

Deliverable 4.1: Descriptions of the workflows between ACTRIS components

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Background and purpose of this document

The overall goal of the ACTRIS Data Centre (DC) is to provide scientists and other user groups with free and open access to all ACTRIS data, complemented with access to innovative and mature data products, together with tools for quality assurance (QA), data analysis and research. ACTRIS data and products should be findable, accessible, interoperable and reusable (FAIR), and the data centre work towards fulfilling the FAIR principles. The numerous measurement methodologies applied in ACTRIS result in a considerable diversity of the data collected. In accordance with these requirements, the ACTRIS DC will be organized in 6 Units, with clear links and procedures for interaction between the data centre Units, National Facilities (NFs) and Topical Centres (TCs). The ACTRIS DC will be coordinated by the DVAS unit leader and all data is linked through the ACTRIS data portal serving as the access point to all data and related information. The units and short names are:

- ACTRIS Data Discovery, Virtual Access and Services unit (DVAS)
- ACTRIS In situ data centre unit (In-Situ)
- ACTRIS Aerosol remote sensing data centre unit (ARES)
- ACTRIS Cloud remote sensing data centre unit (CLU)
- ACTRIS trace gases remote sensing data centre unit (GRES)
- ACTRIS Atmospheric simulation chamber data centre unit (ASC)

More information about ACTRIS DC and the units are in the [ACTRIS Data Management Plan \(DMP\)](#) documents

Production of fully quality assured ACTRIS data needs to follow a well-defined workflow involving NFs, TCs and the DC. The initial workflows have been discussed and established between the ACTRIS TCs, DC and the NFs during the ACTRIS Preparatory Phase (under ACTRIS Preparatory Phase Project) to ensure cost-efficient and clear roles and responsibilities and sharing of tasks.

To guarantee traceability of data from the NFs, the data need to be associated with instrument and data quality documentation produced at the responsible Central Facilities (CFs). The workflows will include steps distributed across NFs, TCs and DC, and a web-based workflow management tool will be selected and implemented to ensure full traceability of all data production steps (ACTRIS IMP Milestone MS18 e due M12).

The purpose of this document is to provide up-to-date information on the current status of the workflows and existing open issues. This document also assists with the selection of a workflow management tool later in the ACTRIS IMP project. A first step of selection of this tool is to identify and assess the needs that the tool has to cover, and then accordingly to summarise the workflows and links between the CFs and NFs within ACTRIS.

Workflows between ACTRIS components

The [DMP](#) documents the key elements of the ACTRIS data life cycle and the plans for the data collected, processed and/or generated. The goal of the DMP is to describe the present situation of the DC that is currently in operation. Furthermore, the DMP should also describe the agreed technical solutions that are currently under implementation and outline the strategy and development needed towards making ACTRIS data FAIR at ACTRIS DC level.

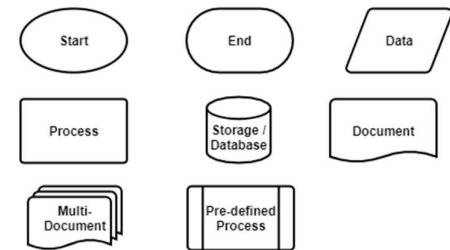
The ACTRIS DMP is an online document which is set up to be machine-actionable as a part of the FAIR data ecosystem. The DMP should be a hub of information on ACTRIS FAIR digital objects. Furthermore, the ACTRIS DMP should follow the glossary of terminology and definitions used in ACTRIS.

The initial workflows are described in annexes of the DMP. These workflows will be revised and updated during ACTRISIMP. There are still some open issues related to the workflows where distribution of tasks and responsibilities are still either not discussed yet or should be identified later in the process. These open issues will be highlighted in this document and will serve as input to meetings and interactions with TCs and NFs for the clarification of the DMP, ACTRIS IMP DeliverableD4.4 due in M46. The symbols used in the workflows are shown to the right.

Colours, indicating responsibility for task operation:



Symbols:



Workflows for ACTRIS in-situ data, and related open issues

The data management of ACTRIS in-situ aerosol, cloud and -trace gas measurements follows a common workflow. The workflow is separated into 2 branches:

- **Online observations:** Measurement done directly on sample air stream immediately after sampling, measurement reported by instrument while sample passes through or immediately after. Instrument QA by on- and off-site comparisons to standard instruments / primary standards. RRT data provision is possible and default.
- **Offline observations:** Measurement done on sample medium in which sample is collected. Sample analysis usually disconnected from sample collection in time and location. Sample handling is documented by a series of reports, leading to final data product. QA on sample handling (e.g. field blanks) and analysis (e.g. round-robin). Rapid delivery of data possible.

[Please follow this link to high-resolution workflow for in-situ data production.](#)

In the high-resolution workflow for in-situ data (above link), the white boxes show where there are different solutions on task distribution for different variables/methodologies. Accordingly, for in-situ data production and for each instrument/methodology there exist workflow implementation tables. For each workflow task, responsibilities include the following roles:

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- **Specification:** defining what is done in the task. Includes step-by-step description, with formulas (e.g Algorithm Description Document (ADD), standard operating procedure (SOP), to be provided later).
- **Implementation:** taking the ADD and SOPs turning it into software or automatic procedures, respectively.
- **Operation:** running the software on a daily basis. Includes documentation of provenance while executing software.
- **Application:** applying the software. Usually automatic, needs to be specified for manual tasks involving humans.

The tables below summarize the workflows (links to schematics provided in the table) and the open issues for each measurement technique.

1.1.1 Aerosol in-situ data

Table 1. Link to ACTRIS aerosol in-situ workflows and summary of the open issues for each measurement technique.

Instrument/methodology	Link to instrument specific workflows and involvement of NFs, TC and DCs	Open tasks to be clarified
Integrating nephelometer	Nephelometer workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> • Review procedure for level 0 data, both Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures at TC, Specification, Implementation, and Operation. • Common workflow handler for online data.
Filter Absorption Photometer	Filter Absorption Photometer workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> • Review procedure for level 0 data, both Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures at TC, Specification, Implementation, and Operation. • Common workflow handler for online data.
Mobility Particle Size Spectrometer	Mobility Particle Size Spectrometer workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> • Review procedure for level 0 data, both Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures at TC, Specification, Implementation, and Operation.

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Instrument/methodology	Link to instrument specific workflows and involvement of NFs, TC and DCs	Open tasks to be clarified
		<ul style="list-style-type: none"> Common workflow handler for online data.
Condensation Particle Counter	Condensation Particle Counter workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> Review procedure for level 0 data, both Specification, Implementation, and Operation. Documenting QC measures at NFs, Specification, Implementation, and Operation. Documenting QC measures at TC, Specification, Implementation, and Operation. Common workflow handler for online data.
Cloud Condensation Nucleus Counter	Cloud Condensation Nucleus Counter workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> Review procedure for level 0 data, both Specification, Implementation, and Operation. Documenting QC measures at NFs, Specification, Implementation, and Operation. Documenting QC measures at TC, Specification, Implementation, and Operation. Common workflow handler for online data.
Aerodynamic / Optical Particle Size Spectrometer	Aerodynamic / Optical Particle Size Spectrometer workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> Templates for level 0, 1, 2 data Review procedure for level 0 data, both Specification, Implementation, and Operation. Documenting QC measures at NFs, Specification, Implementation, and Operation. Documenting QC measures at TC, Specification, Implementation, and Operation. Common workflow handler for online data.

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Instrument/methodology	Link to instrument specific workflows and involvement of NFs, TC and DCs	Open tasks to be clarified
Aerosol Chemical Speciation Monitor	Aerosol Chemical Speciation Monitor workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> • Templates for level 0, 1, 2 data • Review procedure for level 0 data, both Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures at TC, Specification, Implementation, and Operation. • Common workflow handler for online data.
Proton-induced X-ray Emission	Proton-induced X-ray Emission workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> • Common workflow handler for offline data (LIMS). • Templates for sample handling protocols • Review procedure for level 2 data, Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures by TC, Specification, Implementation, and Operation.
Organic Tracers	Organic Tracers workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> • Common workflow handler for offline data (LIMS). • Templates for sample handling protocols • Review procedure for level 2 data, Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation.

Instrument/methodology	Link to instrument specific workflows and involvement of NFs, TC and DCs	Open tasks to be clarified
		<ul style="list-style-type: none"> Documenting QC measures by TC, Specification, Implementation, and Operation.
Organic Carbon / Elemental Carbon	Organic Carbon / Elemental Carbon workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> Common workflow handler for offline data (LIMS). Templates for sample handling protocols Review procedure for level 2 data, Specification, Implementation, and Operation. Documenting QC measures at NFs, Specification, Implementation, and Operation. Documenting QC measures by TC, Specification, Implementation, and Operation.
Scanning Particle Size Magnifier / (Neutral) Air Ion Spectrometer / Nano Mobility Particle Size Spectrometer	Scanning Particle Size Magnifier / (Neutral) Air Ion Spectrometer / Nano Mobility Particle Size Spectrometer workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> Templates for level 0, 1, 2 data Review procedure for level 0 data, both Specification, Implementation, and Operation. Documenting QC measures at NFs, Specification, Implementation, and Operation. Documenting QC measures at TC, Specification, Implementation, and Operation. Common workflow handler for online data.
Particle Size Magnifier	Particle Size Magnifier workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> Templates for level 0, 1, 2 data Review procedure for level 0 data, both Specification, Implementation, and Operation. Documenting QC measures at NFs, Specification, Implementation, and Operation.

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Instrument/methodology	Link to instrument specific workflows and involvement of NFs, TC and DCs	Open tasks to be clarified
		<ul style="list-style-type: none">• Documenting QC measures at TC, Specification, Implementation, and Operation.• Common workflow handler for online data.

1.1.2 Cloud in-situ data

Table 2. Link to ACTRIS cloud in-situ workflows and summary of the open issues for each measurement technique.

Instrument/methodology	Link to instrument specific workflows and involvement of NFs, TC and DCs	Open issues to be clarified
Integrating Cloud Probe	Integrating Cloud Probe workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> • Templates for level 0, 1, 2 data • Review procedure for level 0 data, both Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures at TC, Specification, Implementation, and Operation. • Common workflow handler for online data.
Ice Nucleus Counter	Ice Nucleus Counter workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> • Templates for level 0, 1, 2 data • Review procedure for level 0 data, both Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures at TC, Specification,

		<p>Implementation, and Operation.</p> <p>Common workflow handler for online data.</p>
Cloud Imaging Probe	Cloud Imaging Probe workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> • Templates for level 0, 1, 2 data • Review procedure for level 0 data, both Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures at TC, Specification, Implementation, and Operation. • Common workflow handler for online data.
Cloud Droplet Probe	Cloud Droplet Probe workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> • Templates for level 0, 1, 2 data • Review procedure for level 0 data, both Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures at TC, Specification, Implementation, and Operation. • Common workflow handler for online data.

Cloud Water Collector	Cloud Water Collector workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> • Common workflow handler for offline data (LIMS). • Templates for sample handling protocols • Review procedure for level 2 data, Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures by TC, Specification, Implementation, and Operation.
Cloud Aerosol Particle Sampler	Cloud Aerosol Particle Sampler workflow implementation tables	<p>Open tasks to be defined and/or implemented:</p> <ul style="list-style-type: none"> • Common workflow handler for offline data (LIMS). • Templates for sample handling protocols • Review procedure for level 2 data, Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures by TC, Specification, Implementation, and Operation.

1.1.3 Trace-gas in-situ data

Table 3. Link to ACTRIS trace gas in-situ workflows and summary of the open issues for each measurement technique.

Instrument/methodology	Link to instrument specific workflows and involvement of NFs, TC and DCs	Open issues to be clarified
Volatile Organic Compounds	Volatile Organic Compounds workflow implementation tables	<p>Open tasks:</p> <ul style="list-style-type: none"> • Integration of QC tool into overall workflow. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures at TC, Specification, Implementation, and Operation. • Common workflow handler for online data.
Nitrogen Oxides	Nitrogen Oxides workflow implementation tables	<p>Open tasks:</p> <ul style="list-style-type: none"> • Review procedure for level 0 data, both Specification, Implementation, and Operation. • Documenting QC measures at NFs, Specification, Implementation, and Operation. • Documenting QC measures at TC, Specification, Implementation, and Operation. <p>Common workflow handler for online data.</p>
Condensable Vapours	Condensable Vapours workflow implementation tables	<p>Open tasks:</p> <ul style="list-style-type: none"> • Common workflow handler for offline data (LIMS). • Templates for sample handling protocols • Review procedure for level 2 data, Specification, Implementation, and Operation.

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		<ul style="list-style-type: none"> Documenting QC measures at NFs, Specification, Implementation, and Operation. <p>Documenting QC measures by TC, Specification, Implementation, and Operation.</p>
Ozone	Ozone workflow implementation tables to be added.	<p>Open tasks:</p> <ul style="list-style-type: none"> Clarification of responsibilities with partner networks doing measurement. Clarify responsibilities for workflow tasks, Specification, Implementation, and Operation. Templates for level 0, 1 data Review procedure for level 0 data, both Specification, Implementation, and Operation. Documenting QC measures at NFs, Specification, Implementation, and Operation. Documenting QC measures at TC, Specification, Implementation, and Operation. Common workflow handler for online data.

Workflow for ACTRIS aerosol remote sensing data, and related open issues

The data management of ACTRIS aerosol remote sensing follows as a general concept a fully automatization of the data flow. It is based on fully centralized processing considering this element as the optimum and efficient procedure for full traceability, versioning and possibility of reprocessing. The data workflow guarantees the standard data provision, but it is suitable also for the NRT/RRT data provision.

[Please follow this link to high-resolution workflow for aerosol remote sensing data production.](#)

In the high-resolution workflow description for aerosol remote sensing data production (link above), each task of the process is numbered in the plot. The predominance of blue in the workflow chart is the result of the centralized processing choice for the aerosol remote sensing component. The data flow foresees interactions between NFs, TC and DC about the data ingestion in the processing chain and the QA/QC procedures.

The specific roles of NFs, TC and DC are described in a more detailed way for each task in the table below.

There are no specific open issues in the workflow. However, the timing of the Level1->Level2 process is not yet established because it is highly dependent on the QA/QC procedures to be applied. A consensus on adopting solutions which allows for releasing Level 2 as fast as possible has been reached. For achieving this objective, as many QC procedures as possible will be applied directly in the processing phase, and probably QA test at NFs will be intensified in frequency. This will be better defined in the progress of the ACTRIS IMP project.

Table 4. Link to ACTRIS aerosol remote sensing workflows and summary of the open issues for each measurement technique.

Work-flow Task ID	Short Description	Specification	Implementation	Operation
T1.A	ACTRIS-AERONET processing	CARS CF	CARS CF	CARS CF
T2.A	Data harvest	ARES DC - CNRS	ARES DC - CNRS	ARES DC - CNRS
T3.A	Storing input data on AERIS/ICARE server	ARES DC - CNRS	ARES DC - CNRS	ARES DC - CNRS
T4.A	GARRLIC preprocessing	CARS CF	ARES DC - CNRS	ARES DC - CNRS
T5.A	Data QC feedback to NFs	CARS CF	ARES DC - CNRS	ARES DC - CNRS
T6.A	GARRLIC processing	ARES DC - CNRS	ARES DC - CNRS	ARES DC - CNRS
T7.A	Processing feedback to developers for future improvements	ARES DC - CNRS	ARES DC - CNRS	ARES DC - CNRS
T8.A	Quicklook generation	ARES DC - CNRS	ARES DC - CNRS	ARES DC - CNRS
T9.A	Storing output on AERIS/ICARE server	ARES DC - CNRS	ARES DC - CNRS	ARES DC - CNRS
T10.A	Set up additional data services	ARES DC - CNRS	ARES DC - CNRS	ARES DC - CNRS
T11.A	Data import from CNR to AERIS/ICARE	ARES DC - CNR+CNRS	ARES DC - CNRS	ARES DC - CNRS
T1.B	Checking tools ACTRIS aerosol lidar	CARS CF	CARS CF	Aerosol remote sensing NFs
T2.B	Transcription and annotation of aerosol lidar data	ARES-DC - CNR	Aerosol remote sensing NFs	Aerosol remote sensing NFs
T3.B	Submission to SCC	ARES-DC - CNR	Aerosol remote sensing NFs	ARES-DC - CNR
T4.B	QA procedures	CARS CF	CARS CF	CARS CF
T5.B	QA transcription	ARES-DC - CNR	CARS CF	CARS CF
T6.B	Storing input at CNR	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T7.B	High-resolution preprocessing	CARS CF	ARES-DC - CNR	ARES-DC - CNR
T8.B	Cloud masking	CARS CF	ARES-DC - CNR	ARES-DC - CNR
T9.B	Quicklook generation	CARS CF	ARES-DC - CNR	ARES-DC - CNR
T10.B	Low-resolution preprocessing	CARS CF	ARES-DC - CNR	ARES-DC - CNR
T11.B	Optical processing	CARS CF	ARES-DC - CNR	ARES-DC - CNR
T12.B	Storing outputs at CNR	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T13.B	Data import from ICARE	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T14.B	Data export to EARLINET DB	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T15.B	Set access rights	Aerosol remote sensing NFs	ARES-DC - CNR	ARES-DC - CNR
T16.B	Data and quicklook provision	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T17.B	Data provision services	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T18.B	Archive	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T19.B	Lidar QA update	CARS CF	CARS CF	CARS CF
T20.B	Meteorological field update	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR

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Work-flow Task ID	Short Description	Specification	Implementation	Operation
T21.B	QC procedures	CARS CF	ARES-DC - CNR	ARES-DC - CNR
T22.B	Feedback to data originators	CARS CF	ARES-DC - CNR	ARES-DC - CNR
T23.B	Reprocessing SCC (redoing steps 10B-11B)	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T24.B	Photometer QA update	CARS CF	CARS CF	CARS CF
T25.B	GARRLIC reprocessing (redoing steps 2A-10A + T13.B with recalibrated photometer input data (L2) and L2 lidar data)	ARES DC - CNRS	ARES DC - CNRS	ARES DC - CNRS
T26.B	Level 2 DOI publication	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T27.B	Climatological averaging procedures	CARS CF	ARES-DC - CNR	ARES-DC - CNR
T28.B	Level3 clim DOI publication	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T29.B	Storing outputs at CNR	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T30.B	Data export to EARLINET DB	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T31.B	Set access rights	Aerosol remote sensing NFs	ARES-DC - CNR	ARES-DC - CNR
T32.B	Data and quicklook provision	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T33.B	Data provision services	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T34.B	Archive	ARES-DC - CNR	ARES-DC - CNR	ARES-DC - CNR
T35.B	Data processing and QC procedure documentation	ARES-DC - CNR & CNRS	ARES-DC - CNR & CNRS	ARES-DC - CNR & CNRS
T36.B	Annual data provision documentation	ARES-DC - CNR & CNRS	ARES-DC - CNR & CNRS	ARES-DC - CNR & CNRS

Workflow for ACTRIS cloud remote sensing data, and related open issues

The data management for the ACTRIS cloud remote sensing data follows a well-defined workflow characterised by a fully automated processing chain enabling data provision (usually) in NRT, and in principle, RRT. The automated workflow is designed to incorporate traceability (provenance) and versioning. Finalised products for publishing (non-NRT) may also involve a human aspect in the curation step.

[Please follow this link to high-resolution workflow for cloud remote sensing data production.](#)

The vast majority of the workflow steps are performed by the CLU unit. Data transfer from NF to CLU is automated, with instrument calibration being performed by CCRES (cloud radar, microwave radiometer and Doppler lidar) and CARS (automatic low-power lidar and ceilometer):

Calibration constants will then be transferred to CLU. CCRES will also define processing protocols for ancillary instrumentation typically present at cloud profiling stations such as disdrometer, raingauge, surface meteorological, radiation sensors. Automated ingestion of ancillary data will follow the same workflow steps and be performed by CLU.

Summary of open issues:

RRT data provision will likely require modification of the data transfer protocols due to the data volumes involved. Initially, this will place more onus on the NFs, but a new automated scheme for data transfer is in development.

Although a single processing chain (Cloudnet processing suite) is in action, the current data processing is not yet fully centralised at CLU, with some processing stages performed at NF. Although software versioning across CLU and NFs enables traceability for this decentralised model, it is envisaged that processing will move to the fully centralised model. RRT processing will reduce the current need for at-NF processing for most NFs.

Specific workflow for the instrument calibration procedures is not yet fully defined. This includes tasks such as calibration schedules (and repeat timescale) together with how this information will be transferred from CCRES/CARS to CLU. The goal is for automated transfer, update and reprocessing where required, but responsibility for each segment in this process is yet to be assigned between CLU/CCRES/CARS.

The responsibility for the tasks involved in housekeeping data and QA/QC feedback is also yet to be fully assigned between CLU/CCRES/CARS. As these tasks become automated, more responsibility will move to CLU, since the automated processing will be performed at CLU.

Workflow for ACTRIS trace gas remote sensing data, and related open issues

Summary of open issues in the workflow is lacking by 21 September 2020.

[Please follow this link to ACTRIS trace gases remote sensing data centre unit \(GRES\) data life cycle and high-resolution workflow diagram – FTIR.](#)

[Please follow this link to ACTRIS trace gases remote sensing data centre unit \(GRES\) data life cycle and workflow diagram – LIDAR.](#)

[Please follow this link to ACTRIS trace gases remote sensing data centre unit \(GRES\) data life cycle and workflow diagram – UV-VIS.](#)

Workflow for ACTRIS atmospheric simulation chamber data, and related open issues

The data management of ACTRIS Atmospheric Simulation Chambers (ASC) follows a common workflow.

[Please follow this link to workflow for Atmospheric Simulation Chamber Data Centre Unit \(ASC\).](#)

The workflow for Atmospheric Simulation Chamber data is structured in two sections: The first section provides information on the generation of metadata concerning the protocol used for the experiment in the Atmospheric Simulation Chambers. The second one describes the workflow for the generation of data and associated metadata for the instrumental part. Concerning the latter section, a large variety of instruments may be used during the experiments for the measurement of trace gases, aerosols and clouds and are thus linked to the corresponding Topical Centres. These instruments have been separated in two categories, leading to two branches in the workflow:

- The “base” instrumentation includes instruments for which standard protocols for data acquisition and treatment have been defined by TCs, such as gas monitors (ozone, NO_x ...), PTR-MS, aerosol optical counters, SMPS. However, the exhaustive list of “base” instruments has not been defined yet and will be established in concertation with the TCs.
- The “specific” instrumentation includes instruments for which standard protocols have not been defined by TCs. It includes non-commercial and cutting-edge instruments for very specific and/or challenging measurements, for example for short-lived species (free radicals).

In the same way, two types of experimental protocols have been defined leading to two other branches in the workflow:

- “Classic” protocols which correspond to experimental protocols that are commonly used by the NFs. The exhaustive list of “classic” protocols has not been defined yet.
- “Original” protocols which are developed to address emerging issues and for which no recommendations have been or will be proposed.

The current workflow which is accessible through the link above may be too broad and reflects only general principles. The workflows haven’t been precisely defined for each instrument or for each type of experiment so far. A dedicated workshop that brings together PIs of NFs, TCs and DC was planned in March 2020 to discuss about these issues. However, due to the sanitary crisis, it has been cancelled and postponed to the fall. So, a number of open issues remains:

- The list of “base” instruments has to be established in concertation between NFs, TCs and TCs.
- More specific workflows have to be defined for each “base” instrument in concertation between NFs, TCs and TCs. In addition, several issues should specifically be answered, e.g.: Are the guidelines established for observational platforms compliant with experiments in simulation chambers? Can the data treatment be performed at the NFs level but using

common software and procedures? What are the minimum requirements in terms of traceability, quality control and quality assurance for specific instrumentation?

- The list of “classical” protocols and the protocols themselves have to be established. The work is currently under progress within EUROCHAMP-2020 project and should continue within ACTRIS-IMP under the supervision of the ACTRIS simulation chamber committee.