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Deliverable D23 (D4.2)

Comparison of NRT source apportionment and manual PMF in the pilot cities

RI URBANS

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

By

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Deliverable D23 (D4.2): Comparison of NRT source apportionment and manual PMF in the pilot cities

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Comments	This document describes the results of an evaluation of the performance of near real time source apportionment (NRT-SA) of PM versus of a “regular” manual process, as commonly performed and described in the literature. This is one of the products of WP4-T4.1 on the pilot study on NRT-SA based on online measurements of black carbon (BC) and PM components using a aethalometers and aerosol chemical speciation monitors.

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1. About this document

WP4 aims at testing and to demonstrating solutions for advanced urban air quality (AQ) monitoring systems and evaluation of exposures (WP 1-3) at representative areas and hot spots in Europe. Specifically, implementing 5 testing and demonstration pilots in (originally) 9 cities (Athens, Barcelona, Birmingham, Bucharest, Helsinki, Milano, Paris, Rotterdam-Amsterdam and Zurich, with at least 3 cities in each pilot) and create synergies with WP5 to devise the roadmap for upscaling service tools (STs). These pilots encompass diverse European urban environments and will demonstrate at a real scale the ability to integrate complementary AQ measurement systems in existing AQ monitoring networks (AQMNs), addressing modalities where the research infrastructures (RIs) are engaged with the national/local authorities, proposing innovative solutions such as mobile instrumentation and building on citizens' observatory initiatives, applying tools developed, and improving their operational integration in AQMNs. The pilots include the demonstration of the following STs.

- Near-real time aerosol source apportionment (NRT-SA) of carbonaceous aerosols (T4.1).
- NRT nanoparticle-particle number size distribution (NRT-PNSD) data (T4.2).
- The urban fine scale mapping including innovative modelling, monitoring, and crowdsourcing (T4.3).
- Novel health indicators of nanoparticles and PM components and source contributions (T4.4).
- Quantifying emission sources in/near urban areas and identifying contribution of hotspots to air pollutant exposure (T4.5).

The pilot on NRT-SA of carbonaceous aerosols employs the source apportionment tool (from WP1-T1.2) for the PM compositional data obtained by using the Aerosol Chemical Speciation Monitor (ACSM, Organic Matter, sulphate, nitrate, ammonium and chloride) and the multi-wavelength aethalometer (Black Carbon, BC). Expected outputs: tracers and contributions of primary sources such as traffic, wood burning, and cooking (depending on measurement site); quantification of the secondary organic aerosols (SOA) fraction; automatic transfer of data (organic aerosols matrices and aethalometer BC concentrations) to ACTRIS DC. These are being reported on a monthly basis by the pilot cities (D22 (D4.1)) to allow uniform view on the sources of aerosol particles across European urban environments.

D23 (D4.2) describes the performance of NRT-SA outputs, versus of a "regular" manual process, as commonly performed and described in the literature.

This is a public document that will be distributed to all RI-URBANS partners for their use and submitted to European Commission as a RI-URBANS deliverable D23 (D4.2). This document can be downloaded at https://riurbans.eu/work-package-4/#deliverables-wp4.

2. Purposes of comparing Source Apportionment outputs

Source apportionment (SA) of organic aerosols (OA) can be challenging, given its molecular complexity and the level of expertise which is required in order to carry out advanced statistical analysis. The feasibility of upgrading that process in near real time (NRT) has been demonstrated "offline" in Chen et al. (2022), using a combination of rolling Positive Matrix Factorization (PMF) and Chemical Mass Balance (CMB) models at three

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European cities (Zürich, Athens & Paris). Results were highly consistent with manual PMF analyses over one year of data. During the pilot phase, offline SA should be considered as the reliable "best estimate" of OA fractions, and thus as a reference, compared to the NRT process.

2.1 Introduction

The comparison of NRT-SA outputs with manual SA has been set to be done monthly, concomitantly with the reports which pilot sites need to provide. It has been agreed that SoFi Pro shall be used for manual SA, with a harmonized protocol described hereinafter.

2.2 Harmonized protocol for manual source apportionment

In order to harmonize manual SA analyses, a unique protocol has been designed and shared to all the participants of the pilot phase. This should prevent from having site-specific potential discrepancies between manual and NRT analyses. This protocol, mostly based on the European phenomenology on SA of OA described in Chen et al. (2022), has been shared to all participants and is described below.

Constrains

HOA (hydrogenated OA), BBOA (biomass burning OA, if available), COA (cooking OA, if applicable), any other site-specific primary profiles (if applicable). Primary profiles used must be the same as NRT process.

a-values & number of factors

- HOA/COA: random a between 0.1-0.4 (step 0.1).
- BBOA: random a between 0.1-0.5 (step 0.1).
- Site specific profile: random a between 0.1-0.3 (step 0.1).
- If applicable, OOA (oxygenated OA) can be differentiated following different f44/f43 ratios.

Run parameters

100 repeats, bootstrap enabled.

Criteria

- Explained variation of f60.
- HOA vs BClf (BC from the combustion of liquid fluids).
- HOA vs NOx.
- BBOA vs BCsf (BC from solid fuels) in winter.
- (Optional) maximize COA noon peak (user-defined local hour range).

3. Results

This report does not aim at documenting the results at all sites since the start of the pilot phase. Indeed, over the course of the phase, several updates of ACSM Export Tool & SoFiRT have been made in order to stabilize, as best as possible, data transfer and NRT SA. This document presents instead i) some examples of the performance and consistency of the NRT SA tool, and ii) some causes of discrepancies that have already been identified (Figure 1).

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HOA	COA	OOA

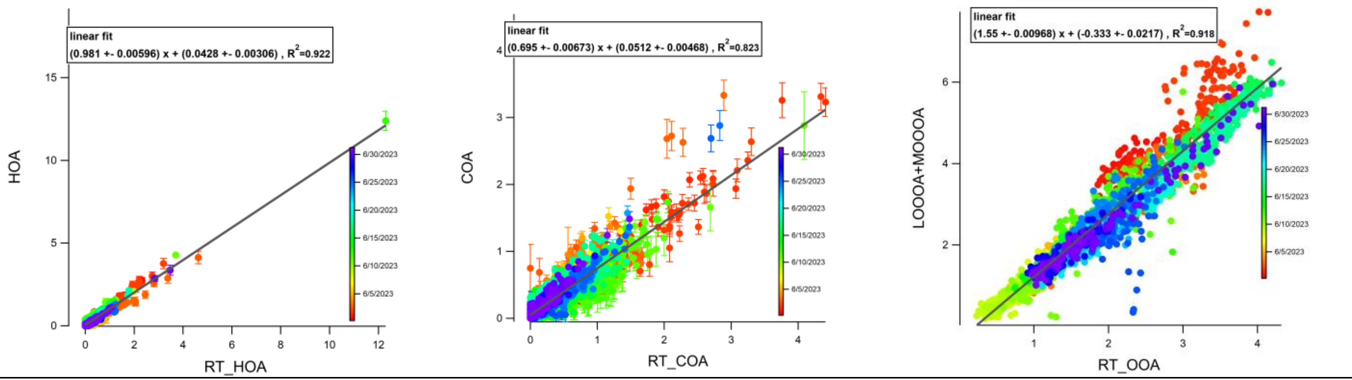

Figure 1. *Correlation between offline PMF results and NRT-SA for Marseille (France) in June 2023*

HOA	COA	OOA

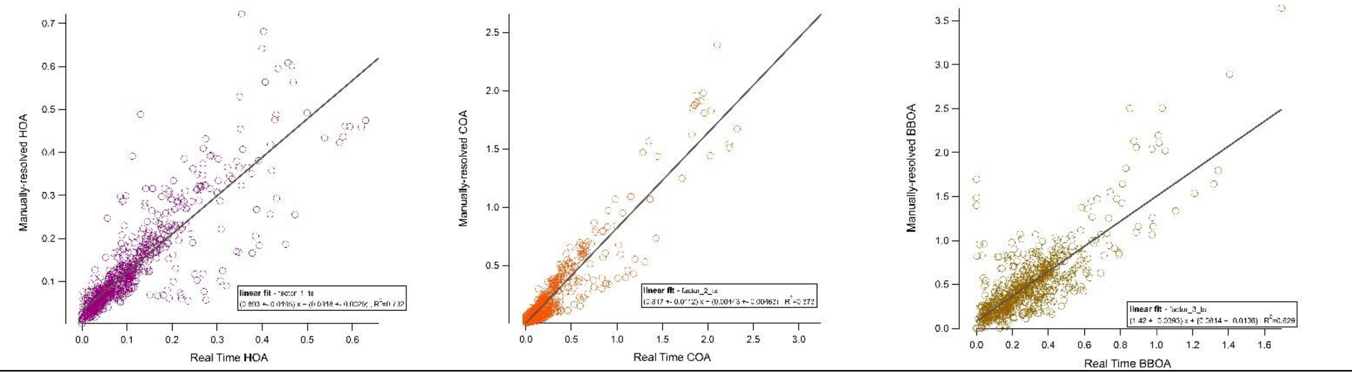

Figure 2. *Correlation between offline PMF results and NRT-SA for Athens (Greece) in April 2023*

HOA	BBOA	OOA

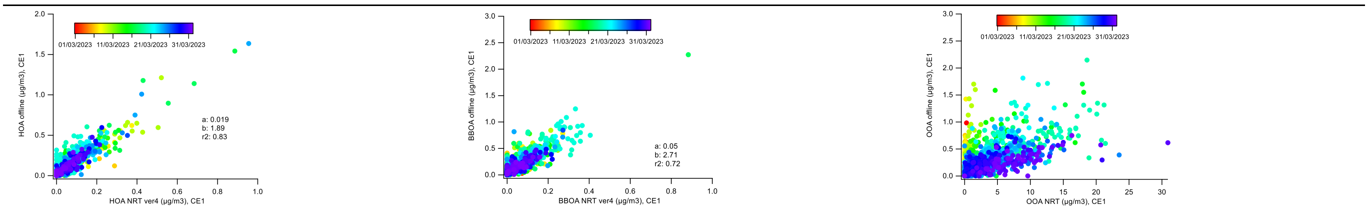

Figure 3. *Correlation between offline PMF results and NRT-SA for Helsinki (FInland) in March 2023*

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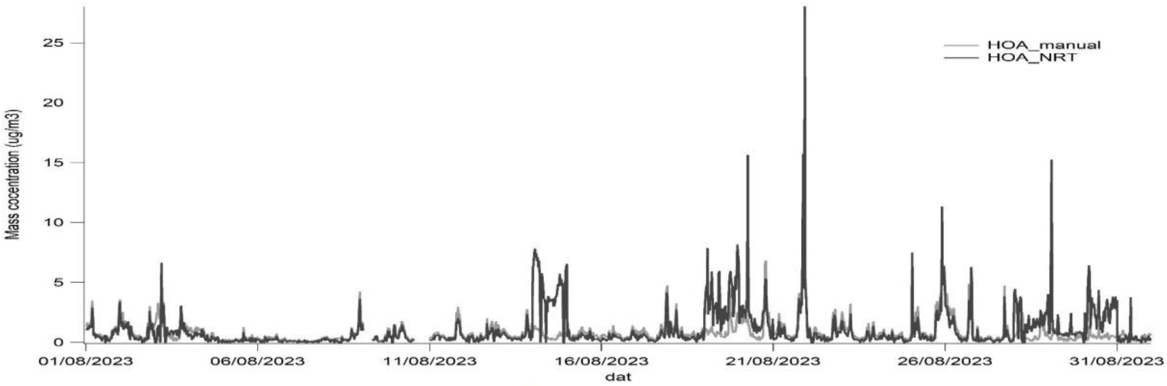
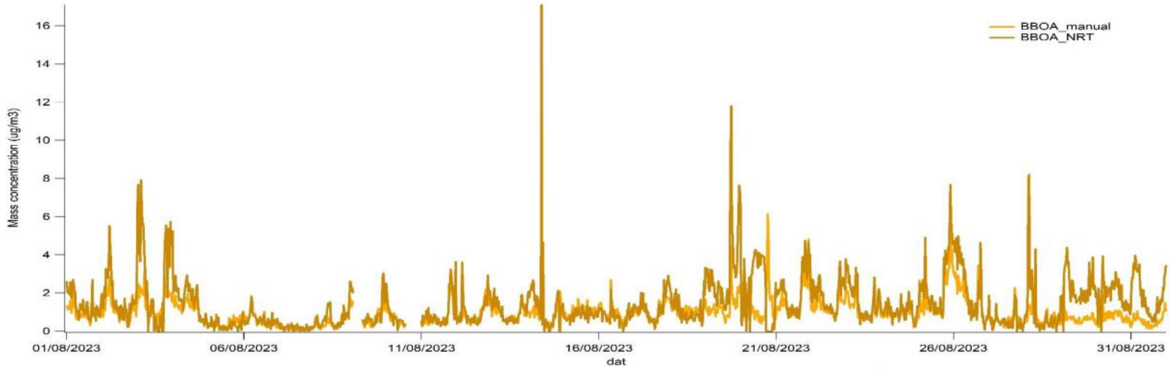
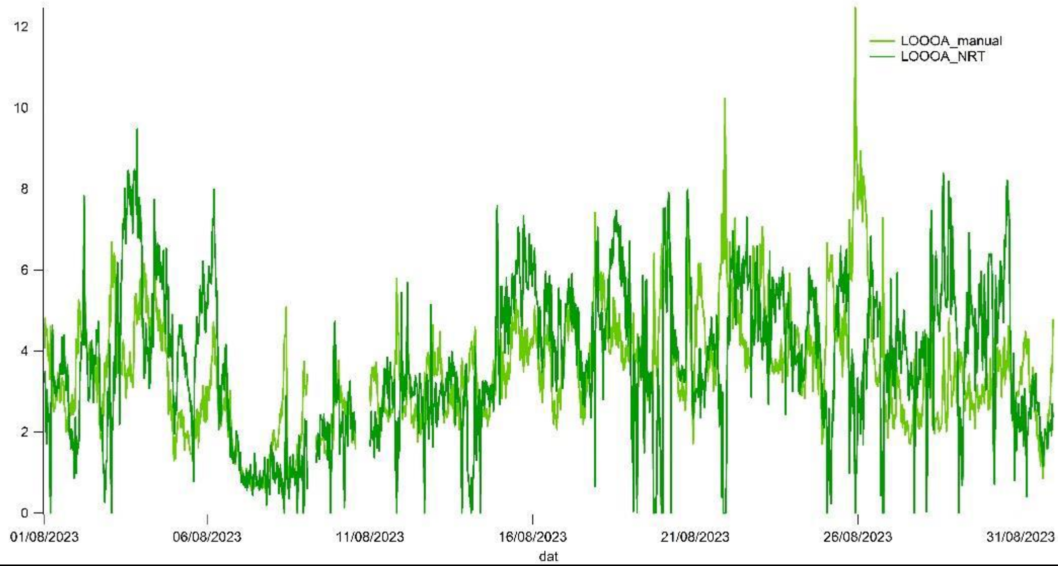
HOA



BBOA



LOOOA



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MOOOA

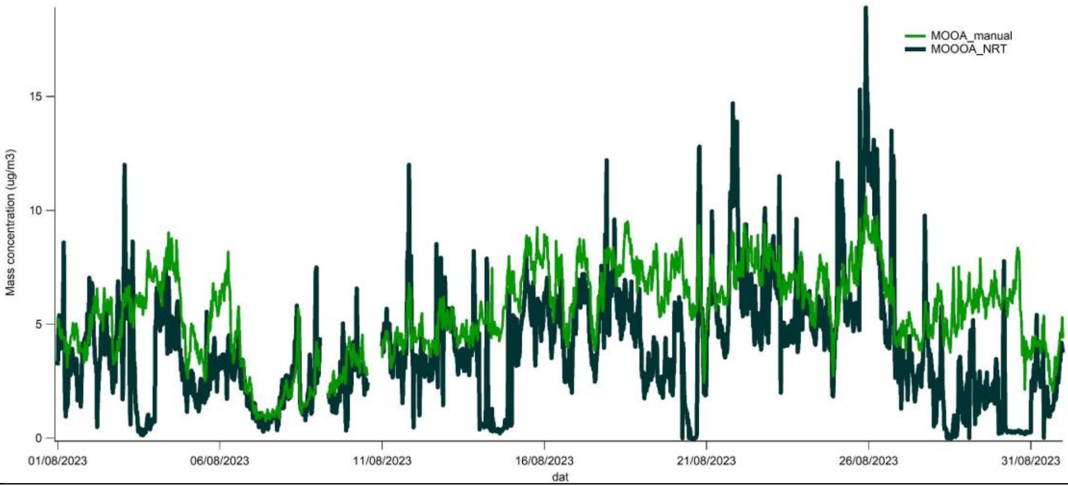

Figure 4. *Timeseries for manually conducted offline PMF and NRT-SA results for Bucharest in August 2023*

From a general perspective, most of the sites show a good consistency for primary factors (HOA, COA, BBOA), although they don't always necessarily exhibit a 1:1 line. Comparison for secondary factors (OOA, LOOOA, MOOOA) usually show a slightly higher dispersion, which should be related to the complexity of this OA fraction. It is noteworthy highlighting that these results may not be representative of the final performances of the NRT SA Tool, but rather demonstrate the potential consistency which can be reached. Indeed, most of the efforts focused on making the whole chain work first, before trying to optimize some of the parameters. To this end, constant interactions between T4.1 and T1.2 have been necessary in order to stabilize data flows, troubleshoot and debug codes.

Below are listed some of the identified reasons for discrepancies:

- Wrong input data lead to wrong SA output: The ACSM Export tool has been updated several times over of the pilot phase in order to make sure that the correct data are being transferred correctly to the SA server. Also, automatic pre-validation of the input data should strongly be considered in order to discard outliers prior to SA. This can be critical for NRT-SA process, given the "rolling mechanism", where bad data could potentially influence the quality of NRT-SA during several days.
- Compare apples with apples: Consistency between NRT-SA and manual SA can only be achieved if input data are consistent. To this end, it is critical to ensure that corrections have been applied correctly and in a uniform way (transmission & air beam corrections, collection efficiency, uncertainty matrix). Also, factor profiles used for constrains need to be consistent with the input OA matrix, especially regarding m/z list. Indeed, ToF-ACSMs and Q-ACSMs don't have the same fragmentation tables, potentially leading to significant underestimation of OA total concentration.
- Gaps in data appeared to play a role in NRT results, which were at first not correctly accounted within the SA tool. Tests and updates have solved this issue.
- Optimizing NRT-SA parameters: Since priority was given to the operationability of the pilot phase at all sites, it has been decided first to keep the NRT-SA as simple as possible. However, some parameters have been identified to potentially lead to null values in NRT-SA results. That is why number of runs, a-value constrains, bootstrapping parameters and temporal windows were recently optimized. The evaluation of the impact of these changes is on-going.
- External tracers: Manual PMF results are optimized with external tracers, especially primary factors such as HOA and BBOA. Based on temporal correlations, NOx, BClf and BCsf are generally used to select the best solutions among the solution space. This aspect is not available on a NRT-SA timeframe yet and is associated

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to additional challenges regarding data transfer and calculations. Additionally, temporal constrains with external tracers is not available on a NRT-SA basis.

4. Conclusions

Results from the pilot phase show that consistency of NRT- SA results and the manual offline SA can be reached, as long as the whole chain is operational, and prior evaluation has been performed. Over the course of the pilot phase, site-to-site discrepancies have been observed, highlighting that some key parameters still need to be framed and harmonized.

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