Milestone M18 (M4.2)

Comparison NRT vs manual PMF in each pilot city

RI-URBANS

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

By

FMI, CNRS & INERIS

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Milestone M18 (M4.2): Comparison NRT vs manual PMF in each pilot city

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Comments	This milestone summarizes and updates (i) the data flow scheme for the near-real-time source apportionment (NRT-SA) in 13 sites situated in 7 countries across Europe, (ii) current status of data flow in different cities and (iii) NRT-SA principles.

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1. About this document

The milestone M18 (M4.2) summarizes and updates (i) the data flow scheme for the near-real-time source apportionment (NRT-SA) in 13 sites situated in 7 countries across Europe, (ii) current status of data flow in different cities and (iii) NRT-SA principles.

This is elaborated in reply to T4.1 (Near-real-time aerosol source apportionment of carbonaceous aerosols, NRT-SA, M02-M40). This task employs the source apportionment tool (from T1.2) for the aerosol chemical speciation monitor, ACSM (aerosol chemical speciation monitor; organics, sulphate, nitrate, ammonium and chloride) and multiwavelength aethalometer (black carbon; BC) data. The outputs are the tracers and contributions of primary sources such as traffic, wood burning, and cooking (depending on measurement site); quantification of the secondary organic aerosol (SOA) fraction; automatic transfer of data (organic aerosols matrices and aethalometer BC concentrations) to the ACTRIS (Aerosol, Clouds and Trace Gases Research Infrastructure) Data Centre.

This is a public document, available in the RI-URBANS website (https://riurbans.eu/work-package-4/#milestones-wp4). The document will be distributed to all RI-URBANS partners for their use and submitted to European Commission as the RI-URBANS milestone M18 (M4.2).

2. Pilot site information

Altogether 13 sites across Europe participate in the NRT-SA piloting. Table 1. contains the information about the pilot sites (stations) located in Paris and Marseille (France), Athens (Greece), Bucharest (Romania), Helsinki (Finland), Po Valley (Italy), Zurich (Switzerland), Barcelona (Spain) and their correspondence to EBAS (i.e., database hosting observation data of atmospheric chemical composition and physical properties; https://ebas-data.nilu.no) and project framework.

Table 1. The contributing pilot sites for the NRT-SA provision in RI-URBANS with respective station identification information and data provision frameworks.

Pilot	Station Name	EBAS Station ID	lat (°)	lon (°)	EBAS Platform ID	EBAS Lab ID	framework	EBAS Station Name
Paris	SIRTA	FR0020R	48.71	2.15	FR0020S	FR01L	ACTRIS / RI-URBANS	SIRTA Atmospheric Research Observatory
Paris	Chatelet	FR0041U	48.86214	2.34462	FR0041S	FR21L	RI-URBANS	Paris Chatelet
Paris	BPEst	FR0042U	48.83857	2.412713	FR0042S	FR21L	RI-URBANS	Paris BPEst
Athens	AthensNOA	GR0004U	37.97312	23.71805	GR0004S	GR07L	ACTRIS / RI-URBANS	Athens NOA
Athens	AthensDEM	GR0100B	37.99532	23.81672	GR0100S	GR05L	ACTRIS / RI-URBANS	DEM_Athens
Bucharest	RADO-Bucharest	RO0007R	44.344°N	26.012°E	RO0007S	RO03L	ACTRIS / RI-URBANS	Bucharest
Helsinki	Supersite	FI0039U	60.19635	24.95222	FI0039S	FI03L	RI-URBANS	Mäkelänkatu
Po Valley	Milano	IT0025U	45.47833	9.23144	IT0025S	IT006L	ACTRIS / RI-URBANS	Milano Pascal
Po Valley	Bologna	IT0022C	44.52366	11.33833	IT0022S	IT006L	ACTRIS / RI-URBANS	ISAC Bologna II
Zürich	Kaserne	CH0010U	47.37759	8.530419	CH0010S	CH02L	RI-URBANS	Zürich-Kaserne

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Marseille	Longchamp	FR0035U	43.30529	5.394716	FR0035S	FR17L	RI-URBANS	Marseille Longchamp
Barcelona	PalauReial	ES0019U	41.38744	2.115306	ES0019S	ES05L	ACTRIS / RI-URBANS	Barcelona
Barcelona	Montseny	ES1778R	41.77934	2.358033	ES1778S	ES05L	ACTRIS / RI-URBANS	Montseny

3. General data flow scheme for the NRT-SA

Figure 1 represents the dataflow scheme for the NRT-SA. Shortly, the ACSM (aerosol chemical speciation monitor) and AE33 (multiwavelength aethalometer, model AE33) data collected in the 13 pilot sites will be, at firstly, transferred to a designated server. The NRT-SA analysis will be done in this server. Visualization of the data and NRT-SA obtained results will be available as an open access data.

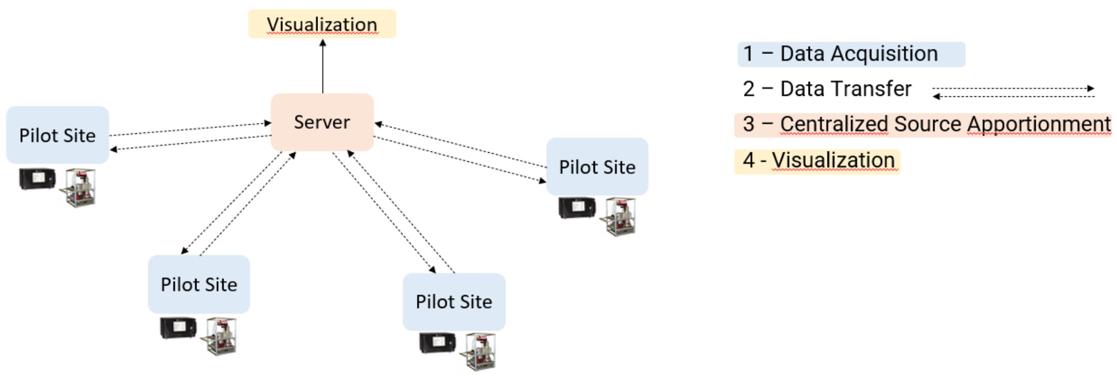

Figure 1. *The dataflow scheme of NRT-SA*

Different software solutions will be used to transfer the ACSM and AE33 data from the pilot sites as the instruments installed and operated at the stations have their own specific data formats.

For AE33 the data logger stores the raw data on the local hard disc as a text/ascii-format file and writes the data into the influxDB time-series database. Next, the NASA-Ames format files (text-based, self-describing, portable format) are generated with a python-tool that extracts data from the influxDB database. The NASA-Ames files are then being automatically submitted hourly to the EBAS database. The data is submitted to EBAS as a level 0 data (i.e., raw data). The NASA-Ames files contain meta information about the measurements (e.g., instrument information, measurement conditions, AE33 parameters) and results for the most recent measurements (previous last hour). For AE33 a recommendation to use NIST-conditions (1013.25hPa and 0^{o}C), GMT time and time base of 60s was given, however as part of the sites belong to local Air Quality Measurement Networks (AQMNs), it is not often possible to change measurement conditions at the site. However, with post processing it is possible to correct for these.

For ACSM a data export tool is used to generate a data package that is subsequently sent to the NextCloud server hosted by the University of Lille (France). All the ACTRIS pilot sites, as well as the Helsinki's device, participated in the intercomparison exercise organized by the Aerosol Chemical Monitor Calibration Centre (ACMCC) in autumn 2022 in order to ensure the comparability of the ACSM results. Both instruments from Airparif, for the Paris city center stations, participated in the intercomparison organized by ACMCC for French air quality monitoring network (AQMN) in spring 2021. Only Zurich and Marseille instruments did not participate in such a metrological workshop in the last 3 years.

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As a whole, the NRT-SA tool provided by WP1 extracts data from these servers and conducts source apportionment automatically, and then, visualizes the results in the internet page https://dataviz.icare.univ-lille.fr/acsm_dataviz. WP4 will conduct source apportionment also manually using Sofi Pro ME-2 software and compare results to automatically conducted SA on a regular basis for each pilot city.

4. Current status of data transfer in the pilot sites

During 2022, the needed data transfer softwares were installed on ACSM and AE33 PCs in each pilot city during autumn 2022 to enable data transfer. For AE33 - a Python based ae33 data logger, for ACSM - Igor based Q-ACSM export tool 4.1, and for ToF-ACSM - Igor based ToF-ACSM export tool v1.0 are used (see Figure 2). Also the stations have established own corresponding accounts in the NextCloud server and the EBAS station codes have been acquired for the new stations.

Figure 2. *Data transfer tools for AE33, ACSM and ToF-ACSM.*

Most sites have had minor issues either with the software or databases, but currently most of the sites are already completely (or almost completely) installed needed software. Table 2 contains the status update on the data transfer and possible issues reported by the pilots in December 2022.

Table 2. *Status update of the measurement and data transfer in different cities at 11.12.2022 for the ACSM.*

Pilot environment	**Athens**		**Barcelona**		**Helsinki**	**Po Valley**		**Paris**			**Zürich**	**Marseille**	**Bucharest**
Name of the pilot site	NOA	NCSRD	Barcelona	Montseny	Supersite	Milano	Bologna	SIRTA	Les Halles	BP Est	Kaserne	Longchamp	INO
NextCloud	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Export tool installed	y	n, soon	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
ACSM Issues	Technical issues (Q-ACSMI, freezing NextCloud	ToF-ACSM detector to be changed											
Software installed	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Data logging	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y

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NASA-Ames template	Y	Y			Y	Y	Y	Y	Y	Y	Y	Y	Y
Nas file checked		Y			Y	Y	in progress	Y	Y	Y	Y	in progress	Y
Nas generator running		Y			Y	Y		Y	soon	soon		soon	Y
Contacted EBAS					Y	Y	Y	Y	Y	Y	Y	soon	new EBAS ID
Ebas submission		soon				soon		soon	soon	soon	soon	soon	Jan
NextCloud sync			soon	soon	Y			Y	soon	soon	Y	soon	Y
AE33 issues	-	-	-	-	-	-	-	-	-	-	PC reinstalled, dataflow not ready	Small issues with data logger	Station info needs to be update

To enable ACSM NRT-SA, the source profiles (i.e. mass spectra) of constrained primary sources such as HOA (Hydrocarbon-Like Organic Aerofol) and BBOA (Biomass Burning Organic Aerosol) and exact number of factors to be searched, are being currently collected in the pilot cities. This is based on pre-existing information from the stations. Most of the stations participated to a study by Chen et al. (2022a), where the sources were studied offline using similar source apportionment methods. For the new stations, with no such existing source apportionment outputs, the manual source apportionment needs to be done first in order to establish the factors.

5. Source apportionment visualization

The source apportionment for ACSM is done using near-real-time procedures described by Chen et al. (2022a,b). For ACSM an aethalometer model described by Sandradevi et al. (2008). The results will be shown in real-time at internet page: https://dataviz.icare.univ-lille.fr/acsm_dataviz. Figure 3 shows an example of visualization of results. The full NRT-SA dataflow from ACSM measurements to visualization was tested for the first time in autumn 2022 in the Paris SIRTA site. This test showed that the procedure works well and can be implemented to all other sites as well.

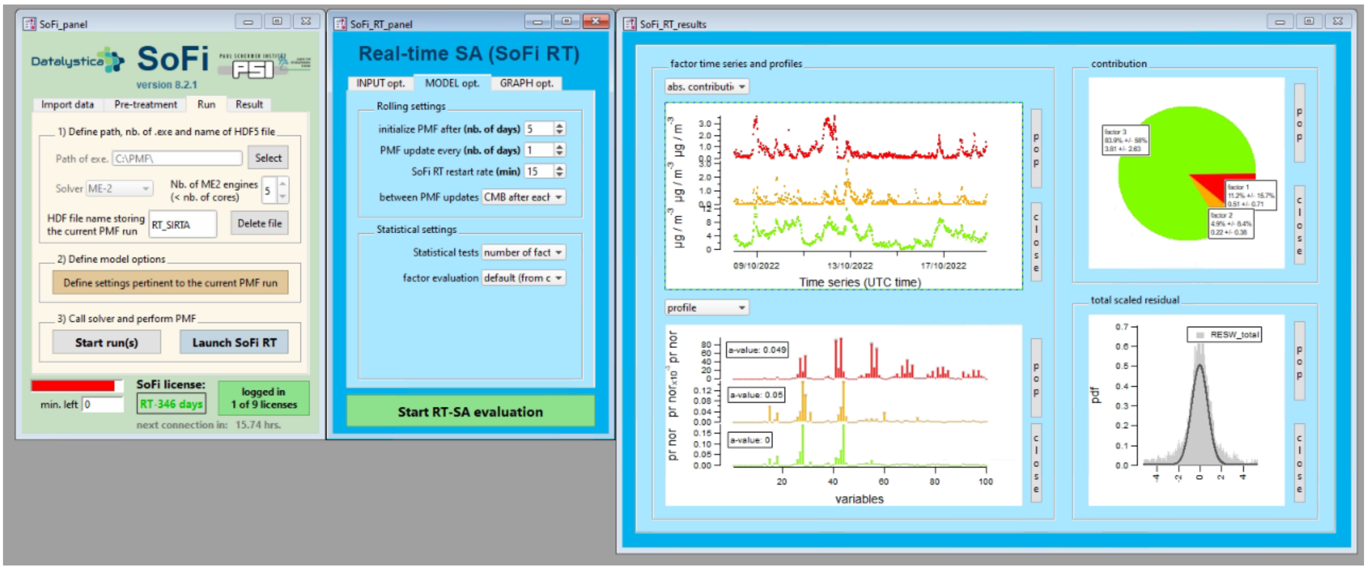

Figure 3. *The snapshot of the SoFI-RT results from the Paris SIRTA site in September 2022.*

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6. Comparison of NRT-SA and manual PMF

Here we present the first comparison of the NRT-SA (using SoFi RT) and manual PMF analysis for SIRTA in Paris, which is one of the forerunner sites in the NRT-SA development and delivery (Chen et al. 2022b). To do so SoFi RT analysis has been achieved a posteriori, simulating NRT conditions, on datasets obtained from February 2016 to May 2017, a period for which manual PMF analysis was already conducted (and presented in Zhang et al., 2019).

In this case study, the agreement between the NRT-SA and manual PMF is excellent, as shown in Figure 4 (pie chart of source contributions to the mean PM) and in Figure 5 (timeseries of source contributions) for each of the source factors identified. Both methods indicate the same number of factors (N=4) relevant for the site over the course of the investigated period. The dominating factors are More Oxidized Oxygenated Organic Aerosols (MO-OOA) and Less Oxidized Oxygenated Organic Aerosols (LO-OOA). In total they constitute more than 75% of the organic aerosol mass at SIRTA. BBOA, mainly originating from residential wood burning primary emissions, logically shows much higher contributions during the cold period than in summer season. The smaller contribution (about 10% on average) originate from Hydrocarbon-like Organic Aerosols (HOA), which is indicated a relatively low influence of primary traffic exhaust emissions at this site. Overall, and on average, the various contributions agree within 1-2 % between the NRT-SA and the manual methods (Figure 4).

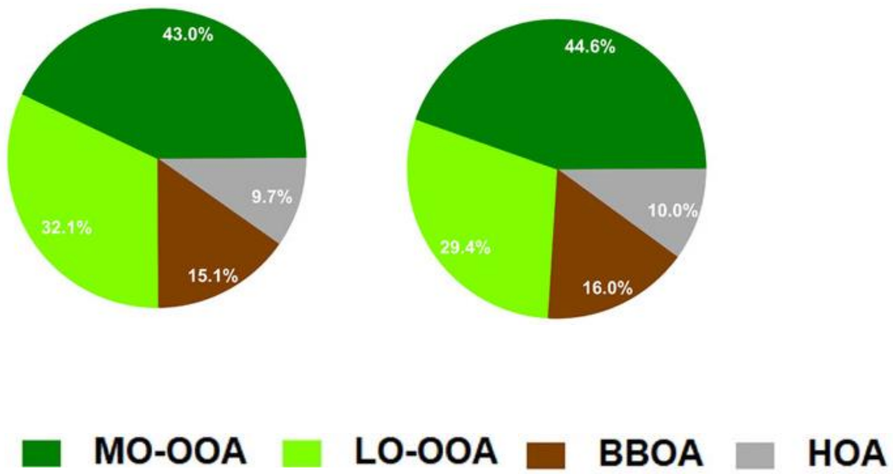

Figure 4. Comparison of average factor contributions obtained from NRT-SA tool (left) and manual PMF (right) analyses in Paris for the period February 2016 – May 2017. Adapted from Chen et al. (2022b).

Following this example, and as soon as the WP4 Task1 pilot phase will start (in January 2023, as planned initially), the quantitative comparison from each site are going to be performed and presented in Deliverable D22 (D4.1) “Monthly reports of concentration levels and PMF for each city during the pilot operation” whereas the NRT-SA service tool is described in Deliverable D4 (D1.4) NRT source apportionment ST for submicron carbonaceous matter (pilots).

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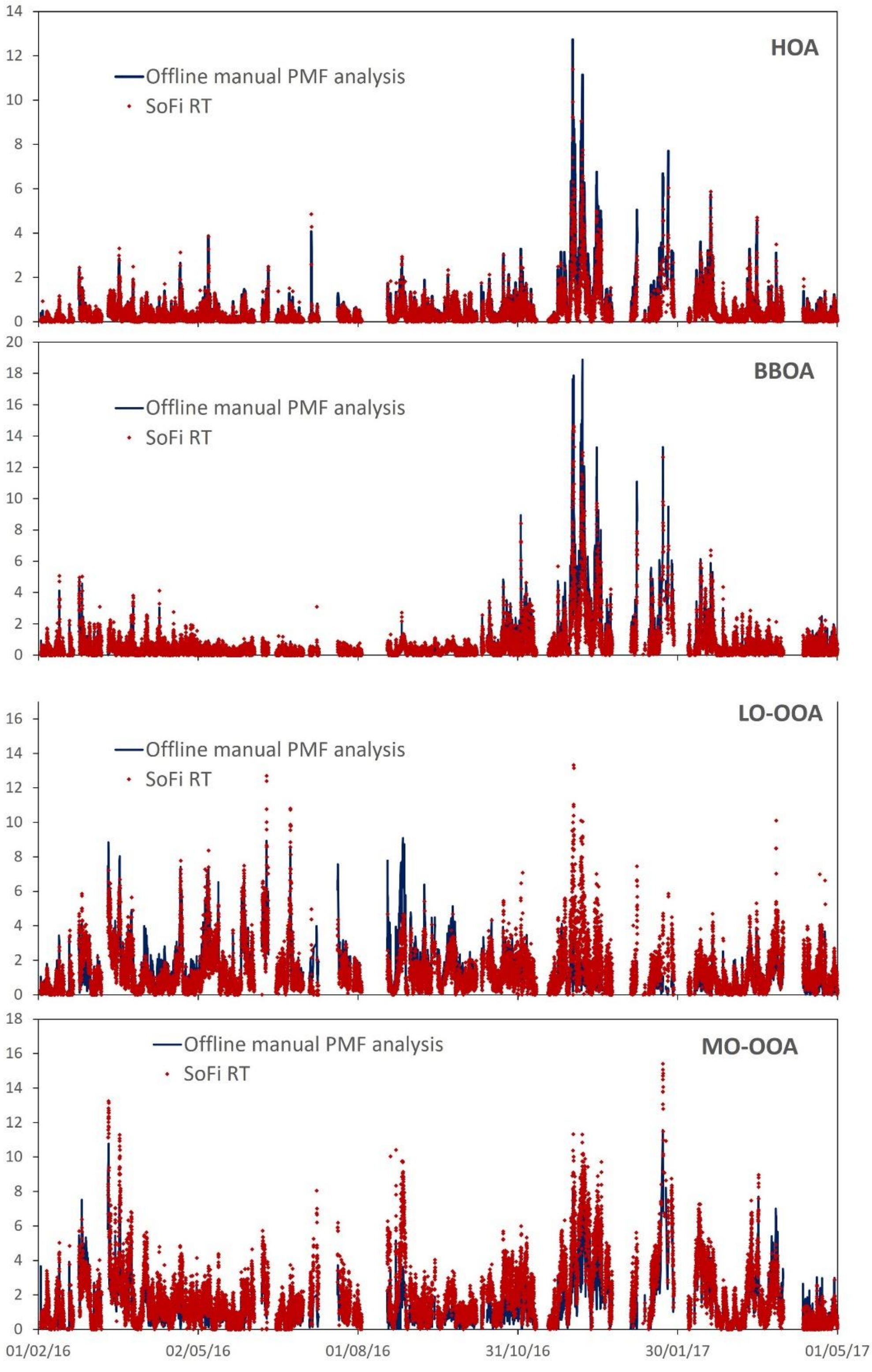

Figure 5. *Comparison between NRT-SA toolkit (SoFi RT) and manual PMF analyses performed for the SIRTA pilot site between February 2016 and May 2017.*

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7. Conclusion and next steps

During the autumn 2022 a lot of work has been made in WP4 to establish the dataflows from the sites to the servers in order to be ready to start the NRT-SA in January 2023. Prior to that, we need to finalize the installation of the NRT-SA software on our centralized computing system (hosted by ACMCC) and establish the expected source profiles and number of factors from the pilot sites. This work is in progress, in close collaboration with all the pilot cities involved in WP4.1. The first comparison of NRT-SA and offline SA yielded very good agreement, which means that NRT-SA can be implemented.

During the next year 2023, a series of frequent meetings will also be held in order to maintain the measurements and dataflows during the pilot period (Jan-Dec 2023). In addition, source apportionment will be conducted again offline in order to compare the NRT-SA with manual PMF results, for each of the pilot sites.

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