climate and climate change studies and modelling (climate variability studies, model verification)
- Air quality and green-house gas modelling (boundary layer observation and prediction)
- Prediction of weather conditions (fog, clouds, precipitation) that impact human activities (e.g. airport traffic planning, renewable energy production)

Expert knowledge on measurements and observations pertaining to clouds and boundary layer processes are also necessary to

- Improve the quality of operational data provision for applied services (e.g. Copernicus program),
- Support Instrument / Measurement industry (standard procedures, new technology).

Currently, in the ACTRIS framework, deriving the relevant parameters rely on measurements based on Doppler millimetre-band radars, automatic low power lidars, microwave radiometers, and Doppler lidars. Requirements for ACTRIS observational platforms contributing to cloud remote-sensing observations are defined in a specific document. Each required instrument must be carefully calibrated before the relevant cloud parameters can be derived. In a network all instruments should be calibrated in a consistent and traceable manner so that retrieved parameters can be derived on a comparable scale and with a known uncertainty. Common algorithms to be applied to all network measurements are also a must to generate network-wide consistent geophysical parameters.

The European FP5 CloudNet program and following activities in ACTRIS-1 and ACTRIS-2 generated a robust set of algorithms that allow the radar-lidar-radiometer synergy to be exploited to retrieve cloud geometrical and microphysical properties. These programs did not however implement consistent calibration methods for Doppler Cloud Radars, hence their calibration uncertainties are not well quantified.

The EG-CLIMET and TOPROF COST actions were instrumental in developing operation and calibration procedures and recommendations for automatic low power lidars and ceilometers, microwave radiometers and Doppler Lidars.

ACTRIS-RI must provide a framework for operation, calibration and data quality monitoring procedures to be implemented network-wide for all pre-cited instruments.

2.3 Mission

The mission of the Centre for Cloud Remote Sensing (CCRES) is to offer operational support to ACTRIS National Facilities operating Cloud remote sensing instrumentation, namely to Doppler W- or Ka-band Radars for cloud profiling, Microwave Radiometers for temperature and humidity profiling, and Doppler Lidars for wind profiling. The CCRES should also provide support for automatic low power lidars and ceilometers used for cloud profiling purposes.

Additionally, the Centre for Cloud Remote Sensing should offer specialized services for the pre-cited instruments and related ACTRIS variables, to ACTRIS users of various types: academia, business, industry and public services.

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3 Operation support provided to ACTRIS National Facilities

The key services and operation support provided by the Centre for Cloud Remote Sensing should be: a) procedures and tools for quality assurance and quality control of ACTRIS measurements and data, b) transfer of knowledge and training to ACTRIS operators and users, and c) improvements of measurement methodologies for clouds and related variables of interest. This TC should provide (1) remote support to NFs (i.e. support that does not require physical access by NFs), related to procedures and performance evaluation; (2) support based on physical access to ensure network-wide calibration and site evaluations when required; (3) training and opportunities for knowledge sharing. During the implementation phase, 65%, 25%, and 10% of the human resources of the TC should be devoted to remote support, physical access, and training, respectively. During the operational phase, these numbers could evolve to 60%, 30%, and 10%.

The Centre for Cloud Remote Sensing should operate at the state-of-the-art, fostering the implementation of validated new techniques in ACTRIS. To sustain a high level of performance and to stimulate the advancement of new techniques and methodologies, the TC should contribute to expert collaboration networks.

3.1 Instruments covered by the Centre for Cloud Remote Sensing, and related ACTRIS variables

The Centre for Cloud Remote Sensing should deliver a service for Doppler W- or Ka-band Radars for cloud profiling, Microwave Radiometers for temperature/humidity profiling and liquid water path, and Doppler Lidars for wind profiling. The Centre should also provide support for automatic low power lidars and ceilometers used for cloud profiling purposes. These four instruments are necessary to derive vertical profiles of cloud macrophysical and microphysical properties and related atmospheric variables based on several synergetic algorithms.

Critical issues relevant for cloud observations are instrument calibrations, continuous data quality monitoring as well as harmonized data processing. These points must be addressed to derive network-wide consistent atmospheric quantities, such as cloud classification, liquid water content profiles as well as temperature and humidity profiles.

3.1.1 Millimetre-wave Doppler Cloud Radar

A Doppler Cloud Radar (denoted DCR) is an active remote sensing instrument operating in the millimetre wavelength range and providing vertical profiles of reflectivity and Doppler velocity of hydrometeors. The ACTRIS Cloud remote sensing network is composed of different types of DCRs:

- Vertically pointing DCRs at 35 GHz (e.g. MIRA 36 by METEK);
- Scanning DCRs at 35 GHz (e.g. some models of MIRA 35/36 by METEK);
- Vertically pointing DCRs at 94GHz (e.g. 94 GHz BASTA by MODEM; RPG-FMCW-94 by RPG);
- Scanning DCRs at 94GHz (e.g. 94 GHz BASTA-mini by MODEM).

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CCRES should be able to calibrate, provide measurement and data quality assurance procedures for these four types of DCRs. Each DCR type may require particular calibration techniques (e.g. absolute calibration or cross-comparisons, using metallic or natural targets).

3.1.2 Microwave radiometer

Passive microwave radiometers (MWR) are used to measure several atmospheric quantities, such as the cloud liquid water path, column-integrated water vapour, as well as temperature and humidity profiles of the lower troposphere. For the TC, the liquid water path is the most important variable since it can only be measured using this technique with sufficient accuracy.

Most of the MWR within the ACTRIS Cloud remote sensing network are instruments that measure in two frequency bands (Ka-Band, 22-30 GHz) and V-Band (51-58 GHz) and have an elevation scanning capability. This is also considered as optimal setting for deriving all above mentioned parameters.

The minimum requirement within ACTRIS is a vertically pointing two channel radiometer (23/31 GHz) to measure only cloud liquid water path and integrated water vapour.

CCRES should be able to provide standard operation, calibration and quality check procedures as well as quality assurance for the MWRs of the two main manufacturers. It will provide guidelines for minimum requirements for potentially newly developed instruments.

3.1.3 Doppler Wind Lidar

A Doppler wind lidar (DWL) is an active remote sensing instrument that provides profiles of Doppler velocity from atmospheric tracers of the wind such as aerosol particles and cloud droplets.

The DWL operating within the ACTRIS Cloud remote sensing network are long-range (maximum range beyond 2 km) instruments operating at a wavelength of 1.5 um, and have scanning capability enabling the provision of horizontal winds and turbulent properties throughout the full extent of the boundary layer.

CCRES should be able to provide standard operation, calibration and quality check procedures as well as quality assurance for the long-range scanning DWLs from the two main manufacturers. It will provide guidelines for minimum requirements for potentially newly developed instruments.

3.2 Estimation of the need

Instrument	Number of instruments/groups to which the TC is providing operational support		
	Now	by 2025	
		Min.	Max.
Millimetre-wave Doppler Cloud Radar	15	15	30
Microwave Radiometer	15	15	30
Doppler Wind Lidar	8	15	30

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3.3 Timeline for implementation of the mandatory operation support

Considering the ACTRIS roadmap, the CCRES should consider the following implementation plan for the mandatory operation support (including general tasks, scheduled and on request operation support:

Operation support	CONCERNED INSTRUMENTS	TYPE	Preparation phase	Implementation phase	Operation phase
			< 2020	2020 - 2025	> 2025
SOPs (site requirements, instrument deployment, instrument operation).	DCR, MWR, DWL	General task	Basic SOPs, based on experience from past projects	First version of ACTRIS SOP at end of Y1 of implementation phase	Continuous review of SOPs
Instrument-specific calibration	DCR, MWR	Scheduled	Run calibration experiments involving ACTRIS NF DCRs. Develop recommendations for all calibration types, all instruments.	Provision of calibration procedures, guidelines. Development of calibration monitoring software. Calibration intercomparisons. Calibration campaign	Updates and new
Measurement QA criteria & procedures	DCR, MWR, DWL	General task	Basic data flagging (instrument stability) and basic maintenance schedule	Development and implementation of automatic quality checks (analysis of standard housekeeping data). Development of extended data flagging, Definition of extended maintenance schedule	Review of QA/QC methods based on experiences in implementation phase
In-house check-up tools	DCR, MWR, DWL	General task	Recommendation for instrument housekeeping data storage	Development codes to analyze the housekeeping parameters	Updates and new
Data evaluation procedures and plausibility test	DCR, MWR, DWL	General task	Evaluate plausibility ranges for DCR, MWR, DWL measurements	Development of evaluation of DCR, MWR, DWL data by using other observation methods and models	Updates and new
Site performance audits based on remote analysis or mobile systems		Scheduled		Development of questionnaire for site audit, and tools to review log books provided by NFs	Updates and new
NF / instrument performance assessment	DCR	Scheduled	Annual CCRES workshop in the framework of ACTRIS-2	Annual workshop with NFs for discussion of measurement performance, data quality and instrument issues, Performance evaluation for new NFs	
Documentation and traceability		General task		Traceability of data products (level 0 > level 3) by complete documentation of data flow and metadata	
Training	DCR, MWR, DWL	Scheduled	Development of material for future training sessions.	Regular training sessions (at least once per year) on pre-defined subjects, such as calibration, training of new operators, implementation of SOPs and data quality procedures	
	DCR, MWR, DWL	Scheduled		Transfer of expertise during regular exercises to assess the performances of the NFs	
	DCR, MWR, DWL	General task		Documentation available on the CCRES website: instrument setup, QC, QA protocols, operation and optimization of the instruments and data management	
	DCR, MWR, DWL	On-request		Regular webex sessions as follow-ups of the face-to-face training (quarterly)	
Consultancy		On-request		Upgrading of the instruments	
		On-request		Establishment of new observing stations (site selection, specific instrument location)	
Testing of new instruments and procedures		On-request		Testing of prototypes against reference instruments	
Development of strategies to increase duty cycle	DCR	General task		Setup of user forum to detect reasons for instrument downtimes	Continuation
Development of new technological products and methods	DCR, MWR, DWL	General task	Monitoring of new developments	Discussion with manufacturers and operators on optimizing instrument performance	
Development of retrieval algorithms, including the exploitation of instrument synergies	DCR, MWR, DWL	General task	Review of existing algorithms	Review new retrieval algorithm developments (DCR and DCR + auxiliary), make recommendations for implementation by the DC	Updates and new

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3.4 Operation support for quality assurance and quality control

3.4.1 Definition and establishment of standard operation procedures

The Centre for Cloud Remote Sensing should establish and distribute documents that describe operation procedures that users must follow to get an ACTRIS Cloud remote sensing label (minimum and optimal requirement). These Standard Operation Procedures (SOPs) are defined to ensure the correct deployment and the optimal routine measurements at ACTRIS National Facilities (NFs). The same SOPs should be recommended for operation of Cloud remote sensing instruments external to ACTRIS. The SOPs should cover site requirements, instrument deployment protocols to prevent signal contamination from external sources, instrument operation procedures, maintenance, and calibration requirements.

[redacted] Millimetre-wave Doppler Cloud Radar

The following SOPs must be established for DCRs with the objective of reaching consistent operation quality within the DCR network. This should include:

- SOP for site requirements (quality of environment, open view of horizon, wave-length, emission frequency regulations);
- SOP for instrument deployment to prevent signal contamination and to have maximum employment of standard procedures vs non-standard procedures (90/10).
- SOP for instrument operation, to adjust the temporal sampling, and define pointing and scanning or ancillary measurement or type of processing and to have continuous operation 24/7.

Milestones:

- First version of SOP to be provided by end of Year 1 of implementation phase (e.g. end of 2020)

[redacted] Microwave radiometer

The following standard operation procedures must be established for MWR with the objective of reaching consistent operation quality within the MWR network. This should include:

- Site requirements (open view to horizon, preferably in northern direction to perform elevation scans)
- Minimum requirements for observations (temporal resolution of data, noise level of BT observations, stability, available frequencies/channels)
- Firmware requirements
- Calibration and Maintenance requirements (regular inspection, housekeeping data)
- Consistent retrieval algorithms for atmospheric parameters (cloud liquid water path, temperature profiles)
- Data flow implementation (common procedure from instrument to data centre)

The TC should provide guidelines and routines for the NFs and should regularly check the implementation of the guidelines via routine quality checks. The responsibility of implementation is at the level of the NF.

Milestones:

- First version of SOP to be provided by end of Year 1 of implementation phase. These SOP should be further developed in the implementation phase.

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[redacted] Doppler Wind Lidar

The following SOPs must be established for DWLs with the objective of reaching consistent operation quality within the network. This should include:

- SOP for site requirements to determine scanning capability (open view within a cone of specified elevation angle from zenith necessary to obtain a wind profile, and preferably open view to horizon to enable low-elevation scans)
- SOP for scanning sequence selection to ensure that required parameters are obtained with sufficient regularity
- SOP for instrument operation, including temporal sampling, telescope focus calibration, pointing angle determination
- Calibration and firmware requirements (housekeeping data)
- Data flow implementation (common procedure from instrument to data centre)

Milestones:

- First version of SOP to be provided by end of Year 1 of implementation phase (e.g. end of 2020)

3.4.2 Development and provision of instrument-specific calibration

A major objective of the TC is to ensure network-wide accurate calibration of each DCR and MWR installed in ACTRIS NFs following harmonized protocols and tools. Regular calibration of each instrument is necessary to put all measurements on a common absolute scale.

The calibration of each instrument covered by the TC should be based on tested and traceable procedures possibly including multiple techniques: e.g. (1) absolute calibration based on calibrated targets, (2) relative calibration using calibration transfer from a reference instrument, (3) absolute calibration using geophysical targets with known characteristics. The TC should be responsible for the development and delivery of procedures for specific calibration of DCRs and MWRs at each ACTRIS NF. The calibration service could be provided at the TC facility or at NFs, depending on the feasibility. It should offer low-uncertainty reference calibration according to robust calibration techniques. Regular calibration workshops open to NF operators should be organized at the TC.

[redacted] Millimetre-wave Doppler Cloud Radar

At least three types of calibration should be proposed for the DCR:

Cross-check recommendations: (1) autonomous-user calibration procedure based on natural targets (using recommended ancillary measurements);

Low-uncertainty reference calibration: (2) calibration at TC facility based on reference targets; (3) calibration at NF facility using TC reference equipment (calibration kit).

The TC should maintain reference equipment for DCR calibration at the TC facility and also in a mobile setup to implement “low-uncertainty reference calibration”. The TC should support NF operators through training of DCR calibration techniques based on natural targets.

The TC should offer low-uncertainty reference calibration to NFs once every 2 years.

- Develop external calibration procedures with specific experimental set-up for each instrument: sensitivity, accuracy, stability;
- Quantify the stability of the mobile reference DCR after several calibration exercises on NFs.

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Milestones:

- Recommendations for all calibration types (natural and metallic target)
- Calibration monitoring software and guidelines
- Calibration intercomparisons of different methods to quantify uncertainties and variability over time.

Technical requirements (minimal and optimal) for DCR as described in the NF document. TC should establish these requirements.

- One reference cloud radar with the best sensitivity in vertical pointing: to calibrate the cloud radar with a reference with the highest performance.
- One cloud radar in scanning mode: to be able to align on the mast or drone metallic target and validate the cloud radar calibration.
- One calibration mast with well-characterized metallic target: to know the reference value of reflectivity we should have
- One drone with well-characterized metallic target: to know the reference value of reflectivity we should have
- One standard meteorological station (pressure, temperature, humidity, wind, precipitation and horizontal visibility): to characterize the environmental set-up.
- One disdrometer: to characterize the drop size distribution necessary for calibration during rain events.
- Equipment for external monitoring of transmitted radar power and attenuation due to radome wetting by rain.

[redacted] Microwave radiometer

For MWR, guidelines for calibration procedures should be provided by the TC to the NFs. Regular calibration workshops for NF operators should be performed at the TC (see 3.4.1).

- Absolute calibration using liquid nitrogen (LN2) should be performed every 6 months or when spurious data are detected. Details should be provided by the TC. An extended calibration QC compared to the manufacturer’s standard is important, by observing cold-load brightness temperatures before and after the calibration.
- Automatic routine for detector noise levels and cross-correlation
- Relative calibration (hot-load/noise-diode) should be part of the standard operation procedures.
- Automatic documentation of relative calibrations has to be guaranteed (storage of quality flags, data, noise level, etc.), manual documentation of absolute calibration, instrument maintenance (e.g. radome change) and instrument site changes
- Calibration schedule depending on instrument type

Milestones:

- Instrument specific recommendations for all calibration types
- Calibration monitoring software and guidelines
- Calibration intercomparisons of different instrument types and generations should provide more instrument-specific calibration procedures

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[redacted] Doppler Wind lidar

Azimuthal pointing angle calibration necessary to ensure reliable wind retrievals can be achieved by scanning across a hard target of known location in the far field, such as a mast, or through consistency checks via intercomparison of retrieved winds with ground-based anemometers or radiosonde profiles. Both methods also ensure that the instrument is providing reliable radial velocities. For DWL, guidelines for calibration procedures should be provided by the TC to the NFs.

- Azimuthal pointing angle calibration should be performed on a routine basis by including a specific scan once per day or once per hour

Milestones:

- Location specific recommendations for calibration
- Calibration monitoring software and guidelines

3.4.3 Definition of measurement quality-assurance criteria and procedures

Standard procedures for quality assurance and quality check (QA/QC) should be developed and provided to NFs to ensure that instrument operators have the means to monitor measurement quality, can take corrective actions when measurement quality changes, and control the calibration quality. A list of housekeeping data and QA/QC flags should be developed to identify measurements that are not compliant with requirements for Doppler Cloud Radars, Microwave Radiometers, and Doppler Wind Lidars. Criteria and procedures should be made available at the end of the ACTRIS-PPP.

The TC should provide QA/QC guidelines to the NFs and should regularly check the implementation of the guidelines via routine quality checks (see 3.3.4). The responsibility of implementation is at the level of the NF.

[redacted] Millimetre-wave Doppler Cloud Radar

The following QA/QC procedures are necessary for DCR operation:

- Instrument stability monitoring on transmitter and receiver side
- Detailed instrument monitoring and documentation (housekeeping data)
- Check of hardware components (radome, amplifier, antenna);
- Flagging for data quality (near-range)
- External hardware to measure transmitted power outside the instrument, hence including water on the radome.
- Analysis of log data (housekeeping) provided by the firmware

Milestones:

- Data flagging method and support to analyse the QC.
- Maintenance schedule

[redacted] Microwave radiometer

The following QA/QC procedures are necessary for MWR operation:

- Detailed instrument monitoring and documentation (housekeeping data)
- Calibration quality control (e.g. clear-sky radiosondes)
- Regular check of hardware components, cleaning of radome, radome coating

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- Camera inspection
- Flagging for data quality by spectral consistency checks: If one or more channels of the MWR are faulty, this check can detect inconsistencies (caused e.g. by external radio frequency interference, rain, wet radome or failed calibration) by comparing to typical atmospheric spectra.

Milestones:

- Implementation of housekeeping data visualization
- Data flagging procedure, spectral consistency check implementation
- Maintenance schedule

[redacted] Doppler Wind Lidar

The following QA/QC procedures are necessary for DWL operation:

- Detailed instrument monitoring and documentation (housekeeping data), especially background monitoring
- Azimuthal pointing angle calibration
- Telescope focus correction

Milestones:

- Implementation of housekeeping data visualization
- Implementation of routine pointing angle calibration

3.4.4 Development and provision of in-house check-up tools

Instrument housekeeping data and calibration data should be collected by NFs for each cloud remote sensing instrument. Instruments should produce housekeeping data automatically. Instruments should produce calibration data when operated in calibration mode (specific mode to be defined). Continuous analysis of this data should allow instrument operators to check the quality of their measurements. To perform this analysis, the TC should provide software tools and visualization tools to check the instrument performance and possible calibration trends. This should include In-house check-up tools that operators at NF can execute to analyze the housekeeping parameters automatically stored by the instrument in order to monitor the instrument performance and stability. The TC should develop such in-house check-up tools in an open-source programming language (i.e. Python).

3.4.5 Development of data evaluation procedures and plausibility test

Doppler cloud radar and microwave radiometer data should be sent by NFs to the ACTRIS Cloud Remote Sensing Data Centre. The DC should then be responsible for processing data to produce retrievals of relevant Cloud geophysical properties. Data evaluation, based on various tests should then be implemented to qualify the retrieved data. Methods to test retrieved data should be established by the TC (e.g. evaluating plausible range, internal consistency, multi-instrument intercomparisons,…) and data evaluation procedures should be developed by the TC and provided to the DC for implementation. This software should be developed as open-access software.

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[redacted] Millimetre-wave Doppler Cloud Radar

Data evaluation and plausibility check is a critical issue for DCRs.

- Should come up with plausible range of Reflectivity values based on statistics, and also some constraints based on MWR LWP and Cloud geometrical depth, and possibly Doppler velocity.
- Horizontal wind speed derived with scanning cloud radar can be compared with radiosonde measurement.

Milestones:

- Implementation of reflectivity consistency checks
- Implementation of liquid water closure
- Implementation of data flagging procedure

[redacted] Microwave radiometer

Data evaluation and plausibility check is a critical issue for MWR. These checks should be performed directly after measurement at the NF/DC, to detect inconsistencies and other problems.

- Comparison of retrieved atmospheric parameters to other observations (e.g. IWV of GPS)
- Comparison of observed brightness temperatures to products or forward-modelled brightness temperatures of NWP models to detect systematic biases (O-B)

Milestones:

- Implementation of comparison to other observations and/or models
- Implementation of data flagging procedure

[redacted] Doppler wind lidar

Data evaluation and plausibility checks are necessary for DWLs.

- Horizontal wind speeds derived from scanning can be compared with ground/mast-based anemometers or radiosonde.
- Turbulent parameters can be compared at the surface with sonic-anemometers
- Comparison of retrieved atmospheric parameters to other observations (e.g. aerosol or low-power lidars)

Milestones:

- Implementation of comparison to other observations and/or models
- Implementation of data flagging procedure

3.4.6 Realization of observational site performance audits with reference samples or mobile systems

The TC should realize observational site performance audits. To limit the human resources required for such audits, the audit method should be based on a questionnaire that should be filled by NFs. The questionnaire should include important aspects such as instrument installation, operation, quality control, preventive maintenance, calibration, and data availability. Semi-automatic review procedures should be developed to review log books and metadata about instrument stability monitoring, calibration, measurement quality, data quality control.

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[redacted] Millimetre-wave Doppler Cloud Radar

A mobile reference DCR should be available and used to evaluate measurements at NF sites that reveal data quality problems that cannot be solved by other methods.

[redacted] Microwave radiometer

The site audit with reference systems should not be preferred method for MWRs since the calibration of any system has to be performed after each transport. A mobile MWR unit could only determine the repeatability of absolute calibrations of a MWR at the NF.

A reference system could consist of a mobile radiosounding system for direct clear-sky comparisons to the MWR system, if no operational radiosonde station is situated close to the MWR location. However, this cannot be done for all MWR in a network on a regular basis.

The standard method should be to have remote access to the instrument/host PC in case of problems with providing QC data, as site visits cannot be standard procedure.

3.4.7 Organization of regular exercises to assess the performances of the NFs, including instrument performance workshops

Once per year, the TC should organize a workshop that gathers all NF operators to discuss measurement performance, data quality issues, instrument issues. This workshop should allow for new methods to be presented (by the TC and NFs) that aim at improving the overall quality of the cloud remote sensing data. This workshop should be organized at the TC or at NFs, providing opportunities to visit observation sites.

3.4.8 Contribution to documentation and traceability of level 0 to level 3 data products

The TC should contribute to the documentation and the traceability of all the data product levels based on quality assurance, calibration and quality control steps (see section 3.3.2, 3.3.3 and 3.3.5). Discussion should be conducted with the ACTRIS Data Centre to codify this traceability for raw data (level 0), pre-processed data (level 1), fully controlled atmospheric products (level 2), and their climatological aggregations (level 3). This traceability is necessary for all the procedures starting from the instrument deployment to the QA/QC analysis. Homogeneous and complete documentation of the metadata file is essential to develop data flags with the ACTRIS DC.

3.4.9 Contribution to CEN, ISO, or similar standardization activities

The standardization process should not be a significant TC activity even if some work could be done to normalize processes that can be useful for commercial use. Some recommendations could be made to manufacturers to have a standard for atmospheric measurement techniques, concerning the Doppler cloud radar and microwave radiometer.

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3.5 Operation support for knowledge transfer and training

3.5.1 Training of operators and scientists

Training of operators and scientists should be organized to fulfil different requirements: calibration procedures or techniques, training of new operators, support to implement standard operation procedures, data quality control procedures. These training events should have a limited number of participants and could be organized at the different TC units depending on the topics. Workshops on instrument calibration should include background and hands-on training, and hence each training session should have a limited number of participants. Scientists at NFs should get more insight into QA/QC procedures and learn how to detect problems and other issues of their instruments. An online forum for exchange between the NF operators and scientists could also cover this topic.

The TC should propose one additional workshop per year for a wider audience that will focus on new or improved procedures concerning measurement and calibration techniques, data processing algorithms. Space should be provided to share operator and scientist experience and needs related to specific activities.

3.5.2 Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs

The TC should propose consultancy on Doppler cloud radars and microwave radiometers to the NFs that would like to have new observational or exploratory platforms, and new instruments. Based on its experience, the TC should provide consultancy during visits, discussions, workshops and supports to the manufacturers. The TC should propose support to NFs that plan to install new DCRs and MWRs to ensure that new instruments are deployed following current state-of-the-art procedures. This support should be proposed at the end of the preparatory phase (2019).

For Doppler cloud radars and microwave radiometers, similar consultancy should be proposed with:

- A service for instrument location definition and site selection support;
- A draft of technical requirements and standard operational support;
- A methodology to analyze instrument performance and selection.

3.6 Operation support for improvement of measurement methodologies

3.6.1 Testing of new measurement instruments and procedures

The TC should provide space and infrastructure to test new instruments. Performance, accuracy, stability and calibration procedures can be assessed by comparing them to established and well-characterized instruments. This service should be proposed to NFs and ACTRIS users. All the techniques, procedures and supports are presented in section 3.3.3. These supports to test new instruments and procedures should be proposed at the end of the preparatory phase (2019).

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3.6.2 Development of strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime

The TC should develop strategies to increase the duty cycle of instruments operated at the NFs, and to reduce breakdown and maintenance downtime. A forum for NF operators (as already described in 3.4.1) can help identify solutions to upcoming problems. The experience of many NFs should help to provide a clearer view on instrument performance and deficiencies and might also allow the development of improved components together with the manufacturers. A list of components most likely to breakdown or wear out should be compiled and provided to users.

3.6.3 Development of new technological products and methods

New technological products and methods should be developed and proposed for Doppler cloud radars and microwave radiometers deployed by ACTRIS NFs and external users. Different aspects should be foreseen such as new experimental set-up, new instruments, and new algorithms. Discussion with manufacturers and operators on optimizing instrument performance should be conducted.

3.6.4 Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies

The TC should take an active role in the development and evaluation of retrieval algorithms and tools for producing level 1 to 3 data, including the exploitation of instrument synergies. It should promote community development of open-source retrieval algorithms. The TC should:

- have retrieval algorithm development expertise,
- help coordinate the scientific community involved in retrieval algorithm development,
- assess what algorithms should be implemented by the cloud remote sensing DC,
- propose a retrieval generation framework

For a harmonized and consistent data set across the different NFs, a central development of retrieval algorithms for atmospheric quantities is necessary. This is however a further step after implementing standard operation, quality check, and calibration procedures.

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3.7 Provision of the operation support

3.7.1 Scheduled support

This TC should provide (1) remote support to NFs, related to procedures and performance evaluation; (2) support based on physical access to ensure network-wide calibration and site evaluations when required; (3) training and opportunities for knowledge sharing. Support requiring physical access and support for training and sharing of knowledge will be proposed as scheduled support advertised on the ACTRIS website and through direct communication with NF operators. Support concerning operation and quality control procedures should be released on a regular basis as updated documents and tools become available.

Instrument	Type of support	Specific support	Frequency	Comments
DCR and MWR	Provision of instrument-specific calibration	DCR: comparison with reference DCR or using reference targets.	DCR: Once every 1 or 2 years MWR: Once every 6 months	And after each major upgrade
	Site performance audits with reference samples or mobile systems*	Performance audit based on analysis of recorded data. Performance audit based on site visit.	Once per year based on data. One site visit per NF.	Additional visit if replacement of instrument.
	Organization of regular exercises to assess the performances of the NFs, including instrument performance workshops*		Once per year	
DCR, MWR, DWL	Training of operators and scientists*		Once per year	Co-located with instrument performance workshops

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3.7.2 Operation support on request

This TC should provide additional support on request for site performance audits in case of major changes at the NF, consultancy for setting up new observation platforms and testing new instruments.

Instrument	Type of support	Specific support	Comments
DCR and MWR	Direct comparison with fixed or mobile reference systems		Requires physical access support at CCRES or NF
DCR, MWR, DWL	Evaluation of new instruments and firmware		Based on physical access support or remote support
	Evaluation of new algorithms		Based on remote support
	Specific training		Requires physical access support at CCRES or NF

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4 Services provided to ACTRIS users

An ACTRIS user is a person, a team, or an institution using either ACTRIS data or any other ACTRIS service. ACTRIS users originate from academia, business, industry and public services, from ACTRIS member countries as well as from countries, which are not ACTRIS members, inside and outside Europe.

ACTRIS Cloud remote sensing users are operators of DCRs, MWRs or DWLs from academia (e.g. research institutes and universities operating observational sites), public services such as operational agencies (e.g. meteorological services, air quality agencies,..), businesses (e.g. airports,…), and industry (e.g. instrument manufacturers), that are NOT operating an ACTRIS observational platform (NF).

The CCRES should provide (1) remote service to ACTRIS users, related to procedures and performance evaluation and (2) training and opportunities for knowledge sharing. It is unlikely that the capacity of the CCRES would be sufficient to provide physical access service to ACTRIS users.

A possible business model could be that the CCRES trains instrument manufacturers to provide physical access services to ACTRIS users following procedures established by the CCRES.

Access to some ACTRIS services is open and free, most importantly the access to ACTRIS data, data products, and digital tools provided by the DC, which is the point of entry for free ACTRIS data services. Other access to ACTRIS services is considered competitive access based on capacity or excellence and will require a review process that is centrally managed by the HO/SAMU. SAMU is the single point of entry for user access to all TC services and to some specific services and data products provided by the DC. Access is regulated by both the ACTRIS access policy and the ACTRIS data policy, respectively.

4.1 Estimation of the need

An estimation of the number of users who could benefit from the services of CCRES is presented below.

Type of ACTRIS user	Number of users to which ACTRIS is providing services		
	Now	by 2025	
		Min.	Max.
Academia: DCR MWR DWL	2	5	10
	2	5	10
	2	5	10
Business: DCR MWR DWL	0	5	15
	0	5	15
	0	5	15
Industry: DCR MWR DWL	3	3	5
	3	3	5
	3	3	5
Public services: DCR MWR DWL	2	5	10
	2	5	10
	2	5	10

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4.2 Provision of measurement quality assurance and quality control procedures and tools

The CCRES should provide procedures and tools (open source software) for QA/QC of MWR and DCR data to ACTRIS users. The procedures and tools should be the same as the ones developed for ACTRIS NFs. Recommendations for deployment specifications, calibration techniques and algorithm assumption. However, no regular quality assessment by the TC can be guaranteed.

4.3 Instrument-specific calibration

Some methods, techniques and instruments should be offered by the CCRES to the ACTRIS users. One training event should be provided to the ACTRIS users to show and explain how a calibration can be performed at their sites depending on which system should be calibrated (scanning radar and zenith-fixed radar for example). A first set of these requirements should be available at the end of the implementation phase (2019)

Established calibration procedures and standards should be provided to users. No regular quality assessment by the TC can be guaranteed.

4.4 Knowledge transfer and operator training

The TC should focus its support to the NFs but some support should be offer on request to ACTRIS users. Priority should be given to NF operators and ACTRIS users could also benefit from the following support:

- DCR and MWR calibration training at the TC but also at sites;
- DCR and MWR standard operation procedures;
- Retrieval algorithm workshop to derive cloud microphysical properties;
- Consultancy for new observational and exploratory platform or instruments;

4.5 Improvement of measurement and retrieval methodologies for aerosols, clouds, and reactive trace gases

One goal of the TC is to improve the measurement and retrieval methodologies for clouds. To reach this objective, direct and intensive discussions with the DCR and MWR manufacturers should be established. Some parts of training events, workshops and meetings can be dedicated to these fruitful discussions, in order to improve and develop new techniques and methods to optimize measurement, calibration and hence the associated retrievals.

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5 Governance and management structure of the Centre for Cloud Remote Sensing

The Units of the Centre for the Cloud Remote Sensing shall be organized according to the specific role of the CF, assuring that the CF complies with the requirements and obligations described in sections 6 and 7 of this document, and considering the general principles described in the *Baseline document for the concept of the Central Facilities*. The Centre for Cloud Remote Sensing shall be organized such that:

- It has a well-defined structure of Units,
- It has a well-defined decision-making process,
- It is coordinated by a CF Director and managed by a CF Management Board, which consists of the CF Director and the CF Unit Heads,
- It has clear and cost-efficient task sharing between the Units,
- It has a risk management strategy,
- It participates in the ACTRIS decision making by sending representative(s) to the ACTRIS legal entity bodies, e.g. to the RI committee.

6 Requirements for the Centre for Cloud Remote Sensing

6.1 General requirements

In order to be labelled as Centre for Cloud Remote Sensing, the candidate shall:

- Commit for long-term operation, at least 10 years starting with the next year after the implementation as a CF,
- Set-up an appropriate structure of Units, to ensure an adequate functionality of the CF, cost-effective operation, and scalability with respect to the user demands and advancement of the state-of-the art technology,
- Demonstrate the capacity (in terms of material and personnel resources), to ensure the provision of the needed services and operation support, as described in section 6.2
- Provide a feasible implementation and operation plan for the first five years, starting with the next year after the selection as CF,
- Commit to provide a minimum amount of user services, as described in section 4
- Commit to provide the mandatory operation support to the ACTRIS NFs, as described in section 3.

6.2 Technical requirements

6.2.1 Facilities

The TC should have capacity to host and organize workshops for groups ranging 10-50 participants. The TC should include one or more facilities that have the capacity to host users and their equipment for field tests.

[redacted] Millimetre-wave Doppler Cloud Radar

For DCR calibration, the TC should include and have the capacity to operate the following equipment:

- One or more cloud radars with scanning capability that will be maintained at a TC facility and serve as reference cloud radar.
- One calibration mast and well-characterized metallic targets that will serve as reference to calibrate cloud radars with scanning capability.
- One drone able to carry a reference target that will serve as reference to calibrate cloud radars without scanning capability
- A set of well-characterized metal targets to be used for absolute calibration
- One or more standard meteorological stations (pressure, temperature, humidity, wind, precipitation and horizontal visibility): to characterize the environmental set-up.
- One or more disdrometers: to characterize the drop size distribution necessary for calibration during rain events.
- A mobile well-characterized Doppler cloud radar with scanning capability that will serve as reference instrument for calibration transfer to DCRs at NFs.

[redacted] Microwave Radiometer

For MWR calibration, the TC should include and have the capacity to operate the following equipment:

- One or more MWR with scanning capability that will be maintained at a TC facility and serve as reference instrument.
- Sufficient standard calibration equipment for operator workshops (supply liquid nitrogen, latest version of cold calibration targets)
- One or more standard meteorological station (pressure, temperature, humidity, wind, precipitation and horizontal visibility): to characterize the environmental set-up.
- A state-of-the-art radiosonde station to assess calibration accuracy by independent clear sky radiosonde comparison

6.2.2 Human resources

The TC staff should include expert scientists, qualified operators and technicians with several years of experience in operating DCRs, MWRs and DWLs. Ideally the staff should have experience in instrument development, instrument calibration, data processing, development of retrieval algorithms. The TC staff should also include management and administrative staff to support the organization of the TC and logistical aspects (hosting, transport,…). Experience in provision of support and service to a wide range of users is also important.

The TC should operate with about 10 full-time equivalent positions distributed in 3-4 units.

7 Selection of the Centre for Cloud Remote Sensing site(s)

The site(s) hosting the Centre for Cloud Remote Sensing are selected based on a set of criteria covering:

- The **level of commitment** for long-term operation
- The **capacity** to provide the operational support and the services described in sections 3 and 4
    - o The availability of the necessary laboratories, instruments, equipment
    - o The availability of human resources (no., expertise)
- The **efficiency** in providing the operational support and the services
    - o The feasibility of the implementation plan (costs, resources, timeline)
    - o The feasibility of the operation plan (methodology, costs per service)
- The **level of maturity**
    - o Status of the development of the Units
    - o No. of existing users
    - o Adequacy of the decision-making
    - o Risk management strategy

8 Obligations of the Centre for Cloud Remote Sensing

8.1 General obligations

The following general obligations shall apply to the Centre for Cloud Remote Sensing while operational:

- To organize its activities in a cost-efficient way, timely, and with high quality,
- To actively participate in the governance and sustainable development of ACTRIS,
- To provide services to users, according to the access procedures, availability of time, and material resources,
- To provide operation support to the NFs, according to the identified needs, agreed schedules, and procedures,
- To implement efficient user interaction activities by:
- Organizing workshops, to interact with users,
- Collecting user feed-back,
- Maintaining the CF and ACTRIS websites,
- To document its activities, accesses provided, key performance indicators, and finances, and provide this information to the HO,
- To contribute to minimize and assess the uncertainties related to data and data products, according to their role and in collaboration with each other.

8.2 Technical obligations

8.2.1 Technical obligations in relation with the ACTRIS National Facilities

[redacted] Guidelines, quality assurance criteria and procedures

The Centre for Cloud Remote Sensing is responsible for the quality assurance procedures and guidelines of the ACTRIS measurements conducted at the NFs operating Millimetre-band Doppler Cloud Radars, Microwave Radiometers and Doppler Wind Lidars. For this, the TC should implement the following operation support for each of the instrument types under its topics:

- Definition and establishment of standard operation procedures (as described in sections 3.3.1)
- Definition of measurement quality-assurance criteria and procedures (as described in sections 3.3.3)

All the procedures, guidelines, quality assurance criteria, plausibility tests, etc. should be documented and accessible to all related NFs. Specific training sessions with the related NF operators should be organized to ensure a smooth and correct implementation of the above.

[redacted] Tools, tests and consultancy for quality control of the measurements

It is duty of the Centre for Cloud Remote Sensing to assist the related NFs in the quality control of their measurements by providing the following operation support for each of the instrument types under its topics:

- Development and provision of instrument-specific calibration (as described in sections 3.3.2)
- Development and provision of in-house check-up tools (as described in sections 3.3.4)
- Development of data evaluation procedures and plausibility test (as described in sections 3.3.5)
- Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs (as described in sections 3.4.2)
- Testing of new measurement instruments and procedures (as described in sections 3.5.1)

This operation support should be offered to the related NFs whenever there is a need, or a significant progress in the development of these tools, and accompanied by the appropriate training.

[redacted] Assessment of performances, measurement flagging

The Centre for Cloud Remote Sensing is mandated to assist the Data Centre and the related NFs in the quality control of the measurements and data, by:

- Realization of observational site performance audits based on semi-automatic review procedures and possibly based on the deployment of mobile reference instruments at NFs (as described in sections 3.3.6)
- Organizing regular exercises to assess the performances of the NFs, including instrument performance workshops (as described in sections 3.3.7)
- Contributing to documentation and traceability of level 0 to level 3 data products (as described in sections 3.3.8)

The activities involving directly the NFs operating Cloud Remote Sensing instruments covered by the TC (e.g. Doppler Cloud Radars and Microwave radiometers) should be scheduled by the TC and provided regularly. The corresponding NFs should participate in these activities according to the plan proposed by the Centre for Cloud Remote Sensing and agreed together with the ACTRIS Scientific Advisory Board (SAB).

[redacted] Transfer of knowledge and training

In addition to the training organized for the implementation of guidelines, procedures, and tools developed in support of the quality control of the measurements, the Centre for Cloud Remote Sensing should organize training sessions with the NFs operating Cloud Remote Sensing instruments as needed (see sections 3.4.1).

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[redacted] Improvement of measurement methodologies for cloud remote sensing

Although it is not an obligation, the Centre for Cloud Remote Sensing should work to sustain a high level of performance and to stimulate the advancement of new techniques and methodologies in the cloud remote sensing field by:

- Development of strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime (as described in section 3.5.2)
- Tests of new technological products and methods (as described in section 3.5.3)
- Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies (as described in section 3.5.4)

8.2.2 Technical obligations in relation with the ACTRIS Data Centre

Regarding ACTRIS data produced by DCRs, MWRs and DWLs, the following general share of responsibilities between the CCRES and the ACTRIS Data Centre applies:

Responsibilities of CCRES	Responsibilities of ACTRIS DC
The CCRES is responsible for **developing and facilitating the implementation of** • **level-0 data QA/QC tools to be implemented by ACTRIS NFs** to keep control on the quality of their measurements • **level-1 to level-3 QA/QC tools to be implemented by ACTRIS DC** Evaluating the NF performance summaries	ACTRIS Data Centre is responsible for • Implementing QA/**QC tests of ACTRIS data** (level 1 to level 3 data), which are made available through the ACTRIS data portal • Producing NF performance summaries based on QA/QC test analyses
The CCRES is responsible for • **auditing the ACTRIS NFs** and reviewing their calibration databases • **Deciding on data flag status**	ACTRIS Data Centre is responsible for • Maintaining calibration and metadata databases for each ACTRIS NF, based on information provided by NFs • Providing the **traceability and full documentation of the data quality** of the ACTRIS data • Maintaining the ACTRIS Cloud remote sensing database
The CCRES is responsible for **testing and evaluating new retrieval algorithms or tools** for producing level 1 to 3 data, including the exploitation of instrument synergies	ACTRIS Data Centre is responsible for **implementing the approved retrieval algorithms or tools** into the ACTRIS Data Centre operation

8.2.3 Technical obligations in relation with Centre for Aerosol Remote Sensing)

There is a close link to the Centre for Aerosol Remote Sensing (CARS) because low-power lidars and ceilometers (ALCs) are supported by CARS, while they belong to the minimum required instrumentation of NFs for cloud remote sensing. All quality assurance activities concerning cloud products from ALCs are covered by the CCRES, but should be strongly supported by CARS. An intensive communication between CARS and CCRES is mandatory to ensure that all recommended SOPs and methods are compatible for the quality of both aerosol and cloud related products from ALCs.

8.2.4 Technical obligations in relation with the ACTRIS users

The CCRES should commit to provide a minimum amount of user services as described in section 4. The provision of services will be made on a case-by case situation.

8.3 Evaluation of the activity of the Centre for Cloud Remote Sensing

Once established and operational, the Centre for Cloud Remote Sensing should be annually evaluated for its performances, against the following KPIs:

No.	Criteria	Indicators	Score	Weight
1	Usefulness for ACTRIS NFs	No. of operational support units provided to ACTRIS NFs (incl. calibration)	1 … 10	40%
		Level of involvement in developing and disseminating SoPs, QA/QC tests, tools	1 … 10	
		No of training sessions and workshops open to ACTRIS NFs	1 … 10	
		Average of Usefulness for ACTRIS		
2	Usefulness for ACTRIS users	Level of involvement in developing and disseminating SoPs, QA/QC tests, tools		20%
		No of training sessions and workshops open to ACTRIS users		
		Average of Usefulness for external users		
3	Impact on science & technology	No. of peer-review papers facilitated		30%
		Level of involvement in testing new retrieval algorithms and methods		
		Average of S&T Impact		
4	Integration into ACTRI-RI	Level of collaboration with other nodes and ACTRIS structures (NFs, DC, SAMU, …)		30%
		Quality and readiness of the reports		
		Average of Integration into ACTRI-RI		
Total score				

Glossary

ACTRIS data - are the ACTRIS variables resulting from measurements that fully comply with the standard operating procedures (SOP), measurement recommendations, and quality guidelines established within ACTRIS.

- **ACTRIS level 0 data:** Raw sensor output, either mV or physical units. Native resolution, metadata necessary for next level.
- **ACTRIS level 1 data:** Calibrated and quality assured data with minimum level of quality control.
- **ACTRIS level 2 data:** Approved and fully quality controlled ACTRIS data product or geophysical variable.
- **ACTRIS level 3 data:** Elaborated ACTRIS data products derived by post-processing of ACTRIS Level 0 - 1 -2 data, and data from other sources. The data can be gridded or not.
- **ACTRIS syntheses product** (*Proper name to be defined later*)**:** Data product from e.g. research activities**,** not under direct ACTRIS responsibility, but ACTRIS offer repository and access.

ACTRIS Data Centre (DC) - the Central Facility responsible for ACTRIS data curation, preservation, and distribution of data, value-added products and tools**,** and hosting the ACTRIS data portal.

ACTRIS data originator - entity operating instruments at a National Facility or Topical Centre, resulting in ACTRIS data and delivering ACTRIS data to the Data Centre.

ACTRIS data provider - the Data Centre offering the ACTRIS data and value-added data products and tools to users.

ACTRIS digital tools and services - tailored codes and software for processing and visualization of ACTRIS data, production of ACTRIS data products, and for data analysis and research.

ACTRIS exploratory platform - National Facility (simulation chambers, laboratories, or mobile facilities) operating on campaign basis and delivering dedicated data to the Data Centre.

ACTRIS General Assembly (GA) - a council of ministry- and funding organization representatives of ACTRIS members after ACTRIS legal entity has been established, superior decision-making body of ACTRIS.

ACTRIS Head Office (HO) - a Central Facility coordinating and representing ACTRIS, and holding the statutory seat.

ACTRIS label - earmarks a data set or a measurement site as ACTRIS data or ACTRIS National Facility.

ACTRIS observational platform – ACTRIS National Facility performing long-term, regular observations and delivering standardized data to the Data Centre.

ACTRIS Topical Centres (TCs) – a Central Facility offering services and operation support for QA/QC of measurements and data (including training, calibration, QA/QC tools, and development of standard operation and evaluation procedures)

ACTRIS variables - the measured atmospheric variables as described in the ACTRIS Data Management Plan[1].

[1]The ACTRIS data management plan and list of variables were approved by ACTRIS-2 scientific steering committee, October 2015. These documents are expected to be refined during ACTRIS-PPP (WP5).

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Central Facility (CF) - a European level ACTRIS component that offers ACTRIS data or other ACTRIS services to users as well as operation support to ACTRIS National Facilities.

Central Facility Unit – part of a Central Facility located at, and operated by a research performing organization (RPO) or by ACTRIS ERIC.

CF Director – the person responsible for the coordination and representation of a Central Facility.

CF Unit Head – the person responsible for the coordination and representation of a Central Facility unit.

CF Management Board – consists of the CF Unit Heads and the CF Director; this board manages the Central Facility.

Data curation - the activity that stores, manages and ensures access to all persistent data sets produced within the infrastructure.

Data traceability - an unbroken chain of uniquely identified process steps leading from raw data to any kind of processed data, where identification of process steps follows the data.

Interim ACTRIS Council - a council of ministry- and funding organization representatives of ACTRIS members before ACTRIS legal entity has been established (during the ACTRIS Preparation and Transition Phase), superior decision-making body of ACTRIS.

Measurement traceability - an unbroken chain of comparisons relating an instrument's measurements to a known standard, in the ideal case SI units.

National Facility (NF) - an observational or exploratory platform providing data and/or physical access to the platform within ACTRIS.

Quality assurance and control: Quality assurance is process oriented and focuses on defect prevention; quality control is product oriented and focuses on defect identification:

- **Quality Assurance (QA):** The process or set of processes used to ensure the quality of a product (e.g. data series, instrument, sample, measured value of a variable, etc.),
- **Quality Control (QC):** The process and activities of ensuring products and services meet the expectations.

RI committee – consists of up to two representatives from each Central Facility and [three] representatives from the National Facilities Assembly; the RI committee supports the (Interim) Director or Board of Directors in operating the RI.

Service and Access Management Unit (SAMU) - a part of ACTRIS Head Office facilitating the access to ACTRIS services.

User - a person, a team, or an institution making use of ACTRIS data or other ACTRIS services, including access to ACTRIS facilities.

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Reference documents

ACTRIS-PPP proposal

ACTRIS Data Management Plan, approved by ACTRIS-2 SSC 23 October 2015

ACTRIS Concept Documents

ISO 10012:2003: Measurement management systems — Requirements for measurement processes and measuring equipment

ISO 9000:2015: Quality management systems—Fundamentals and vocabulary

Baseline document for the Concepts of ACTRIS Central Facilities

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Section 7

Concept of the Centre for Reactive Trace Gases in Situ Measurements (CGas-SiM)

ACTRIS PPP WP 4 Task 4.1

22.2.2018

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1 Purpose of the document

This document describes the relevance, mission, requirements and obligations of the ACTRIS Centre for Reactive Trace Gases in Situ Measurements.

2 Description and role of the Centre for Reactive Trace Gases in Situ Measurements

2.1 Framework

ACTRIS is the European platform for fostering the use of research data and data analysis tools in the field of atmospheric aerosols, clouds, and reactive trace gases. ACTRIS Central Facilities (CFs) represent the key operative entities of this Research Infrastructure (RI) and have a fundamental role as they provide operation support to the National Facilities (NFs) i.e. the observational and exploratory platforms as well as services to the users according to the ACTRIS access policy. CFs are operated at the European level and are part of the governance and decision-making structure of the RI. Each CF may have several operational Units that can be located in the same or different locations, and are operated by research performing organizations (RPOs) or by ACTRIS ERIC.

The **C**entre for Reactive Trace **Gas**es in **Si**tu **M**easurements (CGas-SiM) is one of the six ACTRIS Topical Centres (TCs) organized around the main scientific themes of ACTRIS: aerosols, clouds, and reactive trace gases, each with a particular focus on either remote sensing or in situ measurement techniques.

The CGasSiM is related to the ACTRIS tasks for the Reactive Trace Gases Calibration Centre specified in the ACTRIS ESFRI proposal, i.e. "Science Case" and the "Terms of reference" by Global Atmosphere Watch (GAW) of the World Meteorological Organisation (WMO) for the World Calibration Centres (WCC). These needs have passed the ESFRI evaluation process and the selection and evaluation of expert teams, the GAW Scientific Advisory Group for Reactive Trace Gases (SAG-RG) and the Commission of Atmospheric Science (CAS) by WMO. Thus, these needs are the outcome of well justified processes and are high level approved.

Within ACTRIS and ACTRIS-2 projects, the services have been further tested and implemented. Currently, the WCC for VOC and NOx are able to provide limited services to users owing to the very limited resources available. It is foreseen that more resources are made available within the ACTRIS RI to achieve a higher coverage and higher level of the services in cooperation with the NFs to provide the highest quality level of the data. In addition, with the introduction of several units, the load of the services will be shared by several institutions in Europe which are well recognized for their high expertise in reactive trace gas measurements and quality management.

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2.2 Scientific relevance

Reactive trace gas species in the Earth's lower atmosphere are a large group of compounds with lifetimes between minutes to a few months. These gases are the players of atmospheric chemistry and determine among others the abundance of free radicals, reactive climate gases, toxic pollutants, aerosol precursors and compounds relevant for atmospheric deposition. Assessing the role and impacts of reactive trace gases in the atmosphere requires knowledge of the global distribution and long-term changes in their abundance especially under a climate change context. Observations of their background levels are also essential for understanding long-range pollution transport, which in turn is crucial for assessing the success of regional to local emission reduction plans (see Schultz et al., 2015).

Key Reactive Trace Gases, which are readily observable, are tropospheric ozone, carbon monoxide, volatile organic compounds (VOCs), reactive nitrogen gases (e.g. NO, NO_2), and reactive sulphur gases. The CGas-SiM in particular should consider the ACTRIS variables volatile organic compounds (VOC), nitrogen oxides (NO, NO_2) and specific inorganic and organic precursors for particles with measurement techniques described in Chapter 3.1 of this document.

ACTRIS network wide in situ observations of key organic and inorganic compounds in the atmosphere are essential for providing reliable scientific data of the chemical composition of the atmosphere, its natural and anthropogenic change, and improving the understanding of interactions within the atmosphere. This requires high data compatibility within the ACTRIS observation network and thus a well-developed quality assurance and quality control (QA/QC) program. For key-VOC and NOx, this is further elaborated in the WMO-GAW program (WMO-GAW, 2017). In ACTRIS-1 and ACTRIS-2, specific VOC and NOx data have successfully been improved and better inter-linked by a comprehensive QA/QC program than before (see Hörger et al., 2013). The ACTRIS RI will provide such high quality data more and more requested by data users e.g. for validating "chemical weather" forecast models, Near Real Time (NRT) assimilation into Global-Chemistry-Climate Models, validating satellite retrievals for e.g. formaldehyde, validating ground remote sensing data products on e.g. ethane. In addition, process studies of VOC oxidation in simulation chambers with near real ambient conditions may benefit from common QA/QC procedures.

For ACTRIS the CGas-SiM should ensure traceability and compatibility of network data and should comprise the WMO-GAW World Calibration Centres for Volatile Organic Compounds (WCC-VOC) and for NOx (WCC-NOx). Both centres have been approved by the international science community and form one corner stone of the QA/QC framework defined within WMO-GAW and thus already include substantial capacities and know-how.

ACTRIS-RI should make use of that knowledge as a basis to implement the CGas-SiM as pan-European effort with units in Germany, Finland, Switzerland, and France at the frontier of science and technical innovations.

2.3 Mission

The key-mission of the CGas-SiM should be to offer operational support to ACTRIS NFs operating instrumentation for continuous long-term measurements of VOC, volatile and semi-volatile aerosol precursors, guide research and service development in the reactive gases field, and develop towards future user needs utilizing newly emerging methodologies. While the main activities should focus on the ACTRIS and GAW communities, specialized services should be offered to users from academia, business, industry, and public services depending on the respective resources.

The core services of CGas-SiM should be to ensure (1) sustainable and traceable high quality data and data products with known accuracy, (2) to implement advanced technologies and data evaluation algorithms, and (3) to assist in sustaining the high competence of the operative staff by implementing and training in advanced measurement technologies and data evaluation algorithms. Additionally, CGas-SiM should provide customized services to NFs and users including testing of prototypes. The key activities of the CGas-SiM for observational platforms are highlighted in Figure 1.

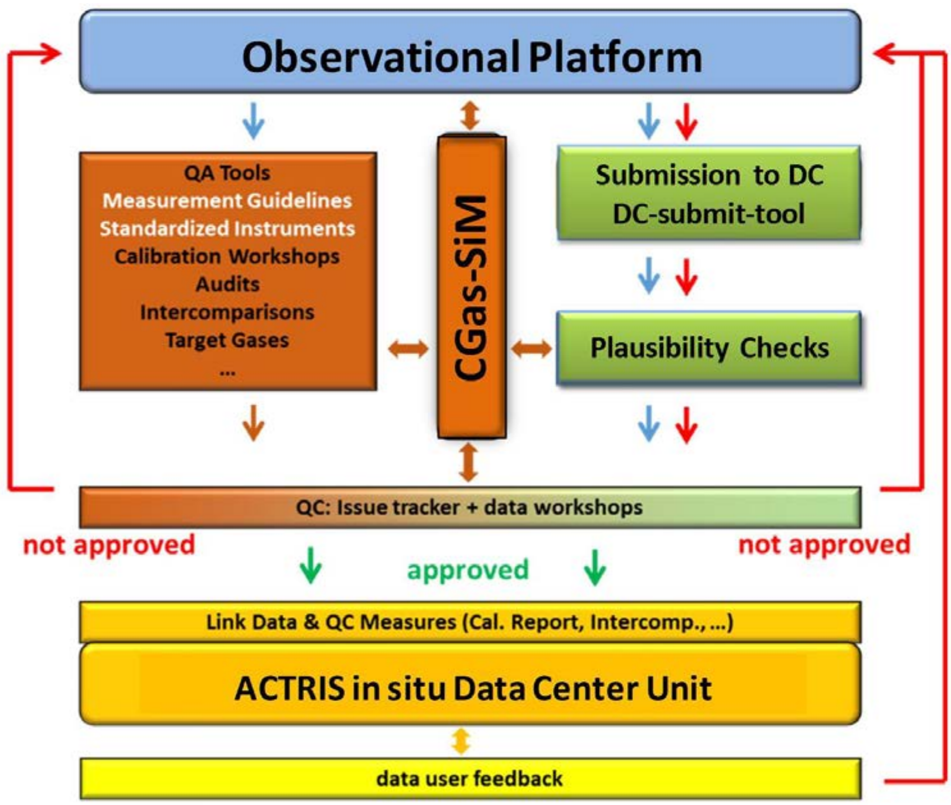

Figure 1: Scheme of the QA/QC system for observational platforms envisioned for the CGas-SiM. The CGas-SiM together with the station assembly should develop the QA Tools (white: developed in cooperation with GAW), should provide plausibility checks performed by stations and CGas-SiM, should control the issue tracker by setting up issues, should discuss and control actions by stations, and should close the issues upon successful finalisation by stations.

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The CGas-SiM activities should

1. establish adequate procedures and methodologies for measurement of VOCs, , volatile and semi-volatile aerosol precursors in close cooperation with international bodies (e.g. GAW) and the NFs;
2. perform quality assurance and quality control of the measurements and data in the RI in close cooperation with NFs and the DC and provide tools for the data providers for checking the data before submission;
3. review yearly submitted data after first submission and provide guidance for improvement;
4. organise yearly a data quality workshop, where data is finally quality checked before submission to the data base;
5. ensure the traceability of data from the NFs to the primary standard (see Figure 2);
6. check the consistency of data and measurement methods by organising intercomparison exercises;
7. ensure a high performance of NFs by conducting station audits and training sessions;
8. promote technological development and knowledge transfer to NFs and users;
9. foster up-to-date capacity-building in the RI by conducting own high quality research with latest technologies contributing to research and development projects.

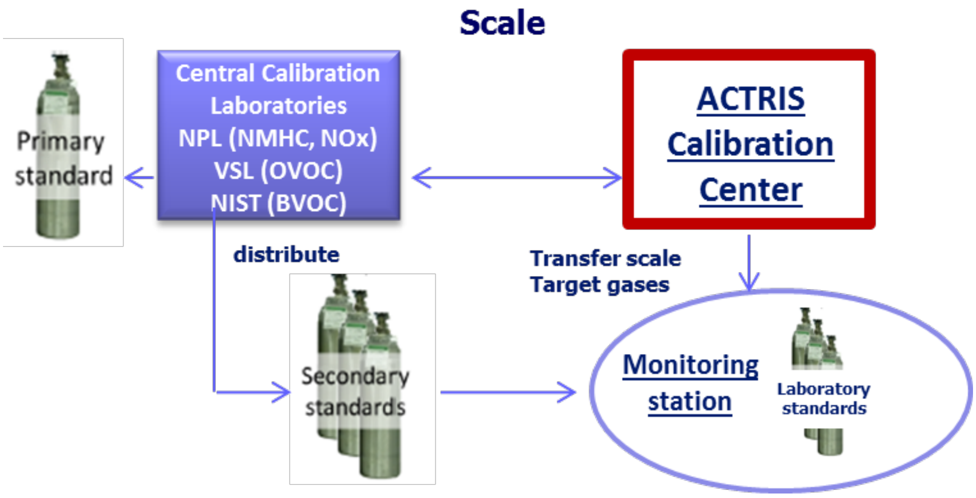

Figure 2: Scheme demonstrating how the SI traceable scale of reactive trace gases should be maintained and transferred to the National Facilities.

The CGas-SiM then should act as a living organisation with adapting its procedures and performance to future needs resulting from research and development projects with focus on analytical methods and traceability of new components in cooperation with NFs and other TCs within their capacity and depending on their available resources

3 Operation support provided to ACTRIS National Facilities

The operation support to NFs which should be provided by the CGas-SiM include: a) procedures and tools for quality assurance and quality control of measurements and data, b) transfer of knowledge and training to operators, and c) improvements of measurement methodologies. The operation support should focus on ACTRIS variables and measurement techniques described in this concept document, also listed in the *Technical Concepts and Requirements for ACTRIS Observational and Exploratory Platforms*.

The CGas-SiM is obliged to put in place and offer to NFs the specific operation support marked with * in this document. Other operation support described in this document is not mandatory for the TC, but recommended.

The operation support can be scheduled or on request. Participation at the scheduled activities is mandatory for the NFs. Measurements not following the mandatory actions are not considered as ACTRIS-conform and do not yield ACTRIS data.

In addition, NFs may request operation support which is not scheduled, depending on the identified need. Specific operation support offered as scheduled or offered on request is detailed in *Annex: Provision of the operation support.* This annex will be updated each time as it is necessary (e.g. development of new testing or calibration methods and tools).

The CGas-SiM should operate at the state-of-the-art, fostering the implementation of validated new techniques in the RI. To sustain a high level of performance and to stimulate the advancement of new techniques and methodologies, the CGas-SiM should contribute to research and expert collaboration networks.

3.1 Measurement techniques covered by the Centre for Reactive Trace Gases in Situ Measurements, and related ACTRIS variables

The ACTRIS variables covered by reactive trace gases in situ measurements should include tracers for anthropogenic/biogenic activities as well as chemical process indicators in the atmosphere. The compounds considered here focus on: (1) non-methane hydrocarbons (up to 40 NMHCs; e.g. ethane, ethyne, propane, i-/n-butane, i-/n-pentane, isoprene, benzene, toluene), (2) the biogenic VOCs (BVOC) with the monoterpenes (e.g. α-/β-pinene, 3-carene, 1,8-cineol, limonene), (3) the oxyVOC (e.g. formaldehyde, methanol, ethanol, acetone), (4) the direct aerosol precursors sulfuric acid and highly oxygenated molecules (HOM), and (5) NO and $N0_2$. In order to detect and quantify the target compounds in ambient air, specific sampling and analytical techniques should be implemented.

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3.1.1 NMHC Gas chromatographic System

The measurement of NMHCs in air by gas chromatography (GC) is described in more detail in the corresponding Measurement Guideline (MG) document (SOP-VOC, 2014). Briefly, measurements can generally be performed in a series of steps with (1) taking a sample, (2) pre-concentration (PC), (3) thermo-desorption (TD), (4) gas chromatographic separation, (5) detection, and (6) data processing and data delivery. For taking an air sample, two options should be implemented: (a) taking the sample air directly to the pre-concentrating system with subsequent analysis (on-line) or (b) via a canister or adsorption trap and later analysis (off-line). The air sample treatment before analysis is prone to loss of target substances and artefact formation and needs careful assessment. For off-line sampling with stainless steel canisters the standard operation procedure of GAW (GAW-Report 204, WMO 2012) should be followed. The detection of NMHC by GC can be by flame ionization detection (FID) or mass spectrometry (MS).

The preferable technique should be on-line sampling for lower risk of artefacts. The QA/QC for NMHC-gas chromatographic system is complex and listed in the MG, it includes a.o. regular zero, calibration and target gas measurements with traceable standards. This measurement guideline should be updated according new developments.

3.1.2 BVOC Gas chromatographic System

The measurements of BVOC namely isoprene and monoterpenes (isoprenoids) in air samples can follow similar procedures as described for NMHC (see Chapter 3.1.1) by using a PC-TD-GC preferably with MS detection. FID is also possible with some peculiarities to consider.

The BVOC system should be tuned with respect to (a) pre-concentrating, (b) thermo-desorbing, (c) detecting, and (d) quantifying the target compounds. For pre-concentrating isoprenoids on adsorbents, special care is required to achieve total scrubbing of the target compounds and to avoid oxidation of the already adsorbed compounds during the sampling process. Further, during the thermo-desorption process isoprenoids may degrade when in contact with hot active adsorbents or metals surfaces which impact complete recovery. The complex compound matrix in ambient air may affect a sound identification of the isoprenoids. Thus a mass selective detection can be recommended, but in highly resolving GC systems also detection by FID can be acceptable. The sensitivity changes and drift of a MS detector can be accounted for by more frequent calibration. For this technique well advanced QA/QC procedures including calibration, artefacts, performance assessments and specific data validation processes should be developed and provided in dedicated measurement guidelines.

3.1.3 Oxy-VOC Measurement Systems

Oxygen containing volatile compounds in air can be analysed using GC-FID, GC-MS, or GC-FID/MS as described above. But, great care should be taken to minimize surface adsorptive losses and releases and to suppress oxidation reactions in the analytical system of VOC that can react with ozone or oxygen to form additional OVOCs as artefacts.

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Some light oxy-VOC including formaldehyde, other aldehydes and ketones can be measured using an off-line method. Ambient air is sampled though a silica gel adsorbent coated with 2,4-Dinitrophenylhydrazine (DNPH). The corresponding derivates can then analysed after liquid extraction with high performance liquid chromatography and UV detection (HPLC-UV). While sensitive, this method is subject to interferences and artefacts which should be carefully evaluated. Formaldehyde specifically can be measured on-line using the Hantzsch reaction. The detection of formaldehyde is based on the liquid phase reaction of formaldehyde with acetyl acetone (2,4-pentadione) and ammonia. This reaction produces 3,5-diacetly-1,4-dihydrolutidine (DDL), which is absorbing light at 410 nm and shows a strong fluorescence around 510 nm, measured by a photomultiplier. This analytical method can achieve a high selectivity, avoiding mostly interferences of other chemical substances in the sample gas. The Hantzsch reaction is conducted in aqueous solution thus gaseous formaldehyde is transferred into aqueous solution first using a stripping coil. Size, temperature and flow rate of the stripping coil should be optimised for a quantitative reaction of HCHO. Details on all processes employed should be provided in a corresponding measurement guideline to be established.

3.1.4 Proton-Transfer-Mass-Spectroscopy

Proton Transfer Reaction-Mass Spectrometer (PTR-MS) is a fast on-line analytical technique for VOCs capable of measuring compounds with higher proton affinity than water molecules, e.g. selected OVOC, unsaturated NMHCs (aromatics, few alkenes, the sum of monoterpenes). In a drift tube VOCs are protonised and subsequently detected by a quadrupole or a time-of-flight (ToF) MS. No specific sample preparation is necessary but isobaric compounds cannot be separated and compounds with a lower proton-affinity than water cannot be detected. Thus, it should be carefully assured that all compounds of interest are detected and no other compound is co-detected together with the target compounds. Details should be provided in a corresponding measurement guideline to be established.

3.1.5 Direct Aerosol Precursor Measurement Systems

The chemical ionisation (CI) atmospheric pressure interface (APi) time of flight (ToF) mass spectrometer can be used to characterise condensing aerosol precursor molecules and clusters comprehensively. This instrument is capable of resolving e.g. the concentrations of atmospheric sulfuric acid, iodic acid and oxidized organic compounds in a quantified manner. It can also resolve the chemical composition of neutral clusters. Various reagent ion chemistries can be applied for charging of the sample molecules and clusters (e.g. NO_3^-, I^-, CH_3COO^-). With the nitrate ion chemistry at ambient pressure, it is possible to ionize and quantify concentrations of e.g. sulfuric acid or iodine oxide containing clusters and detect Highly Oxygenated Molecules (HOM, e.g. $C_{10}H_{14}O_9$) in air samples, online and with fast time resolution. Details should be provided in corresponding measurement guidelines to be established.

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3.1.6 Nitrogen Oxides Measurement Systems

NO in air can be measured using the chemiluminescence detection (CLD) method. Ambient NO reacts with added ozone to yield excited NO_2, and emitted luminescence photons are detected by a photomultiplier.

NO_2 can be measured using either photolytical conversion (PLC) to NO subsequently measured as described above or employing the cavity attenuated phase shift (CAPS) technique.

The photolysis of NO_2 is conducted in a conversion cell. NO_2 is photolytically converted into NO and O. The NO is then detected by a chemiluminescence instrument while the O reacts with O_2 to yield O_3. For this photolytic conversion, either UV emitting lamps, e.g. Xe-lamps, or high-power-light emitting diodes (blue light converter; BLC) can be used.

The CAPS technique relies on producing very long optical paths (up to 2 km) using very high reflectivity mirrors in a sampling cell that is less than 30 cm in length. These monitors utilize a light emitting diode (LED) as an optical source and measure the resultant signal in the frequency domain using a phase shift technique. The CAPS technique is in theory an absolute method, since it provides a direct absorption measurement of nitrogen dioxide at 450 nm, but needs in reality calibration and offset correction. Details of the methods described are in part already reported in the NO_X measurement guidelines (SOP-NOx, 2014) and should be updated according new developments.

3.2 Estimation of the need

In Europe, the ACTRIS observational sites are part of the Emission Monitoring and Evaluation of the Long Range Transmission of Air (EMEP) network of the Convention on Long-Range Transboundary Air Pollution (CLRTAP). Currently, 26 Station are operating VOC and/or NOx measurement systems which require extended QA/QC measures for compatible data (Figure 3). Also the ACTRIS exploratory platform EUROCHAMP-2020 with its 18 atmospheric simulation chambers should benefit from the QA/QC activities of CGas-SiM. Already some ACTRIS and EMEP stations contribute QA/QC data to the WMO-GAW program, currently hosting 37 approved global stations and more than 600 regional and contributing stations with 250 in Europe (Figure 4). WMO-GAW with its contributing networks forms the largest global, atmospheric observation network for research and outreach products are used for science, policy and journalism advice.

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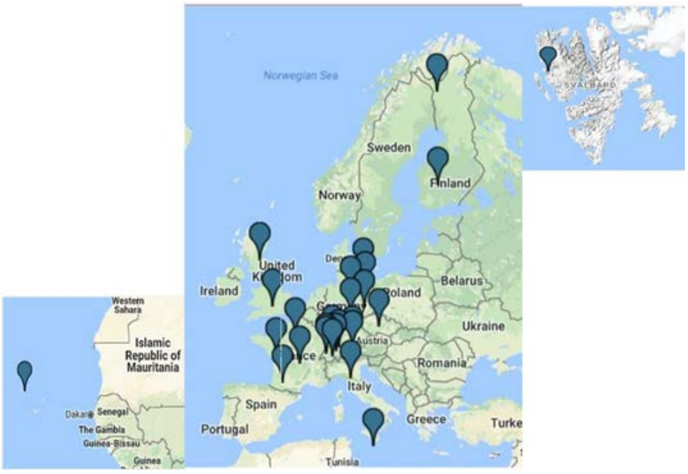

Figure 3: ACTRIS observational sites providing quality assured reactive trace gas in situ data and complying with ACTRIS recommendations in 2016.

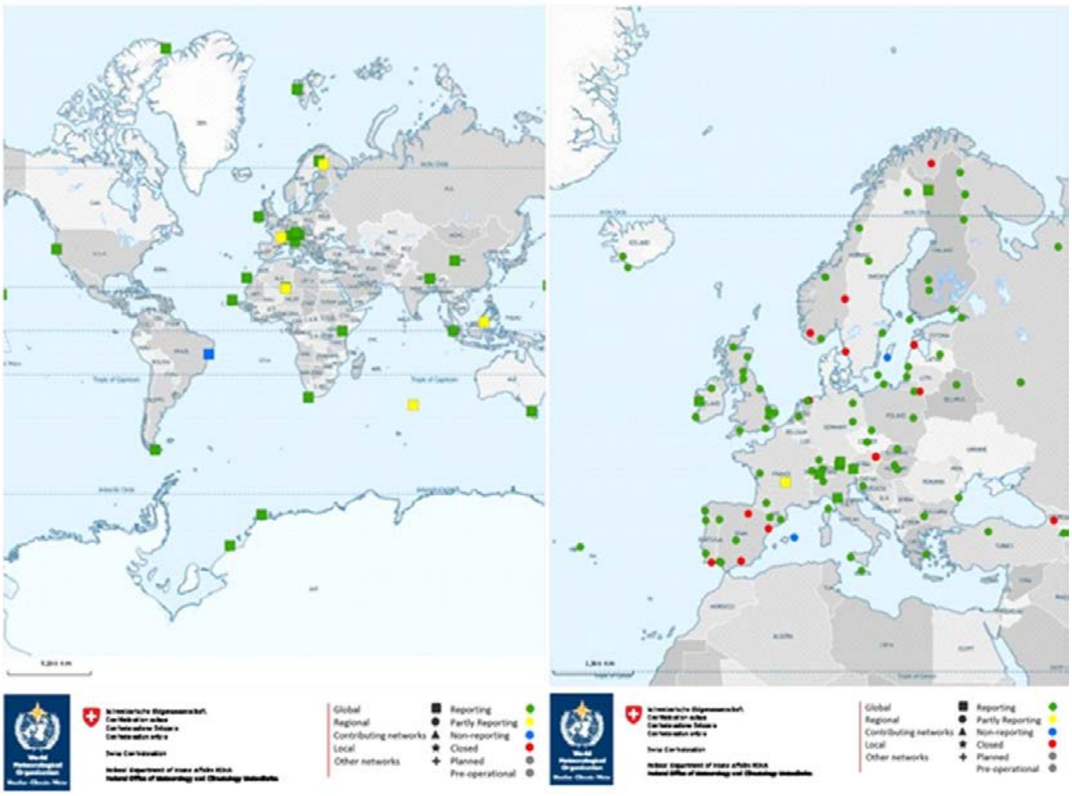

Figure 4.GAW Global stations (left) and the European GAW Global- and Regional stations for VOC and/or (right; https://gawsis.meteoswiss.ch/GAWSIS/index.html).

Details on WMO-GAW are available in the recently published implementation plan for 2016 to 2023 (WMO-GAW 2017).

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Within these networks, currently 92 additional users of the CGas-SiM were identified.

The corner stone for good quality data is a well elaborated QA/QC framework as shown by. WMO-GAW with its central facilities (1) Central Calibration laboratories (CCL), (2) the Quality Assurance – Science Activity Centres (QA-SAC), (3) the World/Regional Calibration Centres (WCCs/RCCs) and (4) the World data Centre (WDCs). In ACTRIS, this quality management framework should form the basis for CGas-SiM. Up to now, for key reactive trace gases only the data quality of non-methane hydrocarbons targets (NMHCs; ethane, ethyne, propane, i-/n-butane, i-/n-pentane, isoprene, benzene, toluene) has been fully assed. The QA/QC for other VOC with biogenic VOCs (BVOC) like monoterpenes (α-/β-pinene, 3-carene, 1,8-cineol, limonene), oxyVOC (formaldehyde, methanol, ethanol, acetone), sulfurVOC (dimethylsuflide DMS), and nitroVOC (acetonitril) as well as NO and NO_2 still is on the agenda. Within the ACTRIS–RI the CGas-SiM should extend the QA/QC checks to the ACTRIS variables measured at ACTRIS observational and exploratory platforms. Table 3-1 provides a summary of the required measurement techniques and a number estimate of groups where potentially operational support is provided.

Table 3-1: Summary of the required potential of the CGAS-SiM

Measurement technique	Number of instruments/groups to which the TC should provide operational support		
	Now	by 2025	
		Min.	Max.
NMHC-GC	15	20	40
BVOC-GC	2	4	8
OVOC-GC	4	6	10
OVOC-DNPH-HPLC	4	6	10
HCHO-HANTZSCH	3	4	10
PTR-MS	4	6	10
CI-APi-ToF	5	10	20
NO-CLD	20	25	40
NO_2-PLC/BLC-CLD	20	25	40
NO_2-CAPS	5	10	20

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3.3 Timeline for implementation of the mandatory operation support

Considering the ACTRIS roadmap, CGas-SiM should consider the following implementation plan for the mandatory operation support (including general tasks, scheduled and on request operation support, see *Annex: Provision of the operation support)*:

Operation support	Type	Preparation phase	Implementation phase	Operation phase
		< 2020	2020 - 2025	> 2025
Measurement Guidelines (MGs) and Standard Operation Procedures (SOPs)	General task	Basic MGs/SOPs including QA/QC procedures for operation of the instruments and data analysis (minimum requirements)	Advanced/New MGs/SOPs including QA/QC procedures for operation of the instruments and data analysis (minimum requirements) (optimum setup)	Updates and new MGs/SOPs
Scale transfer	Scheduled/ On request	Provision of scale to working standards for selected trace gases, on request only	Continue provision of scale to working standards of selected trace gases, on request only and update working standards with new scales	Continue as scheduled support every four years and on request including updates
New Instrument techniques	On request	Direct comparison of selected trace gases with fixed, state-of-the-art, reference instruments	Direct comparison of selected trace gases with fixed, state-of-the-art reference instruments	continue as support on request and consulting for implementing new techniques

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Operation support	Type	Preparation phase	Implementation phase	Operation phase
		< 2020	2020 - 2025	> 2025
Training of operators and scientists	Scheduled/ On request	Training sessions for a specific measurement technique and on pre-defined subjects on request only	Training sessions for a specific measurement technique and on pre-defined subjects on request only	Regular training sessions every two years for a specific measurement technique and on pre-defined subjects as scheduled/on request activity
Provision of target gases	Scheduled	Tests at CGas-SiM laboratories (minimum requirements)	Provide first target gases to stations (minimum requirements), tests at CGas-SiM laboratories (optimum requirements)	Provision of target gases on annual basis
Station comparison (round robin and parallel off-line sampling)	Scheduled/ On request	Selected round robin exercises	At least one regular round robin exercise and one parallel off-line sampling (VOC) per target compound in 5 years (minimum requirements)	Regular round robins and parallel off-line sampling (VOC) at least every two years

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Operation support	Type	Preparation phase	Implementation phase	Operation phase
		< 2020	2020 - 2025	> 2025
Comparison using mobile reference instruments	Scheduled/ On request	Direct comparison with mobile reference system for selected trace gases, in few cases only	Direct comparison with mobile reference system for selected trace gases, in few cases only	Continue at least every four years as scheduled activity and on request
Central side-by-side comparisons	Scheduled/ On request	Selected comparisons for OVOCs, selected BVOC and NOx	Use of existing and establishment of a new platforms (EUROCHAMP) for conducting the comparisons every four years for selected participants	Continue as scheduled activity at least every four years
Station audits	Scheduled		Auditing the performance of the measurement systems at a site (minimum requirements) for selected sites	Continue and extend to optimum requirements as scheduled activity every four years
Survey of target and comparison results; checking compatibility	Scheduled	Assessment of reported target concentrations with QA/QC tools (minimum requirements)	Further developing QA/QC tools and assessment of reported target concentrations (optimum requirements)	Continue annually as scheduled activity
QC data-procedure and review (issue tracker)	Scheduled	Assessment of ambient air data with QA/QC tools (minimum requirements)	Further developing QA/QC tools and assessment of ambient data, operate issue tracker (optimum requirements)	Continue annually as scheduled activity
Consulting in procedures when	General task		Setting up procedures for ACTRIS label award	Consulting how to become an ACTRIS NF and to apply for the

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Operation support	Type	Preparation phase	Implementation phase	Operation phase
		< 2020	2020 - 2025	> 2025
applying for the ACTRIS label				ACTRIS label, control the conformity of existing ACTRIS NF to ACTRIS label

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3.4 Operation support for quality assurance and quality control

3.4.1 Definition and establishment of Measurement Guidelines (MG)

During ACTRIS-2, the first MGs for VOC by gas chromatography and for NOx (NO and NO_2) have been developed (ACTRIS 2011-2017). Since different instrument set ups are deployed at the stations which are generally considered to be appropriate to achieve the DQOs defined in ACTRIS and GAW, the MGs should be generic and not specific to just one instrumental set-up. The MGs for NOx and NMHC Gas chromatography are currently in review by the SAG-RG of WMO GAW and the wider scientific community to achieve high level guidelines commonly agreed upon. During the implementation of ACTRIS-RI, these shall be expanded to cover also the other variables and techniques (BVOC and OVOC by GC, DNPH-HPLC, HCHO-Hantzsch, PTR-MS, NO_2 by CAPS, and CI-APi-ToF), and during future developments of ACTRIS-RI towards further, new analytical technologies.

The objective should be to compile the analytical state-of-the-art into measurement guidelines with the CGas-SiM as competence centre coordinating the expert knowledge transfer in that fields and having a leading role in writing and reviewing state-of-the-art MGs. The MGs should include a description of the measurement techniques and procedures as well as all fields of QA and QC of measurements, calibrations, data evaluation and data delivery. New and updated guidelines should go through a review process and should be approved by the WMO-GAW SAG-RG, the WMO-CAS, and then published. These MGs define how ACTRIS measurements of the corresponding variables should be performed in order to achieve the ACTIRS label. The CGas-SiM will decide in consultancy with the ACTRIS assemblies of NFs and the Research Infrastructure Committee about revisions and the development of new MGs.

3.4.1.1 NMHC by GC

A corresponding MG is in place and currently in the review process (ACTRIS 2011-2017)

3.4.1.2 BVOC by GC

This is partly included in the MG for NMHC monitoring (ACTRIS 2011-2017) and should be revised in a specific BVOC MG during the ACTRIS implementation phase.

3.4.1.3 OVOC by GC, DNPH-HPLC, and HANTZSCH

This is partly included in MG for NMHC monitoring (ACTRIS 2011-2017) and should be revised in a specific OVOC MG during the ACTRIS implementation phase.

3.4.1.4 VOC by PTR-MS

This is currently under development and should be available in the ACTRIS implementation phase.

3.4.1.5 Direct Aerosol Precursors by CI-APi-ToF

This is currently under development and will be available in the ACTRIS implementation phase.

3.4.1.6 NOx by CLD and CAPS

Corresponding MGs exist for NO an NO_2 monitoring with CLD (ACTRIS 2011-2017) and are currently in the review process. A specific MG should be developed for NO_2 monitored by CAPS during the ACTRIS implementation phase.

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3.4.2 Definition of measurement quality-assurance criteria and procedures

Measurement quality-assurance criteria and procedures should be included in the corresponding MGs and Standard Operation Procedures (SOPs). The QA processes are assumed to be similar for the different variables and techniques.

Briefly, QA processes should combine:

- Implementing Measurement Guidelines.
- Following MGs for sampling, calibration, data processing, data corrections and data delivery.
- Assuring documentation and data handling according MGs.
- Using target gas and standard gas addition measurements.
- Participating in round robin and side by side inter-comparisons proposed by CGas-SiM.
- Conducting parallel sampling with or without employing travelling reference instruments coordinated by CGas-SiM.
- Establishing plausibility plots and evaluations.
- Contributing to data quality workshops and to station performance audits.
- Participating in training activities.

In part, QA criteria and procedures for specific ACTRIS variables are already in place as described in the corresponding MGs (ACTRIS 2011-2017). Updated and new QA criteria and procedures should be developed and included in the corresponding MGs during the ACTRIS implementation phase according to needs identified.

3.4.3 Development and provision of instrument-specific calibration

Reactive Trace gases can be calibrated by a combination of high pressure reference gases with corresponding dilution systems, and appropriate zero-gas generation systems. Recommendations and mandatory components as well as procedures should be provided in the corresponding MGs. Furthermore, the CGas-SiM should provide services including (1) the compatibility of laboratory standards with the WMO-GAW CCL scale, (2) offer station audits with test gases to check the calibration, (3) offer round robin test gases and participation in inter-comparison exercises to check calibration and artefact free operation of the respective measurement systems. Depending on needs and availability of suitable instruments, mobile reference instruments should be used by the CGas-SiM in station audits and run in parallel to routine measurements (side-by-side intercomparisons, e.g. using EUROCHAMP capabilities) for a continuous check of calibrations and data quality on-site. Corresponding compliance reports should be provided. Calibration procedures are similar for all ACTRIS variables covered here.

Specifically, the nitrate CI-APi-ToF calibration procedures should include: 1) transmission calibration, 2) controlled fragmentation experiments, 3) concentration calibration with a standardized flow tube experiment or suitable calibration gas, and 4) side-by-side ambient sampling.

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3.4.4 Development and provision of in-house check-up tools

CGas-SiM should provide the MGs, the check of calibrations as listed above, and target gases to investigate the performance of their measurement systems. A set of plausibility check-tools should be made available to the NFs and should be used at the sites. Furthermore, advice should be provided upon request and at the yearly data control workshop. The implementation should proceed in a stepwise manner during the implementation phase after the corresponding MGs become available.

3.4.5 Development of data evaluation procedures and plausibility test

A number of evaluations procedures and plausibility tests have already been developed, tested and partly implemented in ACTRIS and ACTRIS-2 projects. Details are available in the corresponding measurement guidelines (ACTRIS 2011-2017). But data evaluation procedures and plausibility tests should be further developed for all of the mentioned measurement techniques hand-in-hand with the measurement quality assurance criteria in order to enable stations to perform mature plausibility checks and develop a good understanding of the quality of the data. This should be an ongoing activity of the CGas-SiM.

The tests should be designed so that data backup procedure problems and instrumental malfunctioning is eliminated. That includes also situations where everything technically is ok, but instruments are no longer in the range of the calibration conditions. First level of plausibility tests should filter out the most obvious and physically impossible conditions, like negative concentration values, or total ion count is lower than any individual ion count. The plausibility tests should be performed also on operational parameters like inlet voltages, inlet flows, detector pressures and detector operational voltages. Each operational parameter should have its own acceptance window. Instrument specific information is required to perform these tests. Operational parameters should be logged along the data and then processed without specialised software.

The next level of data evaluation procedures should include tests checking the chemical conditions (e.g. recovery rate of target compounds) of the instrument. That requires instrument specific information to be logged. The magnitude and the ratio (e.g. for CI or PTR instruments) of target compounds should be investigated. Significantly altered ratios e.g. in calibration time series, indicate considerable change in the instrument-specific chemistry and thus data are not achieving the required quality level. Performing the tests for instrument-specific chemistry requires data pre-processing and cannot be performed on raw data. That means: The data evaluation procedure should include an automatic data processing procedure. This procedure should be backwards traceable and all parameters used for processing and evaluating should be recorded and stored.

Even though the parameters used for data pre-processing are very much instrument specific, the general evaluation procedures are not. The software for data pre-processing should be able to perform the same tasks with different input parameters in order to incorporate a large number of NFs.

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3.4.6 Realization of observational site performance audits with reference samples or mobile systems

Site performance audits with reference samples or mobile systems should be provided by the CGas-SiM. A period between station visits of 4 years should be envisioned and should be supplemented by calibration checks, round robin exercises, target-gas checks and intercomparisons experiments. New stations and stations encountering problems with data quality and data flow should get more frequent audits upon necessity.

The performance audits check the conformity of a station to the QA requirements as specified in this document and the corresponding MGs. This should include the conformity of the measurements of CGAs-SiM test gases with targeted values within the DQOs (see definitions and procedures of performance and system audits in GAW Report No. 142 (WMO, 2004). The reference for conformity of a station should evolve as the QA system evolves. During the audit at a station the following parts should be evaluated:

- The sampling and instrument set-up.
- The calibration and zero gas systems.
- The QA/QC procedures implemented.
- The training and instructions sessions.
- The calibration, zero gas, target gas, and standard addition data.
- The data delivery.
- The results from intercomparison exercises.
- The uncertainty evaluation.
- The logbooks (instrument, measurements, station).
- The scientific use of the data.
- The overall equipment of the station.

Reference gas samples are already available for currently performed audits within WMO-GAW. Reference instruments are currently available only for a sub-set of reactive trace gases, e.g. formaldehyde and NOx. These instruments should be run in parallel together with the NF instruments during the audit. Results of the audits should be written in a standardized way and provide as comprehensive audit reports.

Specifically, the CGas-SiM should operate a reference CI-APi-ToF in the laboratory, which can be used in side-by-side intercomparison experiments. A standard flow tube experiment should be developed, which should be used to check the performance of instruments participating in intercomparison workshops. For the CI-APi-ToF performance audits, a mobile reference system for generating sulphuric acid vapour can be utilized. That system should be intercompared against the reference system located permanently at the CGas-SiM before and after each station audit. In addition, field deployable permeation systems for generating e.g. fluorinated acids for calibration should be manufactured and used together with the sulfuric acid generator in audits after the implementation phase.

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3.4.7 Organization of regular exercises to assess the performances of the NFs, including instrument performance workshops

Yearly QA/QC workshops checking the plausibility and quality of the NF data should be performed. The objective is the conformity with the DQOs as defined in the MGs. That should include assessments of the year-to-year consistency of the reported data, within network station–to-station consistency, and should consider the impact of emission ratios, chemical processes, lifetime-variability and remoteness of the stations on reported data.

Instrument performance workshops or intercomparison experiments are envisioned on a regular bases aiming at a 4 years period.

Target gases are provided to the stations by CGas-SiM. Building on the experience in ICOS where target gases are successfully used as a major quality control tool, these techniques should be introduced to ACTRIS reactive trace gas measurement stations. CGas-SiM should further optimize the target gas measurement procedures with respect to frequency of measurements and analyses of deviations from reference values as well as in capturing the statistics of the measurements, e.g. repeatability and reproducibility.

In addition, the CGas-SiM should operate a data quality issue tracker system for NFs. That system should be activated on a yearly basis following the initial data submission by a station to the DC. The DC should compile and transfer the submitted data for quality and plausibility checks to CGas-SiM. Issues should then be defined wherever data quality is in question with respect to DQOs and achievable measurement uncertainty by a station. Defined issues should be iteratively solved by the station PI and experts of the CGas-SiM. When CGas-SiM considers conducted actions as sufficient, the issue is closed and revised data can be resubmitted by the station in final form to the DC for publication.

3.4.8 Contribution to documentation and traceability of level 0 to level 3 data products

The CGas-SiM with its different units should be linked to the corresponding international and approved scales maintained at the WMO-CCLs, which are related to SI units. The CGas-SiM should assure the compliance of the stations' laboratory standards with the scale. The CGas-SiM should contribute in key comparisons organized by the community of National Metrology Institutes (NMIs) assembled in the Gas Analysis Working Group (GAWG) of the Consulting Committee of Quantity and Matter (CCQM) of the International Office for Weight and Measures (BIPM).

The CGas-SiM should define together with the DC the data submission templates for the NFs according to the data flow documents developed between the DC and the CGas-SiM. This should include reporting the measurement uncertainty evaluated according the MGs in order assess the quality level of the data and to track any change in data quality. These documents, the MGs, and the data submission procedures regulate the appropriate documentation of the data. All the references on the used calibration gases should inter alia be reported as meta-data together with each data submission. In addition, bias and repeatability/reproducibility of target gas measurements and in round robin measurements, as well as results of intercomparisons should be made available in the data base.

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3.4.9 Contribution to CEN, ISO, or similar standardization activities

The CGas-SiM should contribute to the corresponding standardizations within CEN and ISO and bring in the needs of monitoring reactive trace gases at low air concentrations. By now, the standard operating procedures and measurement guidelines in place focus on urban air quality networks with high concentrations of reactive trace gases not always applicable in remote areas. These documents should further be developed for monitoring background air as in the ACTRIS-RI.

3.5 Operation support for knowledge transfer and training

3.5.1 Training of operators and scientists

For improving and maintaining high data quality in the ACTRIS reactive trace gas network it is essential to train on a regular basis operators and scientists of the NFs. In training centres with thematic training courses, the necessary expertise should be shared with the corresponding station staff. The annual concept of the training schedule should be developed together with the NFs. Objectives of the training should cover all aspects of the MGs, QA/QC procedures and data management. Beside the specific training centres, the yearly data QC workshops, the audits, the side-by-side intercomparisons, and the topical NF assemblies should be used for training. Training is similar for all variables and techniques covered by the CGas-SiM. Besides schooling in technical aspects of the instruments, the training should also provide knowledge about diurnal and seasonal relationships between trace gas species so that the trainees will be able to discover conspicuous features in data series at an early stage either to solve technical problems of an instrument or to be on watch for possibly hazardous events in the environment.

3.5.2 Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs

The CGas-SiM together with the WMO SAG-RG and the UNECE CLRTAP Task Force on Measurement and Modelling (TFMM) should identify gaps in the measurement network in Europe. Thus, CGas-SiM should provide the respective consultancy to the corresponding decision bodies in ACTRIS and GAW. Furthermore, the CGas-SiM should consult new stations in setting up their monitoring infrastructure and quality management system. Consultancy is provided via the MGs, direct communication, reference station visits, and visits of the new to build stations. Consultancy will be available from the beginning of the implementation phase.

3.6 Operation support for improvement of measurement methodologies

3.6.1 Testing of new measurement instruments and procedures

The CGas-SiM should track new developments in measuring and analysing reactive trace gases in air and should be involved in testing and developing new instrumentation for assessing the ACTRIS chemical target variables. Specifically, the suitability of new instruments for long-term monitoring within ACTRIS and the conformity with DQOs should be tested and characterized. Recommendations of the suitability of new measurement technologies for achieving high data quality in the ACTRSI-RI should be provided. For

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this activity specific joint-projects should be envisaged considering further the maturity of the new technologies. During the topical NFs assemblies, initiatives or requirements towards new instrumentation can be discussed and decided.

The presently intended techniques include different ion chemistries for sample ionization in CI-APi-ToF instruments as well as the optical measurement of specific VOC using quantum cascade lasers.

3.6.2 Development of strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime

The CGas-SiM should contribute to development of optimised methods and procedures in order to reduce breakdown and maintenance times to ensure maximum possible operation time of the instruments.

3.6.3 Development of new technological products and methods

New measurement techniques, technological products and methods should be developed by CGas-SiM in collaboration with the NFs. Depending on the situation, the CGas-SiM may recommend to the ACTRIS RI Committee to decide on the implementation of such new techniques at the RI level. The Centre has no obligation to develop the full set of operation support for such new techniques, unless they are embraced by ACTRIS and implemented as part of the NFs.

The CGas-SiM should work on improving data quality verification processes for example based on the uncertainty analysis. Considering the large datasets existing for VOCs measurements, multi-dimensional approaches could be developed to check the consistency of the measurements between sites. For example, factorial analysis (ex. PMF) utilising the co-variability of species commonly observed between sites.

Specifically for CI-APi-ToF instruments, halogen (chloride bromide, iodide) based CI-ion chemistries for charging should be developed and tested. Further, new methods for producing calibration vapours for the CI-APi-ToF should be developed, tested and validated and then distributed to NFs.

3.6.4 Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies

The CGas-SiM should contribute to developments of optimised procedures for level 1 and 2 products, as well for NRT data delivery with automated quality test tools.

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4 Services provided to ACTRIS users

An ACTRIS user is a person, a team, or an institution using either ACTRIS data or any other ACTRIS service. ACTRIS users originate from academia, business, industry and public services, from ACTRIS member countries as well as from countries, which are not ACTRIS members, inside and outside Europe. All user employing or developing instruments for measuring the ACTRIS variables in reactive trace gases may benefit from the QA/QC capabilities developed and available for service by the CGas-SiM.

Access to some ACTRIS services is open and free, most importantly the access to ACTRIS data, data products, and digital tools provided by the DC, which is the point of entry for free ACTRIS data services. Other access to ACTRIS services is considered competitive access based on capacity or excellence and will require a review process that is centrally managed by the HO/SAMU. SAMU is the single point of entry for user access to all TC services and to some specific services and data products provided by the DC. Access is regulated by both the ACTRIS access policy and the ACTRIS data policy, respectively.

Within the CGas-SiM, service provided to ACTRIS users is only provided in a restricted manner considering the limited resources of the TC, the service fee covered by the user, and the priority to ACTRIS NFs support. The units of CGas-SiM will decide about provision of services to GAW, EMEP stations, and other specific users. CGas-SiM should agree on these issues with SAMU. This might include, for example, a service for helping municipalities to set up clean air plans to comply with European air quality regulations for NO_2.

4.1 Estimation of the need

The CGas-SiM is able to schedule some of its potential capabilities for service to ACTRIS users. It is envisaged that up to a maximum of 25% of the availably capacity is made available for use by user. Table 4-1 summarises the current available estimates.

Table 4-1: The CGAs-SiM service estimation for potential ACTRIS users

Type of ACTRIS user	Number of users to which ACTRIS is providing services		
	Now	by 2025	
		Min.	Max.
Academia	0	1	4
Business	0	1	4
Industry	0	1	4
Public Services	0	1	4

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4.2 Provision of measurement quality assurance and quality control procedures and tools

The CGas-SiM can offer all documents and data-plausibility control procedures to users. Furthermore, depending on resources, CGas-SiM can offer participation in round-robin, side-by-side intercomparison and yearly data quality control workshops. In individual cases and on short-term, also calibration of laboratory standards and the provision of target gases may be offered. However, on long-term, such stations should become part of the ACTRIS RI.

4.3 Instrument-specific calibration

The CGas-SiM can offer, depending on resources, calibration of laboratory standards, comparison to travelling reference instruments, and the participation in round-robin and side-by-side intercomparisons which should be used to check the calibration and performance of the instruments including ambient samples under realistic measurement conditions. Besides this, instruments for reactive trace gas monitoring can be calibrated by on-site reference gases, i.e. certified calibration standards, provided by NMIs or, more specifically, by the Central Calibration Laboratories (CCL) of WMO-GAW. Respective standards or gas mixtures traceable to these standards, can be made available on short-term by CGas-SiM.

4.4 Knowledge transfer and operator training

As outlined in 3.4.1, also knowledge transfer and training for users can be offered by CGas-SiM in restricted extent, mainly depending on resources, with priority for ACTRIS NFs support.

4.5 Improvement of measurement and retrieval methodologies for aerosols, clouds, and reactive trace gases

The CGas-SiM can contribute to developments relevant for specific requirements arising from the aerosol-cloud-reactive trace gases interaction, i.e. when processes at the boundaries of respective atmospheric states require the observation of new variables. Between gas- and aerosol-phase, this can already be addressed by the unit on aerosol precursor measurements for organic compounds with very low volatility. This illustrates gap-filling activities provided by the CGas-SiM. The magnitude of the different activities depends on the available resources, the overall importance for ACTRIS, and the network-wide use of such procedures.

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5 Governance and management structure of the Centre for Reactive Trace Gases in Situ Measurements

The CGas-SiM shall be organized in different units according to the specific role of each Unit in addressing the ACTRIS variables, assuring that CGas-SiM complies with the requirements and obligations described in sections 6and 8 of this document, and considering the general principles described in the *Baseline document for the concept of the Central Facilities*. The Centre for Reactive Trace Gases in Situ Measurements shall be organized such that:

- It has a well-defined structure of Units,
- It has a well-defined decision-making process,
- It is coordinated by a CF Director and managed by a CF Management Board, which consists of the CF Director and the CF Unit Heads,
- It has clear and cost-efficient task sharing between the Units,
- It has a risk management strategy,
- It participates in the ACTRIS decision making by sending representative(s) to the ACTRIS legal entity bodies, e.g. to the RI committee.

6 Requirements for the Centre for Reactive Trace gases in Situ Measurements

6.1 General requirements

In order to be labelled as the Centre for Reactive Trace gases in Situ Measurements, the candidate shall:

- Commit for long-term operation, at least 10 years starting with the next year after the implementation as a CF,
- Set-up an appropriate structure of Units, to ensure an adequate functionality of the CF, cost-effective operation, and scalability with respect to the user demands and advancement of the state-of-the-art technology,
- Demonstrate the capacity (in terms of material and personnel resources), to ensure the provision of the needed services and operation support, as described in section 6.2
- Provide a feasible implementation and operation plan for the first five years, starting with the next year after the selection as CF,
- Commit to provide a minimum amount of user services, as described in section 4
- Commit to provide the mandatory operation support to the ACTRIS NFs, as described in section 3.

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6.2 Technical requirements

6.2.1 Facilities

The CGas-SiM should share the tasks between different units. All units should be established in well recognized institutes with long-term experience in the field of continuous long-term monitoring of reactive trace gases in situ in the atmosphere and superior experience in QA/QC. The various units should contribute with their specific and complementary competences to achieve a share of the multiple tasks. Sharing the tasks is necessary because no unit itself has the needed resources. The number of units should be a reasonable balance between available resources comprising personal, competence and capacity, and enhanced coordinative and administrative work. Furthermore, many of the calibration services require independent checks by various laboratories, i.e. the units of the CGas-SiM.

Since high pressure cylinders or air sample canisters should be exchanged between CGas-SiM and stations, the location of the CGas-SiM and its proximity to stations is generally not an issue. With respect to mobile reference instruments and intercomparisons, transport of instruments should be easily feasible in the EU. VOC instruments are more bulky and complex, thus, transport and intercomparison activities are more difficult to achieve. An allocation of units in different European countries would shorten transport time and distance to the NFs. But in general road transportation within Europe is well developed and the location of the units is not a big issue.

All units shall be able to provide calibration, QA/QC, and training services as outlined above. Otherwise, the intended services shall be complimentary, with the coordinating unit having capacity and know-how in the majority of services proposed.

Overall, in each unit laboratory space is needed with parts of the instrumentation covered under Section 3, i.e. at minimum one instrument needs to be present in the laboratory and available for ACTRIS support and users. The CGas-SiM should have training facilities with reference measurement systems (all systems listed in Section 3), side-by-side intercomparison facilities for a reasonable subsets of instruments, i.e. space and logistics for more than 5 VOC systems and more than 10 NOx systems, target gas storage and measurement facilities for compressed gas cylinders for NO and VOC, set-ups for travelling reference instruments or samplers for ambient air measurements, and computing facilities to analyse the corresponding data sets from NFs.

6.2.2 Human resources

The required human resources of CGas-SiM to cover the envisioned services and NFs are estimated to be:

5 full positions expert scientists (>5 years of experience in related field),

5 full positions engineer/qualified operator (>3 years of experience),

3 full positions of technician (> 1 year of experience),

and in the administrative area 0.5, 0.5 and 0.75 full positions of expert manager, qualified officer, and administrative assistance, respectively.

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6.2.3 Other requirements

As the CGas-SiM strongly builds on the experience and resources of the WMO-GAW WCCs for VOC and NOx it is strongly recommended that the WCCs become part of the CGas-SiM. Further, the WCCs are encouraged to head units and coordinate the activities for the respective compound groups. In section 2 and 3, the synergies between GAW and ACTRIS in the reactive trace gases area were identified. ACTRIS procedures and know-how will be used further to strengthen the GAW-WCC activities. It is extremely important to achieve compatible data of reactive trace gases for the ACTRIS-RI and for the GAW-network. By combining QA/QC activities of both networks exceptional synergies are formed thus leading to a world–class centre for QA/QC in the area of atmospheric reactive trace gases, procedure development and training.

7 Basic criteria for the selection of the Centre for Reactive Trace gases in Situ Measurements

The applications to host the Centre for Reactive Trace gases in Situ Measurements are evaluated against a set of criteria covering:

- The **level of commitment** for long-term operation
- The **capacity** to provide the operational support and the services described in sections 3 and 4
  - The availability of the necessary laboratories, instruments, equipment
  - The availability of human resources (no., expertise)
- The **efficiency** in providing the operational support and the services
  - The feasibility of the implementation plan (costs, resources, timeline)
  - The feasibility of the operation plan (methodology, costs per service)
- The level of maturity
  - Status of the development of the Units
  - No. of existing users
  - Adequacy of the decision-making
  - Risk management strategy

These criteria will be detailed in the associated call documents.

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8 Obligations of the Centre for Reactive Trace gases in Situ Measurements

8.1 General obligations

The following general obligations shall apply to the Centre for Reactive Trace gases in Situ Measurements while operational:

- To organize its activities in a cost-efficient way, timely, and with high quality,
- To actively participate in the governance and sustainable development of ACTRIS,
- To provide services to users, according to the access procedures, availability of time, and material resources,
- To provide operation support to the NFs, according to the identified needs, agreed schedules, and procedures,
- To implement efficient user interaction activities by:
  - Organizing workshops, to interact with users,
  - Collecting user feed-backs,
  - Maintaining the CF and ACTRIS websites,
- To document its activities, accesses provided, key performance indicators, and finances, and provide this information to the HO,
  - To contribute to minimize and assess the uncertainties related to data and data products, according to their role and in collaboration with each other,
  - To remain at the forefront of the technology for reactive trace gases in situ measurements.

8.2 Technical obligations

8.2.1 Technical obligations in relation with the ACTRIS National Facilities

Technical obligations of the Centre for Reactive Trace gases in Situ Measurements in relation with the ACTRIS National Facilities refer strictly to the measurement techniques described in this concept document and in *Technical concepts and requirements for ACTRIS Observational Platforms.* The operation of other techniques at the NFs does not imply a technical obligation for the Centre for Reactive Trace gases in Situ Measurements to provide operation support. New techniques / instrument types are only accepted as ACTRIS instruments after the approval of the RI Committee and after the development of the associated QA procedures by the CF.

8.2.1.1 Guidelines, quality assurance criteria and procedures

The Centre for Reactive Trace gases in Situ Measurements is responsible for the quality assurance procedures and guidelines of the ACTRIS measurements conducted at the NFs operating as well as the procedure development as outlines in the previous sections of this concept paper. All the procedures, guidelines, quality assurance criteria, plausibility tests, etc. should be documented and accessible to all related NFs. Specific training sessions with the related NF operators should be organized to ensure a smooth and correct implementation of the above.

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8.2.1.2 Tools, tests and consultancy for quality control of the measurements

It is duty of the Centre for Reactive Trace gases in Situ Measurements to assist the related NFs in the quality control of their measurements by providing the operation support listed in the previous sections, specifically:

- Development and provision of instrument-specific calibration (as described in section 3.3.3).
- Development and provision of in-house check-up tools (as described in section 3.3.4)
- Development of data evaluation procedures and plausibility test (as described in sections 3.3.5).
- Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs (as described in sections 3.4.2
- Testing of new measurement instruments and procedures (as described in sections 3.5.3).

This operation support should be offered to the related NFs whenever there is a need, or a significant progress in the development of these tools, and accompanied by the appropriate training given that sufficient resources are available at the CGas-SiM.

The CGas-SiM shall appoint yearly station workshops for quality control of data. At specified dates prior to the workshop, station PIs have to deliver the data including meta-data according to ACTRIS rules and ACTRIS templates. CGas-SiM will evaluate the data, discuss the evaluation results with station PIs at the workshop, and initiate an issue tracker in case of questionable data. The issues are solved by station PIs and either closed by CGas-SiM or, in case of still open issues, handed back to the station PIs for another review. This dialogue should be openly available at the ACTRIS data centre.

8.2.1.3 Assessment of performances, measurement flagging

The Centre for Reactive Trace gases in Situ Measurements is mandated to assist the Data Centre and the related NFs in the quality control of the measurements and data, by:

- Realization of observational site performance audits with reference samples or mobile systems (as described in sections 3.3.6).
- Organizing regular exercises to assess the performances of the NFs, including instrument performance workshops (as described in sections 3.3.7).
- Contributing to documentation and traceability of level 0 to level 3 data products (as described in sections 3.3.8).

The activities involving directly the NFs operating instruments for measuring reactive trace gases covered by the TC should be scheduled by the TC and provided regularly. The corresponding NFs should participate in these activities according to the plan proposed by the Centre for Reactive Trace gases in Situ Measurements and agreed on with the ACTRIS Scientific Advisory Board (SAB).

8.2.1.4 Transfer of knowledge and training

In addition to the training organized for the implementation of guidelines, procedures, and tools developed in support of QA/QC of the measurements and data, the Centre for Reactive Trace gases in Situ Measurements should organize training sessions with the NFs as needed (see sections 3.4.1).

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8.2.1.5 Improvement of measurement methodologies for Centre for Reactive Trace gases in Situ Measurements

Although it is not an obligation, the Centre for Reactive Trace gases in Situ Measurements should work to sustain a high level of performance and to stimulate the advancement of new techniques and methodologies in the analysis of reactive trace gases in the atmosphere by:

- Development of strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime (as described in section 3.5.2).
- Development of new technological products and methods (as described in section 3.5.3).
- Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies (as described in section 3.5.4)
- Organizing regular events (at least once at 2 years) and other forums, in order to exchange knowledge with the NFs and other scientists.
- Contributing to CEN, ISO, or similar standardization activities (as described in sections 3.3.9).

8.2.2 Technical obligations in relation with the ACTRIS Data Centre

The workflow between CGAs-SiM is graphically shown in Figure 1. Further information is provided in sections 3.3.7 and 3.3.8. Data submitted by the NFs are reviewed by CGAs-SiM on a yearly basis in collaboration with the unit data centre for trace gas in situ data. Jointly with the unit data centre for trace gas in situ data the CGAs-SiM is developing automated QA/QC tools in particular for NRT data submission.

8.2.3 Technical obligations in relation with other TC

The CGas-SiM should establish links to other topical centres where appropriate and ACTRIS variables of reactive trace gases are assessed e.g. Centre for Reactive Trace Gases Remote Sensing.

8.2.4 Technical obligations in relation with the ACTRIS users

The Centre for Reactive Trace gases in Situ Measurements should commit to provide a minimum amount of user services as described in section 4.

8.3 Evaluation of the activity of Centre for Reactive Trace gases in Situ Measurements

Once established and operational, the Centre for Reactive Trace gases in Situ Measurements will be annually evaluated for its performance, against the following Key Performance indicators (KPIs). The KPI and the corresponding scores are listed in Table 8-1.

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Table 8-1: Key Performance indicators for the yearly evaluation of the CGas-SiM activities

Criteria	Indicator	Planned value	Achieved value	Percentage of achievement[1]	Weight
GENERAL SCORE					
Usefulness for ACTRIS NFs	CRITERIA TOTAL SCORE				50 %
	No. of operation support units provided to ACTRIS NFs for quality assurance and quality control				
	No. of operation support units provided to ACTRIS NFs for knowledge transfer and training				
	No. of operation support units provided to ACTRIS NFs for Improvement of measurement and data processing methodologies				
	Average score of satisfaction received from NFs Including utility, fairness and timeliness of the activities for operation support				
Usefulness for ACTRIS users	CRITERIA TOTAL SCORE				20 %
	No. of service units provided to ACTRIS users for quality assurance and quality control				
	No. of service units provided to ACTRIS users for knowledge transfer and training				
	No. of service units provided to ACTRIS users for improvement of measurement and data processing methodologies				
	Average score of satisfaction received from ACTRIS users Including utility, fairness and timeliness of the services performed				
Impac	CRITERIA TOTAL SCORE				

[1] With regard to the planned and approved values

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	No. of new technological products, methods and algorithms developed / improved				20 %
	No. of peer-review CF-related papers published				
	No. of CF-related communications at scientific conferences/workshops				
	No. of CF-related patents promoted				
Integration into ACTRIS	CRITERIA TOTAL SCORE				10 %
	No. of participations to ACTRIS committees and boards				
	No. of activities performed in collaboration with other TCs (joint SOPs, joint workshops, etc.)				
	Average score of satisfaction received from ACTRIS DC for the contribution to documentation and traceability of data products				
	Average score of satisfaction received from ACTRIS HO for the quality and readiness of the reports				

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9 Glossary

***In situ* measurements** - measured or sampled air and instrument are at the same location and in physical contact. In the context of ACTRIS, *in situ* measurements of aerosol, cloud, and reactive-trace-gas properties are performed at observational sites near the Earth surface, on mobile surface-based or airborne platforms, and in simulation chambers and laboratories.

Remote sensing - measured air and instrument are not at the same location and not in physical contact. In the context of ACTRIS, passive (radiometer) and active atmospheric remote-sensing techniques[2] (lidar, radar) for the observation of aerosols, clouds, and trace gases are applied at observational sites or on mobile surface-based and airborne platforms.

ACTRIS data - are the ACTRIS variables resulting from measurements that fully comply with the standard operating procedures (SOP), measurement recommendations, and quality guidelines established within ACTRIS.

- **ACTRIS level 0 data:** Raw sensor output, either mV or physical units. Native resolution, metadata necessary for next level.
- **ACTRIS level 1 data:** Calibrated and quality assured data with minimum level of quality control.
- **ACTRIS level 2 data:** Approved and fully quality controlled ACTRIS data product or geophysical variable.
- **ACTRIS level 3 data:** Elaborated ACTRIS data products derived by post-processing of ACTRIS Level 0 -1 -2 data, and data from other sources. The data can be gridded or not.
- **ACTRIS syntheses product** (*Proper name to be defined later*)**:** Data product from e.g. research activities**,** not under direct ACTRIS responsibility, but ACTRIS offer repository and access.

ACTRIS Data Centre (DC) - the Central Facility responsible for ACTRIS data curation, preservation, and distribution of data, value-added products and tools**,** and hosting the ACTRIS data portal.

ACTRIS data originator - entity operating instruments at a National Facility or Topical Centre, resulting in ACTRIS data and delivering ACTRIS data to the Data Centre.

ACTRIS data provider - the Data Centre offering the ACTRIS data and value-added data products and tools to users.

ACTRIS digital tools and services - tailored codes and software for processing and visualization of ACTRIS data, production of ACTRIS data products, and for data analysis and research.

ACTRIS exploratory platform - National Facility (simulation chambers, laboratories, or mobile facilities) operating on campaign basis and delivering dedicated data to the Data Centre.

[2] In contrast to remote sensing of the Earth's surface (terrestrial and oceanic remote sensing), which is typically done from satellite or aircraft, atmospheric remote sensing is performed from satellite-borne and airborne as well as from surface-based platforms. In ACTRIS, mainly surface-based remote observations are carried out.

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ACTRIS General Assembly (GA) - a council of ministry- and funding organization representatives of ACTRIS members after ACTRIS legal entity has been established, superior decision-making body of ACTRIS.

ACTRIS Head Office (HO) - a Central Facility coordinating and representing ACTRIS, and holding the statutory seat.

ACTRIS label - earmarks a data set or a measurement site as ACTRIS data or ACTRIS National Facility.

ACTRIS observational platform – ACTRIS National Facility performing long-term, regular observations and delivering standardized data to the Data Centre.

ACTRIS Topical Centres (TCs) – a Central Facility offering services and operation support for QA/QC of measurements and data (including training, calibration, QA/QC tools, and development of standard operation and evaluation procedures)

ACTRIS variables - the measured atmospheric variables as described in the ACTRIS Data Management Plan[3].

Central Facility (CF) - a European level ACTRIS component that offers ACTRIS data or other ACTRIS services to users as well as operation support to ACTRIS National Facilities.

Central Facility Unit – part of a Central Facility located at, and operated by a research performing organization (RPO) or by ACTRIS ERIC.

CF Director – the person responsible for the coordination and representation of a Central Facility.

CF Unit Head – the person responsible for the coordination and representation of a Central Facility unit.

CF Management Board – consists of the CF Unit Heads and the CF Director; this board manages the Central Facility.

Data curation - the activity that stores, manages and ensures access to all persistent data sets produced within the infrastructure.

Data traceability - an unbroken chain of uniquely identified process steps leading from raw data to any kind of processed data, where identification of process steps follows the data.

Interim ACTRIS Council - a council of ministry- and funding organization representatives of ACTRIS members before ACTRIS legal entity has been established (during the ACTRIS Preparation and Transition Phase), superior decision-making body of ACTRIS.

Measurement traceability - an unbroken chain of comparisons relating an instrument's measurements to a known standard, in the ideal case SI units.

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[3]The ACTRIS data management plan and list of variables were approved by ACTRIS-2 scientific steering committee, October 2015. These documents are expected to be refined during ACTRIS-PPP (WP5).

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National Facility (NF) - an observational or exploratory platform providing data and/or physical access to the platform within ACTRIS.

Quality assurance and control: Quality assurance is process oriented and focuses on defect prevention; quality control is product oriented and focuses on defect identification:

- **Quality Assurance (QA):** The process or set of processes used to ensure the quality of a product (e.g. data series, instrument, sample, measured value of a variable, etc.),
- **Quality Control (QC):** The process and activities of ensuring products and services meet the expectations.

RI committee – consists of up to two representatives from each Central Facility and [three] representatives from the National Facilities Assembly; the RI committee supports the (Interim) Director or Board of Directors in operating the RI.

Service and Access Management Unit (SAMU) - a part of ACTRIS Head Office facilitating the access to ACTRIS services.

User - a person, a team, or an institution making use of ACTRIS data or other ACTRIS services, including access to ACTRIS facilities.

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10 Reference documents

ACTRIS (2011-2017): Measurement Guidelines and Standard Operation Procedures available at: http://actris.nilu.no/Content/SOP).

ACTRIS Concept Documents

ACTRIS Data Management Plan, approved by ACTRIS-2 SSC 23 October 2015

ACTRIS-PPP proposal

Baseline document for the Concepts of ACTRIS Central Facilities

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Schultz M.G., Akimoto H., Bottenheim J., Buchmann B., Galbally I.E., Gilge S.,, Helmig D., Koide H., Lewis A.C., Novelli P.C., Plass-Dülmer C., Ryerson T.B., Steinbacher M., Steinbrecher R., Tarasova O., Tørseth K., Thouret V., Zellweger C. (2015): The Global Atmosphere Watch reactive gases measurement network. Elementa. Science of the Anthropocene, 3: 000067, doi: 10.12952/journal.elementa.000067.

SOP-NOx, 2014: Deliverable D4.10 of ACTRIS I3 in FP7 (2011-2015): Standardized operating procedures (SOPs) for NOxy Measurements, report available at: http://fp7.actris.eu/Portals/97/deliverables/PU/WP4_D4.10_M42.pdf

SOP-VOC, 2014: Deliverable D4.9 of ACTRIS I3 in FP7 (2011-2015): Final SOPs for VOCs measurements, report available at: http://fp7.actris.eu/Portals/97/deliverables/PU/WP4_D4.9_M42_v2.pdf. Technical concepts and requirements for ACTRIS Exploratory Platforms.

WMO 2004: Strategy for the implementation of the Global Atmosphere Watch Programme (2001-2007): a contribution to the implementation of the WMO Long-Term Plan, GAW Report No 142, available at: http://library.wmo.int/pmb_ged/wmo-td_1077.pdf.

WMO-GAW, 2017: GAW Implementation Plan available at: http://www.wmo.int/pages/prog/arep/gaw/documents/GAWIP2016-2023.pdf.

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Annex: Provision of the operation support

Scheduled support

The CGas-SiM should develop and discuss the scheduled support together with the NFs during the yearly assemblies. Fine tuning should be achieved by teleconferences on request. This support should be managed by the lead unit of the CGas-SiM.

QA/QC activities like round robin or intercomparison experiments which are open to all users, should be announced on the CGas-SiM web-page at least 2 months before the event, with number of potential participants and conditions for contribution. Applications should be selected by the CGas-SiM units in one of the bimonthly teleconferences of the CGas-SiM. Results of these activities should be made openly available on the CGas-SiM webpage. The scheduled support is listed in Table:

Table 9-1: Summary of the scheduled support to NFs by the CGas-SiM

Technique	Type of support	Specific support	Frequency	Comments
Reactive Trace Gas Measurement Techniques	Measurement Guidelines (MGs) and Standard Operation Procedures (SOPs)	Provision of MGs and SOPs	Once	and after each major upgrade
	Scale transfer; Transfer standards	Provision of scale to working standards used at NFs	Once and then every four years	and after each major upgrade
	New Instrument techniques	Consulting for implementing new techniques	Once	and after each major upgrade
	Training of operators and scientists	Not specific at this stage	Every two years for a specific measurement technique used	At training centres or co-located with instrument performance workshops
	Target-gases	Provision of target gases	Every year	Target gases have to be analysed by NFs

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Reactive Trace Gas Measurement Techniques	Station comparison RR/flasks/ads. tubes	Provision of target concentrations	Every four years	Station have to report target gas concentrations
	Comparison using mobile reference instruments	Provision of reference instrument	Every four years	The instrument will be run in parallel with on-going measurements at the NF
	Central side-by-side comparisons.	Provision of a platform for conducting the comparisons	Every four years	At one NF or CGas-SiM unit this kind of intercomparison will be conducted
	Station audits	Auditing the performance of the measurement systems at the NFs	Every four years	Audits will conducted using traceable standards and/or reference instruments
	Survey of target and comparison results; checking compatibility	Provision of QA/QC tools to NFs	Every year	Level 0 data will be reviewed
	QC data-procedure and review	Provision of QA/QC tools to NFs	Every year	Level 1 data will be reviewed
	ACTRIS Label	Consulting NFs in procedures when applying for the ACTRIS label	once	Approval is based on achieving the DQOs for the ACTRIS variables applied for.

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Operation support on request

The operation support on request should managed by SAMU. SAMU should inform the lead unit of CGas-SiM about requests. The requests are discussed in bimonthly teleconferences of the unit heads. SAMU will then be informed about the decisions. The type of support available in CGas-SiM for support on request is shown in Table 9-2.

Table 9-2: Summary of support on request available in the CGas-SiM

Technique	Type of support	Specific support	Comments
Reactive Trace Gas Measurement Techniques	Measurement Guidelines (MGs) and Standard Operation Procedures (SOPs)	Provision of MGs and SOPs	and after each major upgrade
	Scale transfer; Transfer standards	Provision of scale to working standards used at users	and after each major upgrade
	New Instrument techniques	Testing to reference instruments	conducted at CGaS-SiM
	Training of operators and scientists	Not specific at this stage	At training centres or co-located with instrument performance workshops
	Comparison with user instruments RR/flasks/ads. tubes	Provision of target concentrations	Conducted at the user
	Central side-by-side comparisons.	Provision of a platform for conducting the comparisons	At a CGas-SiM unit this kind of intercomparison will be conducted and/or in cooperation with EUROCHAMP
	ACTRIS Label	Consulting user how to become a ACTRIS member and to apply for the ACTRIS Label	Approval is based on achieving the DQOs for the ACTRIS variables applied for.

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Section 8

Concept of the Centre for Reactive Trace Gases Remote Sensing (CREGARS)

ACTRIS PPP WP 4 task 4.1

21.2.2018

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1 Purpose of the document

This document describes the relevance, mission, requirements and obligations of the ACTRIS Centre for Reactive Trace Gases Remote Sensing.

2 Description and Role of the Centre for Reactive Trace Gases Remote Sensing

2.1 Framework

The Centre for Reactive Trace Gases Remote Sensing is one of the six ACTRIS Topical Centres (TC) organized around the main scientific themes of ACTRIS: aerosols, clouds, and reactive trace gases, each with a particular focus on either remote sensing or in situ measurement techniques.

The following documents are completing the current concept of the Centre for Reactive Trace Gases Remote Sensing (CREGARS):

- **The ACTRIS framework** is described in the following documents:
    - ACTRIS ESFRI proposal
    - ACTRIS-PPP project
    - ACTRIS Stakeholder Handbook
    - ACTRIS Science Case document
- **The general rules and principles for the ACTRIS Central Facilities** are described in the Baseline document for the Concepts of ACTRIS Central Facilities.
- **The measurements techniques operated by the ACTRIS National Facilities** for which the operation support should be offered, along with the specific requirements, are described in:
    - Technical concepts and requirements for ACTRIS Observational Platforms
    - Technical concepts and requirements for ACTRIS Exploratory Platforms

2.2 Scientific relevance

Targeted ACTRIS Variables

The Centre for Reactive Trace Gases Remote Sensing (CREGARS) must deal with total columns and/or vertical profiles of a number of atmospheric traces gases that are within the scope of ACTRIS, meaning (1) that they are short-lived climate pollutants, for which ACTRIS will provide the whole value-chain, from the raw measurement data to quality-controlled and traceable geophysical data (L2) and possibly derived higher-level (L3) data, (2) that they are solicited by a large user community, and (3) that they are not yet provided on a sustainable basis by another European Research Infrastructure (RI) or organisation. The variables that are targeted at start are total columns and/or vertical profiles of NO_2, HCHO, C_2H_6, O_3 and NH_3. Aerosol extinction profiles in the lowermost troposphere, as well as aerosol backscatter coefficient profiles and total aerosol optical depth will also be provided. Which products/species are to be provided by the 3 different techniques (FTIR, UVVIS, and O3 DIAL) as "mandatory", "optimum", or "specialising" will be specified in Section 3.1 below. The list of targeted variables will expand when the associated measurement and data analysis techniques and the user demands evolve; e.g., additional Volatile Organic Compounds like CHOCHO, C_2H_2, … may be included in the future, if funding allows.

Rationale

Observations related to reactive trace gases concentrations can be done either in-situ, at the surface or on a tower or on a moving platform like an aircraft, or by remote sensing techniques, again from the same platforms as well as from space-borne platforms. The in-situ observations provide local concentration values of the target reactive trace gases. The remote sensing techniques do not measure the concentrations directly, but they typically measure an electromagnetic spectrum from which the concentrations must be retrieved. The retrieval results generally are vertical profiles (with a variable vertical resolution) or total or partial columns of target trace gases. They are therefore better comparable to the corresponding remotely sensed satellite data than the corresponding local in-situ data, and are used extensively by the satellite community for the validation of their products. Also the atmospheric modelling communities, e.g., the ones involved in the Copernicus Atmospheric Monitoring Service (CAMS) or the ones involved in CMIP (Coupled Model Intercomparison Project) are keen on using observational data of columns and/or vertical profiles of reactive trace gases to validate the models and (re-)analyses of the atmospheric composition. Another important use of the remotely sensed reactive trace gases data is the detection and evaluation of long-term trends, which will be an important application in the Copernicus Climate Change Service (C3S).

Relevant measurement techniques

The remote sensing measurement techniques that will be considered in ACTRIS for the provision of the target variables are:

- the Fourier-transform Infrared (FTIR) solar absorption technique,
- the UV-visible Differential Optical Absorption Spectroscopy (DOAS) technique, called UVVIS hereafter, including the zenith-sky (ZS-) and the Multi-Axis (MAX-)DOAS systems,
- the LIDAR technique for trace gas vertical profiling, in particular for Ozone in the troposphere up to the upper stratosphere, also called O_3 DIAL (Differential Absorption LIDAR)

Because the techniques do not measure the variables directly, but derive (retrieve) them from spectral measurements using dedicated retrieval algorithms, both the observing systems as well as the retrieval algorithms must satisfy stringent specifications for ensuring that the retrieved products are accurate and precise, high-quality profiles or columns, and for ensuring consistency among the different contributing observation facilities.

State-of-the-art

At the international level, the reference network for high-quality remote sensing of reactive trace gases is the Network for the Detection of Atmospheric Composition Change (NDACC). This network started as a research network and evolved bottom-up. For each of the instrumental techniques involved in NDACC, among which FTIR, UVVIS and LIDAR techniques, Instrument Working Groups (IWG) guide the members operating these instruments through various Protocols (http://www.ndsc.ncep.noaa.gov/organize/protocols/) with which the members must comply. The purpose of the Protocols is to ensure the high-quality and intra-network consistency of the NDACC data.

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At present, it is the responsibility of the IWG to establish and update the Protocols and of each PI to comply with the Protocols. However tools and resources are lacking in the IWGs to verify the PIs' compliance. Several research performing organisations (RPOs) contribute to the QA/QC processes but there is no dedicated and sustainable QA/QC service provider.

Europe contributes very significantly to this Network: 45 out of 66 active NDACC Principal Investigators for O3 DIAL, UVVIS and FTIR instruments are affiliated to a European RPO. Also the governance structure of NDACC as a whole and of the IWG is such that all responsibilities are shared among a European and a non-European co-chair.

At many NDACC observatories, collocated in-situ measurements of trace gases and/or in-situ or remote sensing measurements of aerosol, or meteorological measurements are implemented. The synergy and complementarity between in-situ and remote sensing data of reactive trace gases has been the subject of collaborative investigation between both communities, e.g., in the ACTRIS-1 project by Dils et al, Atmos. Chem. Phys., 11, 6735-6748, https://doi.org/10.5194/acp-11-6735-2011, 2011, and 'Derived tropospheric column data' by Henne et al., http://nors.aeronomie.be/projectdir/PDF/D5.2_NORS_DTCD.pdf. Synergies and complementarities also exist between aerosol measurements from dedicated aerosol instruments and UVVIS MAXDOAS instruments, see e.g., Piters et al., 2012[1].

Needs for a Centre for Reactive Trace Gases Remote Sensing (CREGARS) in ACTRIS

As said above, the reactive trace gases remote sensing techniques do not measure the variables directly, but derive (retrieve) them from spectral measurements using dedicated retrieval algorithms, both the observing systems as well as the retrieval algorithms must satisfy stringent specifications for ensuring that the retrieved products are accurate and precise, high-quality profiles or columns, and for ensuring consistency among the different contributing observation facilities.

Another important aspect to be characterised for making correct use of the target products is the representativeness of the data: the remote sensing technique probes a volume of air of which the exact location and extent depend on the technique and the observational conditions. The spatial (horizontal as well as vertical) and temporal resolution associated with the data are directly related to the representativeness.

Therefore, consistency across the RI regarding the reactive trace gases remote sensing data products and their characterisation, including the evaluation of the full uncertainty budget including the representativeness error, requires agreements about instruments and their set-up and operation, as well as standardized retrieval algorithms and agreed procedures for uncertainty and representativeness evaluation.

The Centre for Reactive Trace Gases Remote Sensing (CREGARS) shall serve the need to prescribe and support the instrumental set-up, operations, and retrieval and uncertainty evaluation procedures to achieve harmonised, high-quality, well-characterised remote sensing measurements of the targeted selection of reactive trace gases at the National Facilities (NFs), and to assure and control the quality of the reactive trace gases remote sensing data that will be submitted to the ACTRIS Data Centre.

[1] Piters, A.J.M., et al, Atmos. Meas. Tech., 5, 457–485, 2012, doi:10.5194/amt-5-457-2012

As stated above, NDACC has already established various such protocols for measurements, instrument intercomparisons, data validation and data handling (see http://www.ndsc.ncep.noaa.gov/organize/protocols), however without any guarantee sustainability.

Secondly, additional target- and instrument-specific procedures are required to ensure the intra-network consistency and the long-term quality and homogeneity of the data in the database. E.g., in the Infrared WG (IRWG) and UVVIS WG, work has been done to harmonise the retrieval strategies for HCHO and NO_2 in the context of the S5P satellite validation project, but there is no sustainable follow-up of this effort. The establishment and maintenance of the procedures is another role for the Topical Centre.

Thirdly, the NDACC protocols are quite generic. The provision of tools that support the National Facilities and serve users to comply with the generic protocols and more specific guidelines established in ACTRIS is a third role for the Topical Centre. For example, the CREGARS must provide and maintain verified data retrieval software and associated templates.

Fourth, the TC must contribute to the education of future instrument operators and data providers by providing didactic material and dedicated support (including training) upon request and according to available resources.

For now, there is no official centre that is already operational in the ACTRIS sense. However, as described above, some services that the Centre for Reactive Trace Gases Remote Sensing must provide, are already provided on a voluntary or project-wise basis, and according to available resources, by some RPO involved in NDACC. This implies that currently the need for these services is well recognised, the procedures behind the services do exist in many cases and are known or are being established in the context of short-term projects[2], but the provision of the services is done on an ad-hoc basis and not guaranteed on the long-term in a sustainable manner. This implies that the long-term quality of the remote sensing data of reactive trace gases is not guaranteed in a sustainable manner. The Centre for Reactive Trace Gases Remote Sensing will fill this gap for the ACTRIS target species.

Mission

The mission of the Centre for Reactive Trace Gases Remote Sensing is to offer operational support to ACTRIS National Facilities operating FTIR, UVVIS spectrometers or LIDARS (O_3 DIAL).

Additionally, the Centre for Reactive Trace Gases Remote Sensing should offer specialized services for the above instruments and related ACTRIS variables, to ACTRIS users of various types: academia, research organisations, business, industry, and public services.

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[2] On top of existing NDACC Protocols, recent and currently running EU projects like the FP7 projects NORS (nors.aeronomie.be) and QA4ECV (qa4ecv.eu) and the H2020 project GAIA-CLIM (gaia-clim.eu) include the establishment of quality assurance and harmonisation procedures, as well as procedures for establishing traceability to standards. Also the contract CAMS-27 will implement QA/QC procedures for the rapid delivery data stream from NDACC partners to CAMS.

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3 Operation support provided to ACTRIS National Facilities

The operation support provided by the Centre for Reactive Trace Gases Remote Sensing are:

a) procedures and tools for quality assurance and quality control of ACTRIS measurements and data,
b) centralised processing from level-1 to 2 for UVVIS spectrometers,
c) transfer of knowledge and training to ACTRIS operators,
d) improvements of measurement methodologies for reactive trace gases (and aerosol if measured by the same technique).

The operation support is offered to the National Facilities for the measurement techniques described in this concept document, also listed in the *Technical concepts and requirements for ACTRIS Observational Platforms*.

The Centre for Reactive Trace Gases Remote Sensing is obliged to put in place and offer to NFs the specific operation support marked with * in this document. Other operation support described in this document is not mandatory for the TC, but recommended.

The operation support can be scheduled or on request. Participation at the scheduled activities is mandatory for the NFs. Measurements not following the mandatory actions are not considered as ACTRIS-conform and do not yield ACTRIS data.

In addition, NFs may request operation support which is not scheduled, depending on the identified need. Specific operation support offered as scheduled or offered on request is detailed in the Annex in Section 9. This annex will be updated each time it is necessary (e.g. development of new testing or calibration methods and tools).

The Centre for Reactive Trace Gases Remote Sensing should operate at the state-of-the-art, fostering the implementation of validated new techniques in ACTRIS. To sustain a high level of performance and to stimulate the advancement of new techniques and methodologies, the Centre for Reactive Trace Gases Remote Sensing contributes to expert collaboration networks like NDACC, as well as to dedicated research projects.

Therefore, the ACTRIS Centre for Reactive Trace Gases Remote Sensing will establish procedures and specifications for the ACTRIS target species that are more elaborated than they are in the more generic NDACC protocols, but always compliant with the NDACC Protocols.

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3.1 Measurement techniques covered by the Centre for Reactive Trace Gases Remote Sensing (CREGARS) and related ACTRIS variables

Measurement techniques covered by the Centre for Aerosol Remote Sensing are described in detail in: *Technical concepts and requirements for ACTRIS Observational Platforms* and *Technical concepts and requirements for ACTRIS Exploratory Platforms.*

3.1.1 FTIR solar absorption spectrometry

Typical set-up:

A high-spectral-resolution FTIR spectrometer operating in the mid-infrared spectral region (1900-4100 cm^{-1} for the minimum setup, 700–5000 cm^{-1} for the optimum setup) , and coupled to a sun tracker, preferably operated automatically or remotely controlled. The data are analysed with a standard line-by-line fitting algorithm. In order to perform high quality measurements liquid nitrogen-cooling of the detectors is necessary; preferably the liquid nitrogen filling of the detector is done automatically or remotely controlled.

Data quality:

The data quality is affected mainly by the spectral resolution and alignment of the spectrometer, the S/N ratio and possible artefacts of the recorded spectra (e.g., due to detector non-linearity), the pointing precision of the sun tracker, the temperature stability of the instrument/lab, the accuracy of the pressure-temperature profiles used as input as well as the retrieval algorithm itself and the selection of retrieval and spectroscopic parameters for each target species. FTIR solar absorption spectrometers require cloud-free conditions during the observation time, therefore the quality of the data can be affected by the sky-conditions (e.g., undetected presence of cirrus in the field-of-view).

Retrieval products (FTIR L2 data) targeted in ACTRIS:

-
- C_2H_6 and HCHO total columns (“mandatory”)
- NH3 as well as NO_2 total columns when feasible (“specialising”)
- O_3 partial and total columns when the instrument set-up is optimal (“optimum”)

3.1.2 UVVIS spectrometer

Typical set-up:

A grating spectrometer detecting scattered sunlight, covering spectral bands in the range from 300 to 550 nm, with a spectral resolution better than 1.5 nm. Spectral data are analysed with a DOAS-type algorithm. UVVIS instruments can feature different levels of complexity depending on the target data products, ranging from simple zenith-sky systems (ZS-DOAS) for stratospheric total column measurements at twilight, to thermally controlled multi-axis systems (MAXDOAS) equipped with elevation scanners and/or sun-tracking devices for daytime high-frequency tropospheric column and profile measurements.

Data quality:

The data quality is affected by the accuracy of the calibration of the spectrometer (in particular the wavelength registration and the Instrumental Spectral Response Function (ISRF)), the S/N ratio and

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possible artefacts of the recorded spectra (e.g., due to polarisation sensitivity, stray-light or detector non-linearity), the pointing precision of the elevation scanner for MAX-DOAS instruments and/or the sun-tracker for direct-sun systems, the temperature stability of the instrument, the accuracy of the a-priori profiles used as input for zenith-sky and MAX-DOAS instruments as well as the retrieval algorithms themselves and the selection of analysis settings and spectroscopic parameters for each target species.

Retrieval products (UVVIS-ZS L2 data) targeted in ACTRIS:

- O_3 and NO_2 total columns at twilight

Retrieval products (UVVIS-MAXDOAS L2 data) targeted in ACTRIS:

- O_3, NO_2 and HCHO total columns
- NO_2 and HCHO lower tropospheric profiles
- Total aerosol optical depth (AOD) at discrete UV and visible wavelengths
- Lower tropospheric profiles of aerosol extinction at discrete UV and visible wavelengths

3.1.3 O3 DIAL

Typical set-up:

Dual UV-wavelengths LIDAR, both wavelengths having different ozone absorption cross-sections. Lidar signals are collected by a telescope and spectrally separated by a spectrometer or Rmax filters.

Data quality:

The data quality is affected by the alignment of the laser beams in the telescope field of view and the S/N ratio. Lidar measurements need clear skies so the S/N ratio can be affected by the presence of cirrus clouds but the ozone profiles above or below the clouds are unaffected by the clouds.

For each measurement technique separately, it is the role of the CREGARS to prescribe the instrument requirements and operation procedures, and to provide data retrieval procedures, data characterisation procedures, and data submission protocols, as well as to provide tools to perform QA/QC of the data quality.

Retrieval products (O3 DIAL L2 data) targeted in ACTRIS:

- O_3 vertical profile
- Aerosol backscatter coefficient profile in upper troposphere and lower stratosphere

3.2 Estimation of the need

Measurement technique	**Number of instruments/groups to which the TC should provide operational support**		
	Now	**by 2025**	
		Min.	**Max.**
FTIR	0	11	17
UVVIS	0	20	30
O3 DIAL	0	4	9

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For now, there are 11 FTIR that are operated by European RPO that comply with ACTRIS requirements and that are deployed at proposed ACTRIS National Facilities. When ACTRIS will become operational, CREGARS should also provide operational support to FTIR sites that are not yet supported as National Facilities but that comply with the ACTRIS requirements and that are operated by ACTRIS member countries. Therefore, the expected maximum number of users in 2025 is 17.

As regards UVVIS instruments, there are approximately 20 UVVIS stations (SAOZ, MAX-DOAS or Pandora) that currently operate at candidate national facilities in Europe. All of these systems must benefit from the operational support proposed within the TC. By 2025, it is anticipated that the number of instruments at NFs will grow by a few more units, to a maximum of 30.

Concerning LIDARS, there are currently very few operational systems for ozone in Europe. The potential for tropospheric ozone monitoring in Europe using LIDARs would amount to about 4 to 9 stations (, Payerne, Cabauw, Potenza, …).

3.3 Timeline for implementation of the mandatory operation support

Considering the ACTRIS roadmap, CREGARS should consider the following implementation plan for the operation support.

After being selected as the Centre for Reactive Trace Gas Remote Sensing, CREGARS shall make sure that in the period 2020-2025, it

(1) Prepares and verifies all necessary software, tools and associated documentation for instrument QA/QC and site performance audits
(2) Prepares and verifies all necessary software, tools and associated tools and data for the L1 → L2 data retrieval
(3) Prepares and verifies all necessary software to perform the QA/QC of the L2 data submitted by the NFs
(4) Prepares the data flow to the Data Centre
(5) Prepares the facility(ies) for hands-on training of NF operators, for performing instrument tests and for performing tests of the S/W and the tools.
(6) Acquires an initial amount of spare parts, calibration cells, …
(7) Hires and/or designates the required scientific, technical and management personnel of the TC
(8) Prepares the internal communication tools between the TC units and with the HO/SAMU
(9) Prepares the communication tools with the NFs and the users
(10)

In addition, the UVVIS units shall

(1) prepare an operational processing capacity
(2) establish the dataflow from the TC-unit to the Data Centre
(3) acquire and prepare a traveling standard instrument
(4) prepare the calibration and intercomparison facilities

3.4 Operation support for quality assurance and quality control

3.4.1 Definition and establishment of standard measurement guidelines

For all three measurement techniques, the CREGARS must formulate initial Standard Operating Procedures (SOP) and must provide tools for supporting their implementation at the NFs, by 2021. By 2025, CREGARS must be supporting all ACTRIS beneficiaries in an operational mode.

For all instruments, the SOP and tools will evolve in the course of ACTRIS, in line with technological and scientific developments, and the evolution of the research.

[redacted]FTIR

Guidelines for the operation of the ACTRIS FTIR instruments must be established and updated as needs arise; at start NDACC IRWG Protocols will serve as a basis. These measurement guidelines or Standard Operating Procedures (SOP) must provide specific and detailed information for the operation of ACTRIS FTIR instruments for the observation of the ACTRIS target variables.

These SOP must include

- unified alignment procedures,
- procedures to perform calibration cell measurements and run the associated software (Linefit) to analyse the cell measurement for the retrieval of the Instrument Line Shape function (ILS); establish the criteria that the ILS must comply with;
- The Linefit software, that must be maintained and documented and must be available from the CF, including a user guide.

The CREGARS must also take care of providing the required sets of optical filters and instrument parameter settings (e.g., resolution, bandwidth…) for the measurement of each of the ACTRIS reactive trace gases

The CREGARS shall also have at its disposal an ACTRIS-compliant FTIR set-up as a test facility for the establishment of the procedures and as training facility for the ACTRIS beneficiaries and users.

[redacted]UVVIS

Guidelines for the operation of UVVIS DOAS instruments have been established for zenith-sky systems as part of the NDACC UVVIS IWG Protocols. More recently, procedures covering the operation of MAXDOAS instruments have been developed in the context of EU and ESA projects dealing with the development of automated and quality-controlled UVVIS trace gas measurements in support of satellite validation. Those existing guidelines and protocols must be unified and further developed to SOP for all ACTRIS UVVIS DOAS instruments.

The following key elements will be addressed:

- Procedures for ISRF determination and stray-light level determination
- Procedures for polarization sensitivity characterization
- Procedures for detector performance assessment (noise, dark current, linearity)
- For the initial calibration of new instruments, the CREGARS must provide access to a calibration centre where all necessary reference light sources, filters, positioning elements must be available.

- Specific operation parameters must also be formulated (e.g. frequency of MAXDOAS scans, which angles to use, typical accumulation time, data format, automatic QA, etc.)

[redacted] O3 DIAL

Guidelines for the operation of the ACTRIS O3 DIAL instruments must be established and updated as needed, in complement to the NDACC LIDAR protocols.

These guidelines must include:

- The comparison/harmonization of the retrieval of ozone vertical distribution from the LIDAR signals.
- The implementation of standardized definition of trace gas absorption cross-section, vertical resolution and measurement uncertainty in LIDAR retrieval algorithms
- A reference retrieval algorithm for ozone vertical distribution must be made available from the CF, including a user guide.
- Synthetic LIDAR signals must be made available from the CREGARS based on instrumental characteristics for the purpose of signal to noise ratio check.

3.4.2 Definition of measurement quality-assurance criteria and procedures

[redacted] FTIR

Building upon the network-wide protocols dealing with the requirements for instrument quality and instrument intercomparisons, and the more specific quality criteria for the FTIR instruments that have been established by the NDCC IRWG, the CREGARS must establish specific criteria that the ACTRIS measurement data must comply with as, e.g., signal-to-noise ratio, ILS criteria, stability criteria, comparability with other instruments, etc.

The TC must also establish a procedure to control on a regular basis (e.g., yearly - see Sect. 9 Annex) whether the NFs comply with the quality criteria: well-defined sample spectra must be requested for verification at the CF.

Of course, the quality criteria and associated control procedures will evolve continuously, to keep up with the technological evolution of the instruments and the research requirements.

[redacted] UVVIS

Specific quality criteria for the UVVIS zenith-sky instruments have long been established by the NDACC UVVIS WG and have, more recently, been extended to MAX-DOAS instruments. ACTRIS-specific quality criteria must be defined in terms of instrumental performance (e.g. polarisation response, signal-to-noise ratio, spectral resolution (ISRF), spectral stability generally related to thermal stability of instrument). Quality criteria must also be defined in terms of comparability level with other instruments. These must be established during intercomparison field campaigns where a large number of instruments are jointly operated. The CREGARS shall establish a reference site for UVVIS instrument intercalibrations. Such exercises should be conducted at the frequency of about one campaign every 5 to 10 years (see also Sect. 9 Annex).

Since large scale intercomparison campaigns cannot be organised very regularly (due to obvious reasons of cost and logistics), the TC must also establish a procedure to control on a regular basis (e.g., yearly)

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whether the NFs comply with the quality criteria. This can be obtained through the exchange of sample spectra to be verified at the CF. To quality assure new instruments and/or new NFs, the TC must also rely on certified travelling standard instruments which must be deployed on-site for calibration transfer.

[redacted] O3 DIAL

The CREGARS must establish guidelines to inform the ACTRIS NFs operating O3 DIAL instruments about the specific criteria that the measurement data must comply with as, e.g., signal-to-noise ratio or laser-telescope alignment procedures. The TC must also establish a procedure to control on a regular basis (e.g., yearly – see Sect. 9 Annex) whether the NFs comply with the quality criteria.

3.4.3 Development and provision of instrument-specific calibration

[redacted] FTIR

The CREGARS must be responsible for the delivery of appropriate calibration cells for the FTIR instruments operated at the NFs, and for their regular calibration and maintenance. It must maintain and distribute the S/W (Linefit) including its documentation for the analysis of the cell spectra that are used for the ILS determination.

The gas cells that are distributed to the NFs must be calibrated regularly (annually) at the TC against a well-controlled N_2O cell. To that end, the NF operators must have to turn in their calibration cells on a regular basis to the CREGARS for re-calibrating it against the reference N_2O cell.

Also the ILS measurements taken at the NFs must be submitted to the CREGARS on a regular basis (see Sect. 9) for verification.

[redacted] UVVIS

Each instrument must receive initial calibration in the CREGARS. Such calibration must include:

- Wavelength calibration based on emission lines of spectral lamps (usually gas discharge lamps).
- In-band stray light calibration based on laser lines.
- For direct-sun systems, radiometric calibration based on calibrated high power tungsten halogen lamps.
- Determination of the field of view based on a moving small light source.
- For direct-sun systems, determination of initial reference spectra from solar observations on 2-3 clear sky days.

Once the instrument is at the NF, its calibration must be checked in the following way:

- A mobile Field Calibration Tool (mFCT) will be sent to the station at least once per year to check the radiometric stability of the system.
- A mobile reference instrument (CREGARS Certified Traveling Standard) will be sent to the station and measure side by side with the local instrument to compare the final data products and provide a certification transfer. This should happen every 2-4 years depending on the station and the status of participation to large-scale intercalibration campaigns at the reference site (see Annex).

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[redacted] O3 DIAL

Since ozone DIAL vertical distribution measurements are self-calibrated, their quality is checked periodically with a traveling lidar instrument that must be provided by the CREGARS possibly through an agreement with an external partner. (An option to be investigated is to make an agreement with NASA that provided the international traveling standard instrument since the foundation of NDACC and has participated to more than 15 international intercomparison campaigns). In between intercomparison campaigns, the Centre for Reactive Trace Gases Remote Sensing must assist ACTRIS NFs in checking the quality of their measurements using comparisons with nearby independent ozone profiles, e.g. from ozone sondes or from satellite overpass measurements. These must be made available through the ACTRIS Data Centre.

3.4.4 Development and provision of in-house check-up tools

[redacted] FTIR

The Centre for Reactive Trace Gases Remote Sensing must develop some tools that can be used at the NFs to assure the quality of their measurements, e.g., standardized visualization tools to check the zero baseline and out-of-band artefacts in the atmospheric spectra, tools for doing a preliminary QA/QC check of the data before submission, etc.

The CREGARS must also be a contact point for the instrument and peripheral equipment manufacturers to make the commercially provided equipment operation and handling software and tools evolve in line with the needs of the ACTRIS FTIR community.

And as mentioned above (Section 3.4.1.1) the CREGARS shall have an FTIR set-up at the disposal of the NF operators to experiment and become familiar with the measurement guidelines.

[redacted] UVVIS

The Centre for Reactive Trace Gases Remote Sensing must develop tools that the NFs can use themselves to assure the quality of their measurements, e.g., standardized visualization and tools to check the instrumental spectral response function of the instrument, the wavelength stability, the stability of the signal to noise ratio, etc.

The CREGARS must also be a contact point for the instrument manufacturers to make the commercially provided instrument operation and spectra handling software and tools evolve corresponding to the needs of the ACTRIS UVVIS community.

[redacted] O3 DIAL

The Centre for Reactive Trace Gases Remote Sensing shall develop some tools that the PIs can use themselves to assure the quality of their measurements, e.g., visualization of raw lidar signals, provision of standardized modules to correct for saturation of the lidar photocounting signals, Rayleigh extinction correction, gluing of analogue and photocounting signals, etc... .

The CREGARS must also be a contact point for some instrument manufacturer (e.g. laser or signal acquisition device providers) corresponding to the needs of the ACTRIS Lidar community.

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3.4.5 Development of data evaluation procedures and plausibility test

[redacted] FTIR

Common data retrieval and uncertainties evaluation software, and associated retrieval strategies are inherited from NDACC and related projects and do exist. Their evolution, including best practices for the evaluation of the uncertainties and including the selection of the appropriate reference spectroscopic data, are discussed in the NDACC IRWG, at least on a yearly basis during the annual plenary meetings. It is planned that the Centre for Reactive Trace Gases Remote Sensing will take the lead in this evolution and the corresponding discussions regarding the ACTRIS target species.

The data retrieval strategies must be established such that high-quality data are delivered for all the ACTRIS FTIR sites – knowing that the sites are located at different altitudes and are confronted with different climatological conditions. The CREGARS must therefore verify that the proposed procedures provide good results, not only for all ACTRIS FTIR sites but also for all NDACC FTIR sites worldwide, in order that the procedures established by the CREGARS can be adopted by the whole NDACC FTIR community for the ACTRIS target species.

The Centre for Reactive Trace Gases Remote Sensing must be the housekeeper of the retrieval strategies, of the master copies of the official-version retrieval codes and of the spectroscopic linelists for the ACTRIS target species. It must also verify whether the NFs have applied the strategies as expected before data submission. The CREGARS must actively maintain and enhance the retrieval software codes and their documentation.

Although the NF's are responsible for the data retrieval and the QA/QC, the NF's may delegate the data retrieval and QA/QC to the TC, if the TC has the capacity to perform it.

The CREGARS in collaboration with the ACTRIS Data Centre must also make sure that the NFs have easy access to the required auxiliary data (e.g., NCEP or ECMWF P/T profiles).

It must also provide support for automating the data analysis at the NFs in order to enable the required rapid data delivery (within one month after data acquisition).

[redacted] UVVIS

The evolution towards standardization of retrieval settings and ancillary data sets (e.g. spectral windows, absorption cross-sections, solar reference spectra, data base of reference atmospheric profiles, etc.) has started several years ago in the framework of several European projects such as GeoMon, NORS, QA4ECV and GAIA-CLIM. The most recent developments are taking place within the ESA Pandonia and FRM$_4$DOAS projects, where capacities for centralised processing of multiple instruments using common data retrieval methods, uncertainty evaluation and automated quality control are being developed. It is planned that the ACTRIS Centre for Reactive Trace Gases Remote Sensing must integrate these systems to operationally deliver the ACTRIS target species in NRT mode with a latency of 1 day. The central processing environment must also offer facilities for coherent reprocessing of historical data sets according to retrieval algorithm evolution.

Considering the large variety of the existing UVVIS instruments, data retrieval strategies must be established with enough flexibility to accommodate differences in technical performances and also the large differences in the sites themselves (altitude, location with respect to sources, cloud and aerosol regimes, etc.). The CREGARS must therefore ensure that the procedures in place in the central processing

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systems provide optimal results for a large range of sites. It is the aim that the procedures established by the CREGARS can be adopted by the whole UVVIS community worldwide (beyond the ACTRIS community).

[redacted] O3 DIAL

The evolution of the verified data retrieval and uncertainties evaluation software and retrieval strategies, including best practices for the evaluation of the uncertainties and including the selection of the appropriate reference spectroscopic data, are discussed in the NDACC Lidar WG, during the bi-annual plenary meetings. It is planned that the Centre for Reactive Trace Gases Remote Sensing will play a very active role in these discussions regarding the ACTRIS target species.

The data retrieval strategies must be established such that high-quality data are delivered for all the NDACC Lidar WG sites – knowing that the sites are located at different altitudes and are confronted with different climatological conditions. The CREGARS must therefore verify that the proposed procedures provide good results, not only for all ACTRIS lidar sites but also for all NDACC lidar sites worldwide, in order that the procedures established by the CREGARS can be adopted by the whole NDACC lidar community for the ACTRIS target species.

The CREGARS must be the housekeeper of the retrieval strategies for the ACTRIS target species, and it will verify whether the NFs have applied the strategies as expected before data submission.

3.4.6 Realization of observational site performance audits with reference samples or mobile systems

[redacted] FTIR

The audits of an NF must be done on the basis of submitted sample data:

1. The NFs must be requested to submit their ILS measurements to the CREGARS on a regular basis for the verification of the instrument alignment.
2. The CREGARS must also verify the quality of the spectral data (e.g., Signal to Noise Ratio – time series) collected from the FTIRs at the NFs on a regular basis to assess the instruments performances.
3. The data products submitted by the NFs must be verified on a regular basis for assuring their long-term homogeneity and for verifying the network consistency, e.g., through comparisons of CO_2 and/or N_2 column measurements.

Any deviation from expectations must be discussed between the TC and the FTIR PIs at the NFs, and the TC must provide guidance to improve where needed/possible.

Particular attention must be paid to:

- instrumental line shape parameters retrieved from gas cell measurements
- column measurements of known CO_2 column concentrations
- atmospheric spectra at each site for verification of zero baseline, spectral artefacts like channelling, and out-of-band artefacts

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[redacted] UVVIS

At present, UVVIS instruments are not deployed in a coordinated and systematic way, and therefore instrument performance is essentially verified during large scale intercalibration campaigns, such as the recent CINDI-2 campaign. As part of the ESA Pandonia project, mobile reference systems are being developed with the aim to use them to regularly verify instruments at the different sites of the network. Within ACTRIS, it is planned to extend this approach using certified mobile instruments designed for performance audits of both zenith-sky and MAX-DOAS systems.

Moreover the data products submitted by the NFs must be verified on a regular basis for assuring their long-term homogeneity and for verifying the network consistency, e.g., through comparisons with a global model or with climatological satellite data.

Any deviation from expectations must be discussed between the CREGARS and the NFs, and the CREGARS must provide guidance to improve where needed/possible.

Finally a more global discussion on NFs performances must continue to take place on a yearly basis during the international meetings of the UVVIS remote-sensing community.

[redacted] O3 DIAL

As mentioned in section 3.4.3.3, the quality of NF O3 DIAL measurements must be checked periodically with a traveling lidar instrument. If possible at the lidar site, simultaneous measurements with nearby balloon borne ozonesonde measurements must be reported to identify ozone profile inconsistencies. The Centre for Reactive Trace Gases Remote Sensing must support the NFs to organize and assess these periodic intercomparison campaigns.

3.4.7 Organization of regular exercises to assess the performances of the NFs, including instrument performance workshops

[redacted] FTIR

For each NF FTIR instrument, the CREGARS must perform a ‘peer review’ exercise on a regular basis. To this end, the FTIR NFs will be asked to send pictures of the setup and a sample of recorded spectra for each target species and the corresponding retrieved target gas concentrations and uncertainty budget, as well as a sample of cell spectra and the corresponding ILS parameters, to the CREGARS. The scientific expert at the CREGARS must verify the quality of the spectra and of the retrieved products and their characterisation, by making an independent retrieval at the CREGARS. The CREGARS must then provide feedback to the NF, including recommendations for improvements and possibly for re-processing of data as appropriate.

The CREGARS must have the capacity to do one complete peer review exercise every two years – this will determine the schedule per NF. Additional random checks can be done if a need appears.

[redacted] UVVIS

The main formal assessment process for UVVIS instruments must be based on the participation to large scale intercalibration campaigns, to be organized at the approximate frequency of one every 5 years. The main requirements for a suitable infrastructure hosting such campaigns are (1) the capacity to accommodate a large number of instruments and teams in a single place, (2) to provide a widely open field of view at the horizon in many azimuthal directions and (3) to be equipped with a large set of relevant ancillary measurements.

For each NF UVVIS instrument participating to an intercalibration campaign, the CREGARS must perform a formal peer-reviewed assessment based on pre-established comparison procedure involving calibration steps and in-the-field measurements following a strict acquisition protocol. Typically, intercalibration campaigns must be conducted over a period of two weeks of measurements, weather-permitting; a semi-blind intercomparison protocol must be applied.

For logistical and cost reasons, intercalibration campaigns at the reference site can only be organized at the frequency of once every 5-6 years. As a consequence, an alternative certification approach must be offered for newly installed sites based on the use of certified travelling standard instruments. Additionally, procedures relying on the exchange of raw spectra to be evaluated by the CF will be used. The results of the performance analyses must be discussed at specific workshops on a yearly basis.

[redacted] O3 DIAL

Regular workshops must be organized in order to train the ozone lidar operators to the latest improvement in the hardware and software of ozone lidar systems. In addition, the technical expert at the TC must check each individual lidar profile submitted to the ACTRIS data centre and compare it to nearby ozone profile measurements with adequate methodology. The TC must provide feedback to the NF with recommendation for improvement if needed.

3.4.8 Contribution to documentation and traceability of level 0 to level 3 data products

[redacted] FTIR

The CREGARS must make use of traceability diagrams and associated documentation for the FTIR data products that have been developed in the EU H2020 GAIA-CLIM project (see http://www.gaia-clim.eu/page/ftir-traceability-diagram) to document the traceability of the L0 to L3 ACTRIS FTIR data products. The diagrams must be further completed and updated in agreement with the progress made in the context of ACTRIS. For now, the traceability diagrams cover from L0 to L2; If L3 products will be delivered to ACTRIS DC, then the traceability chains must be extended to the L3 products.

[redacted] UVVIS

The TC must make use of traceability diagrams and associated documentation for the UVVIS observations according to standards developed in the EU H2020 GAIA-CLIM and QA4ECV projects (see http://www.gaia-clim.eu/page/uv-vis-traceability-model-diagram) to document the traceability of the L0 to L3 ACTRIS UVVIS data products. The diagrams must be further completed and updated in agreement with the progress made in the context of ACTRIS.

[redacted] O3 DIAL

The TC must determine standardized procedures to document the level 0 to level 3 data products in cooperation with the ACTRIS data centre. These procedures must use standardized definitions of the vertical resolution and uncertainty of the ozone lidar profiles that have been determined by the NDACC lidar working group.

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3.4.9 Contribution to CEN, ISO, or similar standardization activities

[redacted] FTIR

The need for further standardization of the ACTRIS FTIR remote sensing products, e.g., traceability to WMO or other metrological standards, is recognized – especially for supporting research that relies on a combination of data from different techniques. There are ideas in the community to develop tools for calibration of the FTIR data products to WMO standards. By 2025, the Centre for Reactive Trace Gases Remote Sensing must develop procedures and tools to further contribute to such standardization efforts.

[redacted] UVVIS

Likewise, standardization efforts regarding ACTRIS UVVIS remote sensing products must rely on the development of dedicated tools and procedures aiming to calibrate measurements against WMO standards. This might rely on the operation of in-situ profiling techniques (e.g. sondes) allowing to establish the link between remote-sensing data and established standards. The Centre for Reactive Trace Gases Remote Sensing must contribute to the development of adequate procedures and tools necessary to this aim.

[redacted] O3 DIAL

Standardization efforts regarding ACTRIS O3 DIAL ozone profiles and other remote sensing products must rely on the development of dedicated tools and procedures, in close relationship with what is developed within the WMO GCOS Reference Upper Air Network.

3.5 Operation support for knowledge transfer and training

3.5.1 Training of operators and scientists

Training of operators and scientists who use the ACTRIS data will be provided in three ways:

- By providing didactic material, dedicated guidelines, procedures, user guides, templates, examples, etc. Much material is already available, e.g., for the FTIR and UVVIS instruments operations and data analysis at:
    i. www2.acom.ucar.edu/irwg/links,
    ii. nors.aeronomie.be/index.php/documents
    iii. ndacc-uvvis-wg.aeronomie.be/tools.php
    iv. http://pandonia.net/docs/ http://www.gaia-clim.eu/page/deliverables.

  However, the existing material is not centrally available nor maintained/ updated, therefore the ACTRIS CREGARS must ensure the centralized availability and maintenance of the material and develop missing material as needs arise.
- By providing hands-on training upon request by an ACTRIS PI – if resources permit. Such hands-on training is already provided now by some RPO operating an FTIR, UVVIS or O_3 DIAL on a voluntary basis.
- By having annual workshops during which new or updated procedures, tools, etc. will be presented.

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In case of significant updates to any of the measurement or data analysis procedures, the CREGARS should judge the appropriateness of organizing a dedicated workshop for training the PIs and staff at the NFs. Such workshops must be open to the concerned community, at the world-wide scale.

3.5.2 Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs

The needs to setup new measurements sites and observational capabilities are driven by the distribution of the sources of the trace gases that can be monitored by reactive trace gas remote sensing instruments. It is essential that monitoring sites sample areas close to emission sources, but also background/rural and semi-rural/sub-urban conditions must be met. The characteristics of both natural and anthropogenic sources must be considered in the process of defining new national facilities. In order to provide informed consultancy on the setting up of new observational sites, the CREGARS will use model-based sources of information (e.g. 3D chemical transport models, inverse modelling, statistical methods, evaluation of representativeness areas) as well as satellite data to identify the most relevant observational gaps. Information must be provided to the ACTRIS beneficiaries and users in the form of time-dependent maps of the different trace gases, which will help to assess the relevance of proposed new observational or exploratory platforms.

Examples of such evaluations can be found, e.g., in D1.10 and D1.11 of the GAIA-CLIM project (http://www.gaia-clim.eu/page/deliverables).

The role of the CREGARS must be to maintain the contacts with the research communities and industrial partners to provide a forum for discussing opportunities for new instruments, new observation or exploratory platforms, and possibly to solicit research partners to perform some dedicated studies in support of the evolution of the reactive trace gases remote sensing component of the Research Infrastructure.

3.6 Operation support for improvement of measurement methodologies

3.6.1 Testing of new measurement instruments and procedures

If a new or upgraded instrument is proposed as alternative for certified ACTRIS instruments, the CREGARS must assess its performances by organizing an intercomparison campaign during which the new / upgraded instrument will be co-located with the reference ACTRIS instrument at the CREGARS and in which the TC will play the role of independent referee.

In particular for the UVVIS instruments:

First an initial calibration must be performed in the CREGARS Calibration Centre, which must cover wavelength registration, stray-light characterization, ISRF and field of view determination and radiometric calibration. Further evaluation of the instrument performance must be regularly obtained through participation to intercalibration campaigns (once every 5 years) and/or through on-site comparison with the CREGARS certified traveling standard instrument. This should happen every 2-4 years depending on the station.

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3.6.2 Development of strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime

[redacted] FTIR

For FTIR, it is not possible to have a backup instrument at the CREGARS, but some spare parts like a laser, optics components, and alignment tools... must be available for the ACTRIS beneficiaries. Especially the special optical filters that are required with each FTIR instrument must be available from the CREGARS that must care for grouped purchases. Similarly, the calibration cells must be provided by the CREGARS. Also spare mirrors for the sun tracker might be worthwhile to have at the CREGARS (although these are less standardised). The NFs should reimburse the CREGARS for parts that they obtain from the CREGARS, probably in-kind.

[redacted] UVVIS

It is generally not possible to plan for backup instruments at all sites. However different strategies can be developed to reduce breakdown and maintenance downtime at remote or demanding sites. In particular, it is a common practice to equip remote Antarctic stations with backup instruments (or alternatively key spare parts). Another approach is to operate multi-channel instruments having overlaps in key spectral regions (e.g. the visible blue range where NO_2 is retrieved). This provides an inherent duplication of the measurements reducing the risks of interruption in case of instrumental breakdown affecting only one channel. For zenith-sky sites at Northern latitudes, repair is guaranteed within less than two months and full replacement possible within a six-month delay. The possibility to borrow a spare instrument during the repair period is also offered.

[redacted] O3 DIAL

Considering the cost of O3 DIALs, it is not possible to have a backup instrument at the CREGARS. However optical and electronic parts that could serve as a back-up for NFs in case of breakdown must be available at the CREGARS.

3.6.3 Development of new technological products and methods

New measurement techniques, technological products and methods are developed by the Centre in collaboration with the NFs. Depending on the situation, the Centre may recommend to the ACTRIS RI Committee to decide on the implementation of such new techniques at the RI level. The Centre has no obligation to develop the full set of operation support for such new techniques, unless they are embraced by ACTRIS and implemented as part of the National Facilities.

[redacted] FTIR

The TC must keep contact with the FTIR instruments manufacturers for a bi-directional exchange of information: new developments by the manufacturer will first be assessed at the TC, and vice-versa, the TC will pass on to the manufacturer demands from NF PIs for improvements that appear useful for the whole ACTRIS community. Instruments manufacturers will be invited by the TC to the annual workshops to discuss instrument evolution. Similarly technological developments proposed by individual NFs must be assessed by the CREGARS; if the development is validated, the CREGARS can suggest a path towards implementation at all NFs equipped with an FTIR instrument and/or towards commercialization.

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The evolution of measurement guidelines and data analysis procedures must follow a similar path: initial assessment at the CREGARS and –when the findings are positive – adoption of a path towards acceptance by the CREGARS and implementation at all NFs equipped with an FTIR instrument.

The CREGARS – in collaboration with the ACTRIS community and ACTRIS users – can investigate the option to include additional target species in the list of mandatory ACTRIS trace gases. If such option is agreed by the ACTRIS member countries and the associated funding is secured, it shall develop the required additional procedures and guidelines, and design a roadmap towards implementation at all NFs equipped with an FTIR instrument.

[redacted]UVVIS

It is anticipated that UVVIS instruments will continue to be further developed with the aim to improve their performance and reliability as well as the range of the retrievable data products. E.g. polarization channels might be added to current systems in order to increase their information content for aerosol retrieval. Such developments will typically take place within research organizations, in contact with the TC. The relevance of newly developed techniques must first be assessed at the TC before being transferred to operational instruments and/or central processing systems. The progress with respect to new instrumental developments must be reviewed during annual workshops in order to plan for appropriate and timely evolution of the baselines in place at the TC.

[redacted]O3 DIAL

The TC must keep contact with laser source and electronic cards manufacturers in order to follow all technical developments linked to the lidar technology. New developments are presently made concerning the retrieval of geophysical parameters from the lidar signals using the Optimal Estimation Method (OEM). The TC must follow these developments and if they are found suitable for ozone profile retrieval, a standardized algorithm based on this method must be proposed to the users.

In all cases, new developments that are 'validated' at the CREGARS and for which a roadmap towards implementation has been drawn, must first be proposed by the CREGARS to the ACTRIS RI Committee and Council. Upon approval, the CREGARS must take all the necessary measures for its implementation.

3.6.4 Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies

When new Radiative Transfer developments or improved databases (e.g., for spectroscopic reference data) or new insights in the measurement and data analysis processes become available in the remote sensing community, the TC must contribute to the verification of the impacts of the new/improved knowledge on the ACTRIS data products and upgrade the retrieval algorithms as appropriate, after discussion and consensus agreement in the wider remote sensing community.

If such upgrades happen, the TC must support the NFs to implement these changes and provide updates to the procedures and documentation including the didactic material to maintain compliancy with the new developments. Development of level 3 products and exploitation of instrument synergies require research activities that will be carried out in the context of dedicated R&D projects. As soon as a project comes to a conclusion, and the product becomes mature for operational delivery, the CREGARS must study how this product can be implemented in ACTRIS and what the associated cost would be. The results

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of this study must then be presented to the ACTRIS RI Committee and Council where the decision to implement it will be taken.

4 Services provided to ACTRIS users

The services that CREGARS should provide to ACTRIS users is of the same nature as the operational support provided to ACTRIS NFs. In particular, ACTRIS users will have free access to ACTRIS data, and to the same digital tools and software and associated documentation that CREGARS provides to the ACTRIS NFs. For other types of service that require dedicated manpower from the CREGARS like training, QA/QC, site performance audits…) or services that imply delivery of hardware (spare parts…) the user shall submit a request to HO/SAMU. The request shall be evaluated taking into account the scientific justification and the capacity of the CREGARS.

In the case of the CREGARS, the expected users are:

- The members of the NDACC FTIR, UVVIS and O3 DIAL communities that comply with the ACTRIS requirements
- The candidate NDACC FTIR, UVVIS and O3 DIAL PIs that agree to comply with the ACTRIS requirements
- Any FTIR, UVVIS or O3 DIAL operator who is willing to comply with ACTRIS requirements.

The above users are essentially academic or public service users.

Other users from industry or the business world may request access to CREGARS services; their requests shall be evaluated by HO/SAMU the same way as for any other user.

Access is regulated by both the ACTRIS access policy and the ACTRIS data policy, respectively.

4.1 Estimation of the need

Type of ACTRIS user		Number of users to which ACTRIS is providing services		
		Now	by 2025	
			Min.	Max.
Academia	FTIR	0	14	33
	UVVIS	0	30	40
	O3 DIAL	7	7	7
Business		…	…	…
		…	…	…
		…	…	…
Industry	FTIR	0	0	1
	UVVIS	…	…	…
	O3 DIAL	…	…	…
Public services		…	…	…
		…	…	…
		…	…	…

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The estimated minimum number of users of the CREGARS FTIR units is based on the current number of NDACC FTIR operated by non-European countries and the number of planned NDACC FTIR that are compliant with ACTRIS requirements. The maximum number takes into account the additional number of TCCON FTIR instruments operated worldwide. The manufacturer of the standard NDACC and TCCON FTIR instruments may also become a user.

The number of users of the CREGARS UVVIS units might potentially reach 30 to 40 by 2025 (see section 4).

In the USA a network of five tropospheric ozone lidars has been established in the recent years: they may become users of the CREGARS O3 DIAL unit.

4.2 Provision of measurement quality assurance and quality control procedures and tools

Generally speaking, the CREGARS will offer the same services to the ACTRIS users as the operational support offered to ACTRIS beneficiaries as described in the previous chapter, - at least to the academic/research users affiliated or candidate members of NDACC -, but these services will be offered upon request and will depend on the available resources. Moreover, the services will not necessarily be free of charge.

4.3 Instrument-specific calibration

All calibration tools and procedures described in the previous chapter will be available to ACTRIS users, upon request and as a function of the available resources. The participation to intercomparison campaigns and a site visit with a mobile standard instrument will also be offered to ACTRIS users, upon request and resources permitting. Moreover, the services will not necessarily be free of charge.

4.4 Knowledge transfer and operator training

Training workshops are open to all ACTRIS beneficiaries and users. Dedicated operator training and knowledge transfer will be accessible to ACTRIS users upon request, resources permitting.

Costs for participation or dedicated service may be charged to ACTRIS users (to be decided).

4.5 Improvement of measurement and retrieval methodologies for aerosols, clouds, and reactive trace gases

ACTRIS users requesting more advanced measurements and retrieval methods will have to justify their requests (research arguments). The CREGARS will evaluate the feasibility of the request, in terms of resources (manpower effort, costs), of technical feasibility, and of future perspectives, in consultation with the NFs that are involved. If the request turns out to be acceptable, the CREGARS together with the involved NFs will provide the service, but possibly charge for it.

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5 Governance and management structure of the Centre for Reactive Trace Gases Remote Sensing

The Units of the Centre for Reactive Trace Gases Remote Sensing shall be organized according to the specific role of the TC, assuring that the TC complies with the requirements and obligations described in sections 6 and 8 of this document, and considering the general principles described in the *Baseline document for the concept of the Central Facilities*. The Centre for Reactive Trace Gases Remote Sensing shall be organized such that:

- It has a well-defined structure of Units,
- It has a well-defined decision-making process,
- It is coordinated by a TC Director and managed by a TC Management Board, which consists of the TC Director and the TC Unit Heads,
- It has clear and cost-efficient task sharing between the Units,
- It has a risk management strategy,
- It participates in the ACTRIS decision making by sending representative(s) to the ACTRIS legal entity bodies, e.g. to the RI committee.

6 Requirements for the Centre for Reactive Trace Gases Remote Sensing.

6.1 General requirements

In order to be labelled as the Centre for Reactive Trace Gases Remote Sensing, the candidate shall:

- Commit for long-term operation, at least 10 years starting with the next year after the implementation as a CF,
- Set-up an appropriate structure of Units, to ensure an adequate functionality of the CF, cost-effective operation, and scalability with respect to the user demands and advancement of the state-of-the art technology,
- Demonstrate the capacity (in terms of material and personnel resources), to ensure the provision of the needed services and operation support, as described in section 6.2
- Provide a feasible implementation and operation plan for the first five years, starting with the next year after the selection as CF,
- Commit to provide a minimum amount of user services, as described in section 4
- Commit to provide the mandatory operation support to the ACTRIS NFs, as described in section 3.

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6.2 Technical requirements

6.2.1 Facilities

The CF should have available:

I. For the **FTIR** component of the CF:

I.1. a standard certified ACTRIS FTIR set-up (FTIR instrument coupled to a solar tracker and equipped with the required peripherals (Liq. N2 filling system, dry air flushing,) that complies with the ACTRIS requirements, that is operational and that can be used to perform some tests and hands-on training. This implies that some optical test equipment and expertise in FTIR spectrometry are also available, and that the instrument is not committed to continuous operations as part of a NF;

I.2. the equipment to align the FTIR instrument according to the standard alignment procedures that are mandatory in ACTRIS;

I.3. the equipment and resources to test and deliver calibrated cells to the NFs as well as the equipment and resources to re-calibrate these cells on a regular basis to a well-calibrated N_2O gas cell;

I.4. The required IT infrastructure to develop and verify upgrades of the standard ACTRIS FTIR retrieval software, retrieval strategies and associated tools, like Linefit, GEOMS HDF data formatting tools, data visualization tools, etc.;

II. For the **UVVIS** component of the CF:

II.1. Standard certified reference UVVIS instruments for MAX-DOAS and zenith-sky instrument types

II.2. A Calibration Centre equipped with all necessary light sources and optical elements necessary to characterize UVVIS instruments, for ISRF, wavelength registration, stray-light, polarization response, field-of-view, elevation scanner/sun-tracker accuracy

II.3. Delocalized central processing units dedicated to MAX-DOAS and zenith-sky data processing with Rapid-Delivery capabilities

II.4. The required IT infrastructure and IT and scientific expert skills to develop and verify upgrades of the standard ACTRIS UVVIS retrieval codes, retrieval strategies and associated tools, data formatting tools, data visualization tools, etc.;

II.5. The required expertise to develop, verify, upgrade and maintain retrieval strategies for the current and potential future ACTRIS target species

II.6. A facility allowing for the intercalibration of a large number of UVVIS instruments (>35). This facility should be equipped with all relevant ancillary measurements (sun photometer, in-situ monitors, ceilometer, aerosol extinction profile Raman lidar, and meteorological parameters). Moreover, a wide range of viewing angles needs to be accessible for multiple instruments at the same time. Ideally, full hemispherical view and a view of the horizon at low elevation angles need to be accessible.

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I. For the **O3 DIAL** component of the CF:

III.1. Technical skills to assist DIAL O3 users in the set-up and operation of the lidar (e.g. alignment procedures).

III.2. The equipment and resources to assist NFs in case of lidar breakdown.

III.3 The required IT infrastructure to develop and verify upgrades of the standard ACTRIS lidar retrieval software, retrieval strategies and associated tools, GEOMS HDF data formatting tools, data visualization tools, etc.

6.2.2 Human resources

Skills, expertise

The CREGARS personnel should have the IT, scientific, technical and managerial expert skills required to

- Verify and maintain the instruments' performances
- perform the measurements, data analysis and data submission to the Data Centre
- develop, verify, upgrade and maintain retrieval strategies and spectroscopic reference data (linelists, cross-sections) for the current and potential future ACTRIS target species;
- assure QA/QC of the measurements, the data analysis and the data products delivered by the NFs;
- maintain documentation
- interface to the NFs, to the Data Centre and the Head Office, and maintain appropriate communication channels
- organize trainings, workshops, …
- manage the financial aspects of the CREGARS

The director of the CREGARS shall coordinate the Units that constitute the TC.

Manpower (in FTE):

In the operational phase:

Management / Administration		FTIR	UVVIS	LIDAR	TOTAL
L1 Expert Manager	FTE	0,3	0,55	0,05	0,9
L2 Qualified Officer	FTE	0,1	0,5	0	0,6
L3 Administrative assistant	FTE	0,3	0,2	0,05	0,55
Scientific / Technical					
L1 Expert Scientist	FTE	1,8	1,4	0	3,2
L2 Qualified Operator	FTE	0,1	2,5	0,2	2,8
L3 Technician	FTE	0,75	1,3	0	2,05

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6.2.3 Other requirements

1. The CREGARS should have access to at least one conference facility for organizing the training workshops.
2. Upon request by an NF operating an FTIR instrument, the CREGARS may offer to do the FTIR data processing at the CREGARS; it should therefore have this capability for at least a few NFs that do not have the resources themselves.
3. The CREGARS should have good contact with experts in laboratory spectroscopy – in order to be informed of the latest improvements to the reference spectroscopic data and/or to be able to possibly request some dedicated laboratory spectroscopy experiments or evaluations.

7 Basic criteria for the selection of the Centre for Reactive Trace Gases Remote Sensing

The applications to host the Centre for Reactive Trace Gases Remote Sensing are evaluated against a set of criteria covering:

- The **level of commitment** for long-term operation
- The **capacity** to provide the operational support and the services described in sections 3 and 4
  - The availability of the necessary laboratories, instruments, equipment
  - The availability of human resources (no., expertise)
- The **efficiency** in providing the operational support and the services
  - The feasibility of the implementation plan (costs, resources, timeline)
  - The feasibility of the operation plan (methodology, costs per service)
- The **level of maturity**
  - Status of the development of the Units
  - No. of existing users
  - Adequacy of the decision-making
  - Risk management strategy

These criteria must be detailed in the associated call documents.

8 Obligations of the Centre for Reactive Trace Gases Remote Sensing

8.1 General obligations

The following general obligations shall apply to the Centre for Reactive Trace Gases Remote Sensing while operational:

- To organize its activities in a cost-efficient way, timely, and with high quality,
- To actively participate in the governance and sustainable development of ACTRIS,
- To provide services to users, according to the access procedures, availability of time, and material resources,
- To provide operation support to the NFs, according to the identified needs, agreed schedules, and procedures,
- To implement efficient user interaction activities by:
    - Organizing workshops, to interact with users,
    - Collecting user feed-backs,
    - Maintaining the CF and ACTRIS websites,
- To document its activities, accesses provided, key performance indicators, and finances, and provide this information to the HO,
- To contribute to minimize and assess the uncertainties related to data and data products, according to their role and in collaboration with each other.

8.2 Technical obligations

8.2.1 Technical obligations in relation with the ACTRIS National Facilities

Technical obligations of the Centre for Reactive Trace Gases Remote Sensing in relation with the ACTRIS National Facilities refer strictly to the measurement techniques described in this concept document and in *Technical concepts and requirements for ACTRIS Observational Platforms.* The operation of other techniques at the NFs does not imply a technical obligation for the Centre for Reactive Trace Gases Remote Sensing to provide operation support. New techniques / instrument types are only accepted as ACTRIS instruments after the approval of the RI Committee and after the development of the associated QA procedures by the CF.

[redacted]Guidelines, quality assurance criteria and procedures

The Centre for Reactive Trace Gases Remote Sensing is responsible for the quality assurance procedures and guidelines of the ACTRIS measurements conducted at the NFs operating FTIR, UVVIS or O3 DIAL instruments. For this, the TC should implement the following operation support for each of the Measurement technique under its topics:

- Definition and establishment of standard operation procedures (as described in sections 3.4.1.1 for FTIR, 3.4.1.2 for UVVIS and 3.4.1.3 for O3 DIAL);
- Definition of measurement quality-assurance criteria and procedures (as described in sections 3.4.2.1 for FTIR, 3.4.2.2 for UVVIS and 3.4.2.3 for O3 DIAL

All the procedures, guidelines, quality assurance criteria, plausibility tests, etc. should be documented and accessible to all related NFs. Specific training sessions with the related NF operators should be organized to ensure a smooth and correct implementation of the above.

[redacted] Tools, tests and consultancy for quality control of the measurements

It is duty of the Centre for Reactive Trace Gases Remote Sensing to assist the related NFs in the quality control of their measurements by providing the following operation support for each of the measurement techniques under its topics:

- Development and provision of instrument-specific calibration (as described in sections 3.4.3.1 for FTIR, 3.4.3.2 for UVVIS and 3.4.3.3 for O3 DIAL);
- Development and provision of in-house check-up tools (as described in sections 3.4.4.1 for FTIR, 3.4.4.2 for UVVIS and 3.4.4.3 for O3 DIAL);
- Development of data evaluation procedures and plausibility test (as described in sections 3.4.5.1 for FTIR, 3.4.5.2 for UVVIS and 3.4.5.3 for O3 DIAL);
- Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs (as described in section 3.5.2 for FTIR, UVVIS and O3 DIAL);
- Testing of new measurement instruments and procedures (as described in section 3.6.1 for FTIR, UVVIS and O3 DIAL);

This operation support should be offered to the related NFs whenever there is a need, or a significant progress in the development of these tools, and accompanied by the appropriate training.

[redacted] Assessment of performances, measurement flagging

The Centre for Reactive Trace Gases Remote Sensing is mandated to assist the Data Centre and the related NFs in the quality control of the measurements and data, by:

- Realization of observational site performance audits with reference samples or mobile systems (as described in sections 3.4.6.1 for FTIR, 3.4.6.2 for UVVIS and 3.4.6.3 for O3 DIAL);
- Organizing regular exercises to assess the performances of the NFs, including instrument performance workshops (as described in sections 3.4.7.1 for FTIR, 3.4.7.2 for UVVIS and 3.4.7.3 for O3 DIAL);
- Contributing to documentation and traceability of level 0 to level 3 data products (as described in section 3.4.8.1 for FTIR, 3.4.8.2 for UVVIS and 3.4.8.3 for O3 DIAL);

The activities involving directly the NFs operating FTIR, UVVIS or O3 DIAL instruments should be scheduled by the TC and provided regularly. The corresponding NFs should participate in these activities according to the plan proposed by the Centre for Reactive Trace Gases Remote Sensing and agreed together with the ACTRIS Scientific Advisory Board (SAB).

[redacted] Transfer of knowledge and training

In addition to the training organized for the implementation of guidelines, procedures, and tools developed in support of the quality control of the measurements, the Centre for Reactive Trace Gases Remote Sensing should organize training sessions with the NFs operating FTIR, UVVIS and O3 DIAL instruments as needed (see sections 3.5.1).

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[redacted] Improvement of measurement methodologies for Reactive Trace Gases Remote Sensing

Although it is not an obligation, the Centre for Reactive Trace Gases Remote Sensing should work to sustain a high level of performance and to stimulate the advancement of new techniques and methodologies in the field of remote sensing of reactive trace gases, by:

- Development of strategies to increase the duty cycle of instruments operated at the NFs, to reduce breakdown and maintenance downtime (as described in section 3.6.2.1 for FTIR, 3.6.2.2 for UVVIS and 3.6.2.3 for O3 DIAL)
- Development of new technological products and methods (as described in section 3.6.3.1 for FTIR, 3.6.3.2 for UVVIS and 3.6.3.3 for O3 DIAL);
- Development of retrieval algorithms or tools for producing level 1 to 3 data, including the exploitation of instrument synergies (as described in section 3.6.4 for FTIR, UVVIS and O3 DIAL)
- Organizing regular events (at least once at 2 years) and other forums, in order to exchange knowledge with the NFs and other scientists
- Contributing to CEN, ISO, or similar standardization activities (as described in sections 3.4.9.1 for FTIR, 3.4.9.2 for UVVIS and 3.4.9.3 for O3 DIAL);

8.2.2 Technical obligations in relation with the ACTRIS Data Centre

I. For the **FTIR** component:
   - The data analysis algorithms are maintained by the Centre for Reactive Trace Gases Remote Sensing where the expertise is located.
   - The data processing is done at the NFs, because it are the NF operators who know best the housekeeping data, and who know best how to handle their measurement data (formats, ancillary information, etc.). Moreover, in this way, the NF keeps full responsibility for its retrieved L2 data.
     However, NFs that prefer that the L1 to L2 data processing is done at the TC can request so, and the TC can offer this if it has the required capacity; there is no obligation for the TC to offer such processing capability.
   - A site specific QA/QC of level 2 data is performed at every NF before they are transferred to the TC.
   - In an additional QA/QC step the consistency of the measurement data and of the retrieved data is done at the Centre for Reactive Trace Gases Remote Sensing, to ensure compliance with the instrument SOP and harmonised retrieval strategies and to ensure intra-network consistency.
   - The QA/QC of the data files before submission to the ACTRIS Data Centre is done at the Centre for Reactive Trace Gases Remote Sensing because it requires specific FTIR expertise. Therefore the L2 data will pass from the NFs to the TC for quality control, and then from the TC to the Data Centre. Once the QA/QC procedures of the data files to be submitted are (fully) automated, they could be transferred to the DC, as long as the required expertise is available at the DC.

II. For the **UVVIS** component:

- The data analysis algorithms and the corresponding processing software codes are developed and maintained by the CREGARS in consultation with the UVVIS scientific community.
- The retrieval algorithms and processing tools selected for operational implementation are built as community tools using open-source software freely available to the scientific community.
- The data processing is performed in the UVVIS central processing units of the CF. PIs are responsible for the operation, calibration, maintenance and performance monitoring of their instrument(s) according to SOPs defined by the CF. They are also responsible for the timely delivery of Level-1 data sets (i.e. wavelength calibrated spectral radiance spectra) are to the central processing units, using a standardized file format including all necessary metadata and ancillary data. Although the level-1 to -2 processing is performed within the CF, the PI keeps full responsibility and ownership for the delivered data. Moreover, it has full authority to stop or delay the processing at any time upon appropriateness. The level-1 data sets remain internal to the central processing units are and are not further redistributed unless explicit consent to do so is expressed by the PI.
- The basic QA/QC of the level-1 data set is under the responsibility of the PIs.
- Additional QA/QC is performed at the CREGARS, to ensure compliance with the SOPs, identify possible anomalies with respect to expected instrument performance and to ensure intra-network consistency.
- The final QA/QC of the data files before submission to the ACTRIS Data Centre is done as part of the central processing units. It is however envisaged that once the procedures will be fully validated and automated, they can be transferred to the DC.

III. For the **LIDAR** component:

- The data analysis algorithms are developed and maintained by the CREGARS where the expertise is located.
- The data processing is done at the NFs, by the NF operators, because it are the NF operators who know best the housekeeping data, and who know best how to handle their measurement data (formats, ancillary information, etc.). Moreover, in this way, the NF keeps full responsibility for his retrieved data.
- The QA/QC of the measurement data and of the retrieved data is done at the CREGARS, to ensure compliance with the instrument SOP and harmonised retrieval strategies and to ensure intra-network consistency.
- The QA/QC of the data files before submission to the ACTRIS Data Centre is done at the CREGARS because it requires specific Lidar expertise. Once these QA/QC procedures are (fully) automated, they could be transferred to the DC, as long as the required expertise is available at the DC.

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8.2.3 Technical obligations in relation with other ACTRIS Topical Centres

I. In its attempts to improve the traceability of the remotely-sensed reactive trace gas products to community standards (e.g., the WMO standards), the CREGARS shall collaborate with the Reactive Trace Gases in-situ Centre, in order to use the same standards.

II. Concerning the traceability and quality assessment of the aerosol products of the UVVIS and O3 DIAL components of the reactive trace gases remote sensing component of ACTRIS, the CREGARS shall collaborate with the aerosol in-situ and aerosol remote sensing topical centres.

8.2.4 Technical obligations in relation with the ACTRIS users

The Centre for Reactive Trace Gases Remote Sensing should commit to provide a minimum amount of user services as described in section 4.

As stated in Section 4, the CREGARS will provide the same services to the ACTRIS users than to the ACTRIS beneficiaries, but the services must be provided upon request with a different time schedule, and the charged costs may be different. The CREGARS must keep the SAMU and the Head Office informed about the services that it has provided.

8.3 Evaluation of the activity of the Centre for Reactive Trace Gases Remote Sensing

Once established and operational, the Centre for Reactive Trace Gases Remote Sensing will be annually evaluated for its performances, against the following KPIs:

No.	Criteria	Indicators	Score	Weight
1	Usefulness for ACTRIS NFs	No. of operational support units provided to ACTRIS NFs		35%
		Number of innovative updates to SOPs, documentation, QA/QC procedures, …		
		Number of publications from the ACTRIS beneficiaries		
		Average of Usefulness for ACTRIS		
2	Usefulness for ACTRIS users	No. of service units (calibration, training, data QA/QC, ….) provided to ACTRIS users		25%
		Number of ACTRIS users involved in intercomparison campaigns		
		Number of users involved in workshops		
		Number of RTGRS data units accessed at the DC		
		Average of Usefulness for external users		
3	Impact on science & technology	No. of peer-review papers that make use of ACTRIS data		25%
		Technological progress		
		Scientific progress (e.g., new target species added, enhanced accuracy/precision of a target data product, …)		
		Increase in size of the user community		
		Average of S&T Impact		
4	Integration into ACTRI-RI	Level of collaboration with other nodes and ACTRIS structures (NFs, TCs, DC, SAMU, …)		15%
		Quality and readiness of the reports		
		Average of Integration into ACTRI-RI		
Total score				

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9 List of acronyms

AOD – Aerosol Optical Depth

CF – Central Facility

CREGARS – Centre for reactive Trace Gases Remote Sensing

DIAL – Differential Absorption LIDAR

DOAS – Differential Optical Absorption Spectroscopy

FTIR – Fourier Transform Infrared Spectrometer

ISRF - Instrumental Spectral Response Function

mFCT - mobile Field Calibration Tool

MAXDOAS – Multi-Axis Differential Optical Absorption Spectroscopy

NF – National Facility

NRT – Near Real Time

QA – Quality Assurance

QC – Quality Control

SAB – Scientific Advisory Board

SOP – Standard Operation Procedure

TC – Topical Centre

UVVIS – UV-visible

UV - Ultraviolet

ZS – Zenith-Sky

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10 Glossary

ACTRIS data - are the ACTRIS variables resulting from measurements that fully comply with the Standard Operating Procedures (SOP), measurement recommendations, and quality guidelines established within ACTRIS.

- **ACTRIS level 0 data:** Raw sensor output, either mV or physical units. Native resolution, metadata necessary for next level.
- **ACTRIS level 1 data:** Calibrated and quality assured data with minimum level of quality control.
- **ACTRIS level 2 data:** Approved and fully quality controlled ACTRIS data product or geophysical variable.
- **ACTRIS level 3 data:** Elaborated ACTRIS data products derived by post-processing of ACTRIS Level 0 - 1 -2 data, and data from other sources. The data can be gridded or not.
- **ACTRIS syntheses product** (*Proper name to be defined later*)**:** Data product from e.g. research activities**,** not under direct ACTRIS responsibility, but ACTRIS offer repository and access.

ACTRIS Data Centre (DC) - the Central Facility responsible for ACTRIS data curation, preservation, and distribution of data, value-added products and tools**,** and hosting the ACTRIS data portal.

ACTRIS data originator - entity operating instruments at a National Facility or Topical Centre, resulting in ACTRIS data and delivering ACTRIS data to the Data Centre.

ACTRIS data provider - the Data Centre offering the ACTRIS data and value-added data products and tools to users.

ACTRIS digital tools and services - tailored codes and software for processing and visualization of ACTRIS data, production of ACTRIS data products, and for data analysis and research.

ACTRIS exploratory platform - National Facility (simulation chambers, laboratories, or mobile facilities) operating on campaign basis and delivering dedicated data to the Data Centre.

ACTRIS General Assembly (GA) - a council of ministry- and funding organization representatives of ACTRIS members after ACTRIS legal entity has been established, superior decision-making body of ACTRIS.

ACTRIS Head Office (HO) - a Central Facility coordinating and representing ACTRIS, and holding the statutory seat.

ACTRIS label - earmarks a data set or a measurement site as ACTRIS data or ACTRIS National Facility.

ACTRIS observational platform – ACTRIS National Facility performing long-term, regular observations and delivering standardized data to the Data Centre.

ACTRIS Topical Centres (TCs) – a Central Facility offering services and operation support for QA/QC of measurements and data (including training, calibration, QA/QC tools, and development of standard operation and evaluation procedures)

ACTRIS variables - the measured atmospheric variables as described in the ACTRIS Data Management Plan[3].

Central Facility (CF) - a European level ACTRIS component that offers ACTRIS data or other ACTRIS services to users as well as operation support to ACTRIS National Facilities.

Central Facility Unit – part of a Central Facility located at, and operated by a research performing organization (RPO) or by ACTRIS ERIC.

CF Director – the person responsible for the coordination and representation of a Central Facility.

CF Unit Head – the person responsible for the coordination and representation of a Central Facility unit.

CF Management Board – consists of the CF Unit Heads and the CF Director; this board manages the Central Facility.

Data curation - the activity that stores, manages and ensures access to all persistent data sets produced within the infrastructure.

Data traceability - an unbroken chain of uniquely identified process steps leading from raw data to any kind of processed data, where identification of process steps follows the data.

Interim ACTRIS Council - a council of ministry- and funding organization representatives of ACTRIS members before ACTRIS legal entity has been established (during the ACTRIS Preparation and Transition Phase), superior decision-making body of ACTRIS.

Measurement traceability - an unbroken chain of comparisons relating an instrument's measurements to a known standard, in the ideal case SI units.

National Facility (NF) - an observational or exploratory platform providing data and/or physical access to the platform within ACTRIS.

Quality assurance and control: Quality assurance is process oriented and focuses on defect prevention; quality control is product oriented and focuses on defect identification:

- **Quality Assurance (QA):** The process or set of processes used to ensure the quality of a product (e.g. data series, instrument, sample, measured value of a variable, etc.),
- **Quality Control (QC):** The process and activities of ensuring products and services meet the expectations.

RI committee – consists of up to two representatives from each Central Facility and [three] representatives from the National Facilities Assembly; the RI committee supports the (Interim) Director or Board of Directors in operating the RI.

Service and Access Management Unit (SAMU) - a part of ACTRIS Head Office facilitating the access to ACTRIS services.

User - a person, a team, or an institution making use of ACTRIS data or other ACTRIS services, including access to ACTRIS facilities.

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[3] The ACTRIS data management plan and list of variables were approved by ACTRIS-2 scientific steering committee, October 2015. These documents are expected to be refined during ACTRIS-PPP (WP5).

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11 Reference documents

Please include here the complete list of documents referenced in the text.

ACTRIS-PPP proposal

ACTRIS Data Management Plan, approved by ACTRIS-2 SSC 23 October 2015

ACTRIS Concept Documents

ISO 10012:2003: Measurement management systems — Requirements for measurement processes and measuring equipment

ISO 9000:2015: Quality management systems—Fundamentals and vocabulary

Baseline document for the Concepts of ACTRIS Central Facilities

Technical concepts and requirements for ACTRIS Observational Platforms

Technical concepts and requirements for ACTRIS Exploratory Platforms

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Annex: Provision of the operation support

Scheduled support

The CREGARS must have a repository where guidelines, training support, example data, software, input files for running the software, spectroscopic reference data, etc. are available to all ACTRIS beneficiaries and users.

Technique	Type of support	Specific support	Frequency	Comments
	Provision of measurement guidelines and software for ILS characterization	Provision of Linefit software	With any update	Available from the CREGARS repository
	Provision of retrieval strategies and software	Provision of outline of the retrieval strategy per target species	Upon every update	Available from the CREGARS repository
		Provision of the standard retrieval S/W	Upon every update	Available from the CREGARS repository
		Provision of retrieval control files and reference spectroscopic data	Upon every update	Available from the CREGARS repository
	QA/QC	QA/QC of instrument setup and measurements (operations)	Every 2 year and with any major upgrade of measurement guidelines or Linefit	Sample spectra and linefit results must be requested from each NF
		QA/QC of data analysis	Every 2 year and with any major upgrade of retrieval strategies or S/W	Sample data (L2) must be requested from each NF
		QA/QC of data products before submission to DC	Upon every delivery (at least monthly)	This process must be automated as much as possible and

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				may run at the DC.
		Verification of the calibration cells	Every 2 year	NFs must be requested to send their cell to the CREGARS for evaluation against a calibrated N2O cell.
	Training of operators and scientists		Annual workshop	Co-located with NDACC annual working group meetings

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Technique	Type of support	Specific support	Frequency	Comments
UVVIS	Laboratory calibration of instrument in CREGARS Calibration Center	Wavelength calibration and ISRF determination	Once initially	Before installation at NF
		In-band stray light calibration based on Laser sources	Once initially	
		Radiometric calibration	Once initially	
		Field of view determination	Once initially	
	Provision of measurement guidelines and associated software tools	On-site calibration and monitoring procedures	At start	
		Data acquisition protocol	At start	
	Central processing	Standardised slant column retrieval	Operational	Optimisation needed for individual (non- standard) instrument
		Standardised trace gas column and profile retrieval	Operational	
		Automated QA/QC incl. feedback to data providers	Operational	Access to dashboard displaying processing status, e-mail alerts in case of anomalies
		Generation of final products in standardised GEOMS format	Operational	

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		Rapid-delivery with latency <= 1 day	Operational	Required for satellite validation
	Intercalibration campaign	Provide assessment of performance by intercomparison	Every 5 years	Needs adequate facility to host large number of instruments
		Provide certification label for NDACC/ACTRIS operation	Every 5 years	
		Provide forum for discussion involving the whole community	Every 5 years	Forster advances in measurement technique and data retrieval

Technique	**Type of support**	**Specific support**	**Frequency**	**Comments**
O3 DIAL				

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Operation support on request

Technique	Type of support	Specific support	Comments
FTIR, UVVIS and O3 DIAL	Site performance audits with reference samples or mobile systems*	Peer review verification of NF performance at the CREGARS	NFs must be requested to provide sample L1 and corresponding L2 data – to be assessed by the CREGARS
	Training of operators and scientists*	Organization of dedicated training session at the NF or at the CREGARS	Training for operation of the instrument or training for the data analysis
	Consultancy for setting-up new observational or exploratory platforms and new instruments at the NFs*		Based on existing satellite or model analyses or model analyses upon requests
	Testing of new measurement instruments, operating procedures or data analysis procedures*	Direct comparison with the reference system or standard data analysis at the CREGARS	
FTIR	Provision of measurement guidelines and software (+ H/W) for ILS characterization	Provision of calibration cells	Spare sets must always be available to satisfy requests
		Provision of optical filters	Spare sets must always be available to satisfy requests
UVVIS	Provision of measurement guidelines and associated software tools	Provision of lines sources and optical filters	On-site ISRF, stray-light and polarization tests
		Provision of community retrieval software codes	For local processing
		Provision of level-1 data formatting tools	Support to inclusion in central processing
O3 DIAL			

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