Milestone M5 (M1.6)

Data management for online source apportionment ST

RI-URBANS

Research Infrastructures Services Reinforcing Air Quality Monitoring Capacities in European Urban & Industrial AreaS (GA n. 101036245)

By

CNRS & INERIS

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Milestone M5 (M1.6): Data management for online source apportionment ST

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Work package (WP)	WP1 Novel AQ metrics and advanced source apportionment STs for PM, and nanoparticles
Milestone	M5 (M1.6)
Lead beneficiary	CNRS
Means of verification	Data management for online source apportionment service tool, visualization interface ready
Estimated delivery deadline	M12 (30/09/2022)
Actual delivery deadline	29/09/2022
Version	Final
Reviewed by	WP1 leaders and project coordination team
Accepted by	RI-URBANS Project Coordination Team
Comments	This milestone addresses T1.2 from WP1 on the development of the source apportionment service tool (SA-ST), and more specifically the corresponding data management (DM) for real-time orchestration. SA-ST decomposed into two independent tools: one for organic aerosols (OA) measured by Aerosol Chemical Speciation Monitor (ACSM), and one for Black Carbon (BC) derived from AE33 aethalometers. They will be further implemented at different pilot sites, as part of WP4 (T4.1). Here, the general scheme of data management corresponding to near real time SA-ST; as well as the detailed information for each tool (ACSM & BC); and the visualisation interface that has been set up; are described.

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1. About this document

This milestone addresses T1.2 from WP1 on the development of the source apportionment service tool (SA-ST), and more specifically the corresponding data management (DM) for real-time orchestration. SA-ST decomposed into two independent tools: one for organic aerosols (OA) measured by Aerosol Chemical Speciation Monitor (ACSM, Ng et al., 2011), and one for Black Carbon (BC) derived from AE33 aethalometers (Drinovec et al., 2015). They will be further implemented at different pilot sites, as part of WP4 (T4.1).

This document describes: 1) the general scheme of data management corresponding to near real time SA-ST; 2) the detailed information for each tool (ACSM & BC); and 3) the visualisation interface that has been set up.

This is a public document, available in the RI-URBANS website. The document will be distributed to all RI-URBANS partners for their use and submitted to European Commission as an RI-URBANS milestone M5 (M1.6). This document can be downloaded at https://riurbans.eu/work-package-1/#milestones-wp1

2. General objectives

Atmospheric aerosol particles deteriorate air quality particularly in the urban environment. With on-line and off-line aerosol chemical measurements, the measured aerosol composition can be connected to specific aerosol sources. Such analysis allows the local air quality authorities to:

- Identify the critical emission sources and processes in their environment.
- Selectively impose actions that reduce specific emissions and thus improve local air quality, for example related to traffic or small-scale wood combustion.

Utilizing the on-line observations with the ACSM and aethalometer, the aim in RI-URBANS is to develop a service tool that will provide near-real time (RT) source apportionment (SA). RT OA source apportionment will be based on the RT procedure developped by Chen et al. (in review), and already tested on three different european cities (Zurich, Paris and Athens). During the T4.1 pilot phase (January 1st, 2023 to December 31st, 2023), the OA SA-ST results will be regularly compared to manual SA analyses, individually performed by the pilots, following an harmonized protocol. RT BC source apportionment will be performed following the automatization of the algorithm proposed in Sandradewi et al. (2008).

Here we describe the data management structures pertinent for the ST development.

In order to rationalize computational constrains, and in an effort of performing harmonized analyses, source apportionment calculations were chosen to be centralized, and not carried out at each individual site. The main flow of information is therefore composed of four different main steps:

- Data acquisition (generation of raw data, and formatting if required)
- Data transfer (onto the database)
- Source apportionment calculation
- Visualisation

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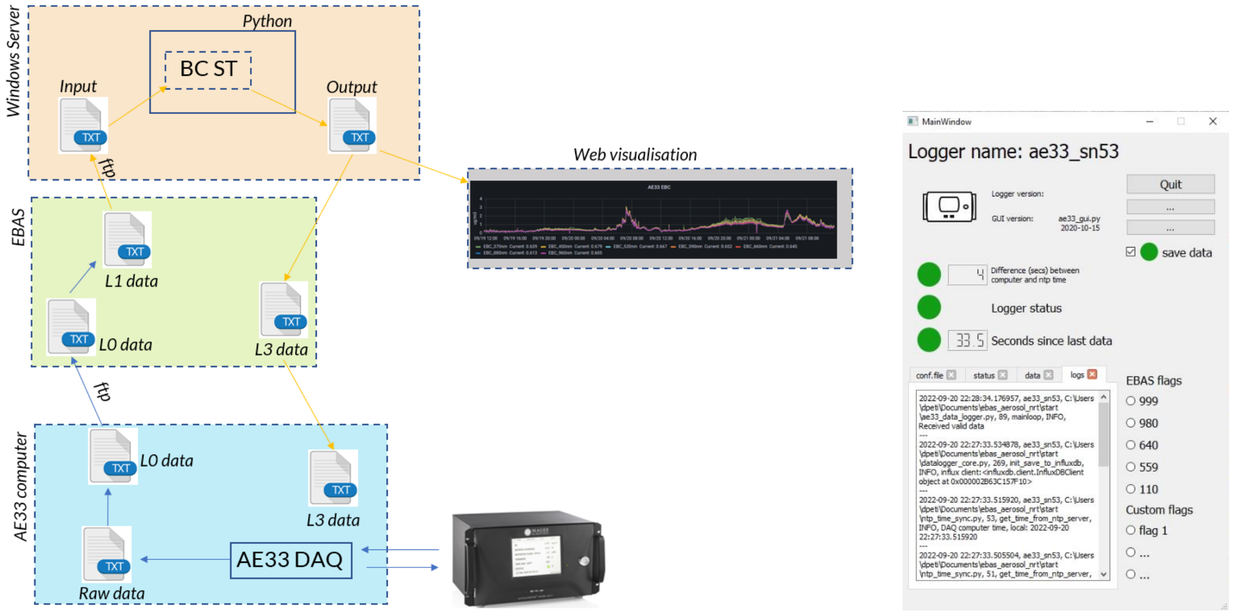
3. Data management for organic aerosols and black carbon source apportionment

3.1 Black Carbon

The data management workflow for BC SA-ST is mainly based on the current ACTRIS near real time workflow for AE33 measurements (Figure 1a).

- Data Acquisition: BC concentrations are retrieved from the acquisition tool developed by the dedicated ACTRIS Central Facility (CF) on aerosol in-situ measurements (CAIS). This tool has already been proven, within the framework of Copernicus CAMS21a project, to robustly provide raw data text files in near real time (Figure 1b). ACTRIS-defined Level0 files are subsequently generated locally from these raw text files using Python routines and pre-defined metadata.
- Data Transfer: Level0 files are automatically transferred to the ACTRIS Data Center (DC, EBAS: ebas.nilu.no). At that stage, they go through an automatic validation procedure, developed by the CF, to produce Level1 ACTRIS data files. Through a ftp sharing process, Level1 data are transferred to a Windows Server (WS).
- Source apportionment: These Level1 files serve as input for RT source apportionment calculation. Outputs will used for web visualization, and creation of Level3 data, back on the ACTRIS DataCenter.



a) b)

***Figure 1**: a) Data workflow for the near real time BC SA-ST. Blue arrows represent secured processes, orange arrows represent unsecured/under development processes. b) Data acquisition panel for AE33 measurements*

At the stage of this milestone, AE33 data acquisition workflow is secured, as the tool is currently being implemented within all pilot sites (Figure 2). Data transfer from stations to DC is planned to be fully operationnal by mid-October 2022. Some other transfers (DC to WS) are under development, and will be settled as soon as effective data transfers occur from pilot sites to DC. Once WS is configured, first SA tests are planned to start with already available data. Also, a dedicated work needs to be undertaken to create corresponding Level3 data on DC, with appropriate template and metadata; this is however not critical for the start of the pilot phase.

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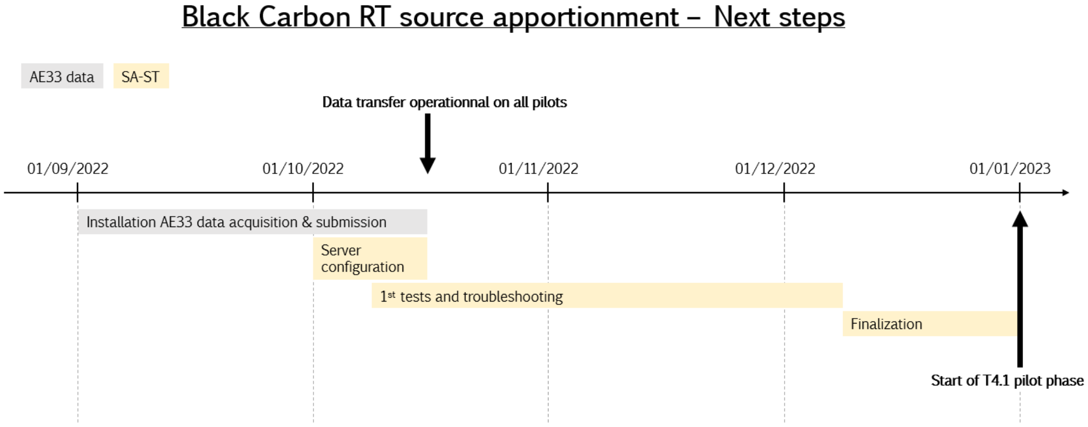

***Figure 2**: Gantt diagramm of BC SA-ST implementation at pilot sites*

BC SA-ST workflow is planned to be on-time for the start of the pilot phase.

3.2 Organic Matter

On the contrary to BC SA-ST, OA SA-ST workflow cannot be fully compliant yet with near real time ACTRIS DMP, mainly because:

- The commercially available SA software to be used in RI-URBANS is not open source, and
- The input data necessary for SA are specific raw data (organic concentration and error matrices) which are currently not covered by the existing tools and templates.

However, a robust architecture has been settled in order to ensure traceable OA SA during the pilot phase (Figure 3).

The steps are as follows:

- Data Acquisition: Raw data are acquired by ACSMs' manufacturer software, and exported by the export tool developed by the dedicated ACTRIS CF (Figure 3b). This tool is currently used for near real time ACTRIS DMP, but a specific add-on ("SoFi-RT") has been coded in order to 1) be able to export the necessary input data for OA SA, and 2) fit the requirements from the SA software. This tool and add-on are fully operational for Q-ACSMs. Further developments are on-going for ToF-ACSMs, especially regarding the generation of the required input data for RT-SA.
- Data Transfer: Raw data files are transferred (synchronized) to a cloud service (NextCloud), which acts as a buffer between the station and the WS where source apportionment calculations are performed.
- Source apportionment: The real time SA will be performed on the WS using SoFi RT. Outputs will be used for visualization, and also transferred back to the station through the NextCloud service.

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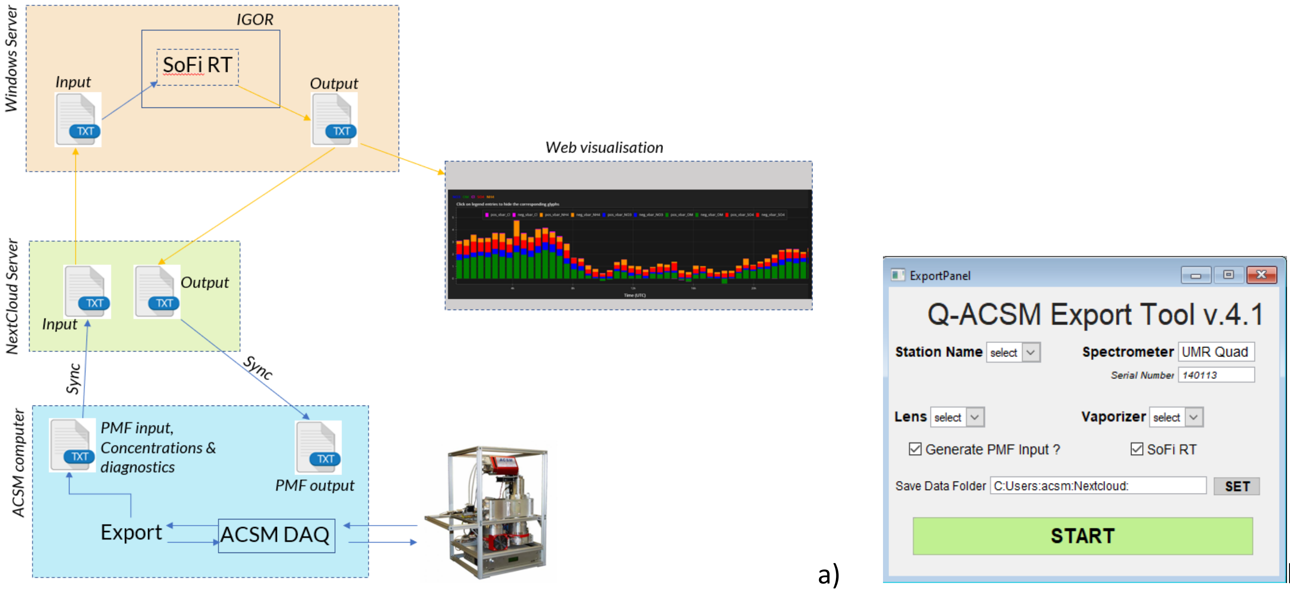

***Figure 3**: Data workflow for the near real time OA SA-ST. Blue arrows represent secured processes, orange arrows represent unsecured/under development processes. b) Data acquisition panel for the ACSM measurements.*

At the stage of this milestone, ACSM data acquisition workflow is secured, as the export tool for all ACSM configurations will be fully operational (Figure 4). Along with the NextCloud client, the export tool is planned to be installed on all participating ACSMs during on-going ACTRIS intercomparison exercises. Some other transfers are under development and will be settled as soon as effective data transfers occur from pilot sites to WS. Once the WS is configured, first tests are planned with already available data.

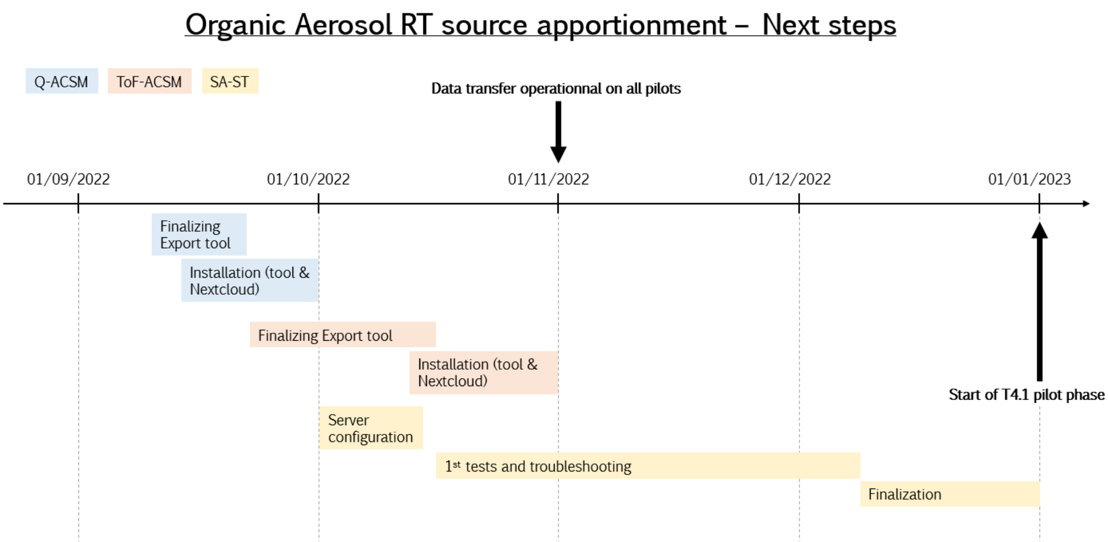

***Figure 4**: Gantt diagramm of OA SA-ST implementation at pilot sites*

OA SA-ST workflow is planned to be on-time for the start of the pilot phase.

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4. Visualisation

A web-based visualization interface has been previously developed for monitoring purposes of European ACSM measurements of non-refractory chemical species (Copernicus CAMS21a WP2), available at: https://dataviz.icare.univ-lille.fr/acsm_dataviz.

It allows to user-friendly select a station and visualize the temporal variations of ACSM components (Figure 5). This interface has been updated to be fed by OA and BC SA-ST outputs (on top of BC and non-refractory chemical species concentrations) as soon as first tests will be triggered.

New stations are added to the list of available sites along with the availability of corresponding data.

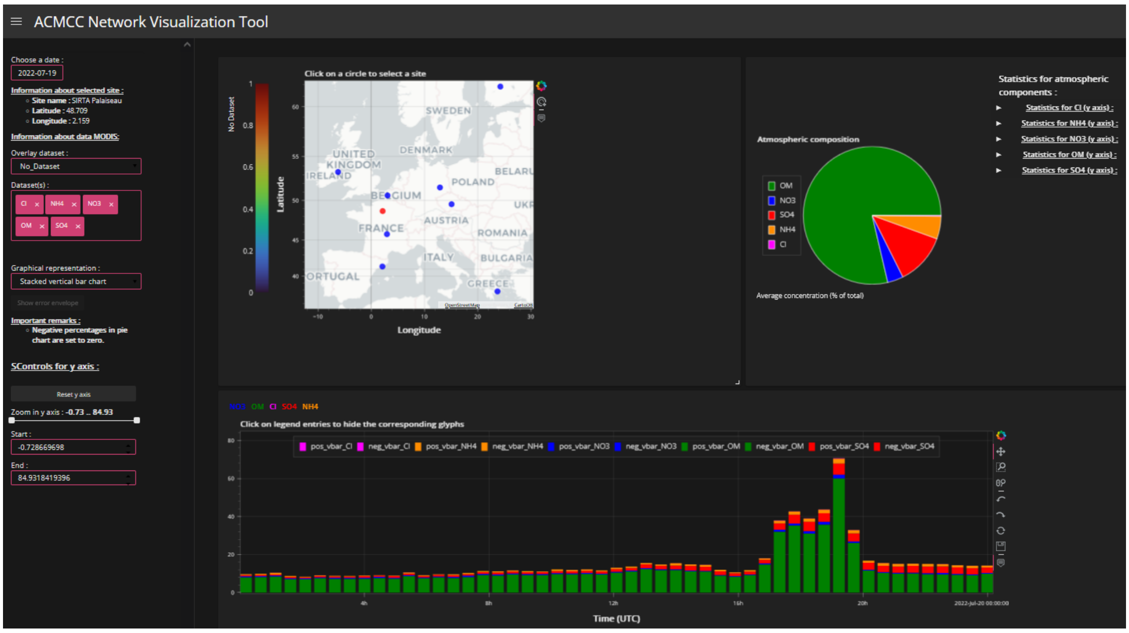

***Figure 5**: Web visualization interface of ACSM data (SIRTA, on 19/07/2022)*

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