PARIS

Process Attribution of Regional Emissions

GA 101081430, RIA

Completion of source apportionment for previous year using Dublin data

Milestone M27	
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Horizon Europe Cluster 5: Climate, energy and mobility
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1. Changes with respect to the DoA (Description of the Action)

N/A

2. Dissemination and uptake

The dissemination of M27 involves the archiving of the source apportionment results of organic matters (OM) from Dublin for 2023 in the EBAS database, ensuring it is publicly accessible. The public availability of the dataset through EBAS promotes transparency, collaboration, and informed decision-making in environmental protection.

While an upload of the source apportionment data to the EBAS database was not originally planned, it was deemed important to do so to ensure open access and promote transparency, collaboration, and informed decision-making. Since currently there is no standardised submission tools or procedures available for the source apportionment data, the PARIS WP7 team has engaged EBAS on this. The working group with members from EBAS, PARIS and another EU project RI-URBANS was created to develop these procedures and data will be submitted after the tools are finalised.

As a temporary solution, the data are shared via email/SharePoint to internal project partners and external parties interested in the data. Efforts are underway (prompted by Paris WP7) to establish a standardized source Apportionment data submission process within EBAS, ensuring long-term, sustainable access to the data.

3. Short Summary of results

Continuous measurements of organic matter (OM) in atmospheric submicron aerosols (PM_1) were conducted in Dublin throughout 2023 using a Quadrupole Aerosol Chemical Speciation Monitor (Q-ACSM) with high time resolution. The OM dataset has been archived in EBAS dataset after rigorous QA/QC procedure.

A new method combining the advanced rolling Positive Matrix Factorization (rolling-PMF) and machine learning techniques was developed for OM source apportionment and was applied to the OM data from Dublin for the year 2023. Six distinct OM factors were identified by rolling-PMF: primary organic aerosols (POA) from peat, wood, and coal burning; hydrocarbon-like organic aerosols (HOA) from traffic and domestic oil burning; and two types of oxygenated organic aerosols (OOA). The newly developed machine learning method enhanced the OM source apportionment by separating the PMF-derived OOA into locally emitted OOA and regionally transported OOA. This detailed source apportionment provides valuable insights into the OM sources and relative contributions of different source sectors.

The innovative source apportionment method developed and tested in Dublin enables its further application to other locations across the Europe, thereby enhancing the understanding of aerosol sources and contributing to better air quality management on a broader scale.

4. Evidence of accomplishment

4.1 Background of the milestone

Atmospheric aerosol particles, also known as particulate matter (PM), have profound impacts on air quality, human health, and climate change. These particles can penetrate deep into the respiratory system, causing respiratory and cardiovascular diseases, and are linked to millions of premature deaths annually (Pope and Dockery, 2012; Lelieveld et al., 2015; Shiraiwa et al., 2017). In terms of climate, aerosols influence both the Earth's radiation balance by scattering and absorbing sunlight and cloud formation processes, which can alter weather patterns and climate dynamics (Ipcc, 2021).

Organic matter (OM) is one of the most significant components of atmospheric PM, constituting between 20% and 90% of the submicron PM (PM_1) mass (Jimenez et al., 2009; Zhang et al., 2011). Furthermore, OM is found to be more toxic than many inorganic aerosol components such as sulfate and nitrate due to the presence of thousands of organic compounds, some of which are hazardous to human health (Wu et al., 2022). Understanding the sources and chemical nature of OM is crucial for mitigating its adverse effects on human health and the environment. Source apportionment of OM is essential for identifying and quantifying the contributions of various sources and formation processes. This detailed information allows policymakers to develop targeted and effective strategies to reduce PM concentrations and implement targeted and effective emission control measures.

The Aerodyne aerosol mass spectrometers, including the Quadrupole Aerosol Chemical Speciation Monitor (Q-ACSM), are powerful tools for real-time chemical speciation of PM in the atmosphere (Allan et al., 2003; Ng et al., 2011). These instruments provide high temporal resolution data, allowing for detailed monitoring of aerosol composition and dynamics. One of the critical advantages of using aerosol mass spectrometers such as Q-ACSM is their ability to provide detailed mass spectra information of OM. This chemical information is crucial for effective source apportionment. By analyzing the mass spectra, specific molecular markers and fragments that are characteristic of different OM sources can be identified. For instance, certain mass-to-charge (m/z) ratios are indicative of primary organic aerosols (POA) from sources like biomass burning, traffic emissions, or cooking activities. Similarly, other m/z ratios can signal secondary organic aerosols (SOA) formed through different atmospheric chemical reactions (Zhang et al., 2011).

Positive Matrix Factorization (PMF) is widely used for the source apportionment of OM. PMF decomposes the observed aerosol data into factors associated with specific sources or processes, providing a quantitative estimate of each source's contribution (Paatero and Tapper, 1994; Zhang et al., 2005). Traditional PMF is generally effective in distinguishing POA factors especially when aided by known reference mass profiles. However, it has limitations in separating SOA, particularly in regions with complex air pollution patterns like Dublin. During extreme air pollution events, such as those occurring during heating hours, all organic aerosol factors spike simultaneously (Lin et al., 2018; Lin et al., 2019), making it challenging for traditional PMF methods to accurately link SOA factors to specific sources or processes.

To address these challenges, a supervised machine learning approach has been developed as a promising strategy for enhancing the characterization of OOA. Machine learning algorithms, increasingly utilized in atmospheric science (Pande et al., 2022; Peng et al., 2023), offer unique advantages in capturing nonlinear effects and discerning subtle patterns within multidimensional datasets. This makes them well-suited for distinguishing between locally produced OOAs and those transported regionally, thereby advancing our ability to accurately characterize air pollution sources and inform evidence-based strategies for air quality management and environmental protection.

4.2 Scope of the milestone

Data Collection and Quality Assurance: Continuous measurements of OM in PM_1 were conducted using a Quadrupole Aerosol Chemical Speciation Monitor (Q-ACSM) in Dublin throughout 2023. Rigorous quality assurance and quality control (QA/QC) procedures were applied to ensure the reliability and accuracy of the collected data. The validated OM dataset has been archived in the EBAS database to ensure public accessibility and transparency.

Data Preparation for PMF: The mass concentration and error (uncertainty) matrix of OM were exported from the standard data analysis software and, after rigorous anomaly checks and quality assurance, were used as inputs for the positive matrix factorization (PMF) model for OA source apportionment.

Application of rolling PMF: An advanced rolling PMF method combined with Source Finder Pro (SoFi Pro) software was performed on OM dataset obtained by Q-ACSM from Dublin in 2023. Reference mass profiles of POA factors from burning experiments were utilized to improve the accuracy of OM source apportionment. The rolling-PMF successfully identified six OM factors in Dublin including four POA factors from peat, wood, coal and oil burning (and traffic emissions), and also two OOA factors.

Development of machine learning approach: A new supervised machine learning approach was developed to address the limitations of traditional PMF in separating OOA. This method enhanced the source apportionment by distinguishing between locally emitted OOAs and those transported regionally, providing a more detailed understanding of OM sources.

Data documentation: All identified OM factors were thoroughly documented with both their mass profiles and temporal variations included. Necessary metadata were associated with the data, ensuring comprehensive documentation ready for sharing. While the relevant EBAS submission procedure is being developed, the documented data is available through temporary solutions, such as SharePoint/email, to ensure immediate accessibility to the data.

4.3 Content of the milestone

Data description: The dataset comprises the source apportionment results of organic matter (OM) in submicron aerosols (PM_1) collected in Dublin throughout 2023. The OM dataset was measured by sophisticated quadrupole aerosol chemical speciation monitor (Q-ACSM), then source apportionment of OM was performed using advanced rolling PMF method combining with Source Finder pro (SoFi Pro), and six OM factors were successfully identified. A machine learning model was developed to further enhance the source apportionment of OOA into locally emitted OOA and regional transported OOA.

Metadata: The dataset is accompanied by comprehensive metadata, detailing information such as the measurement units, station name (Dublin-University College for January to August 2023, or Dublin-Trinity's Botanic Gardens for September to December 2023) and type (urban background site), sampling protocol and period, instruments settings and calibration parameters, contact information of the submitters, the name and descriptions of identified OM factors, and more.

Findability: The dataset is not yet available on EBAS as the submission procedure for OM source apportionment results is still being developed. However, we are actively working on this with EBAS, and the data will be openly available on EBAS in the near future.

Accessibility: While the EBAS submission procedure is being finalized, the documented OM source apportionment data is available through temporary solutions, such as SharePoint/email, to ensure immediate accessibility to the data. Once the submission process is complete, the data will be openly accessible via the EBAS database.

Interoperability: The dataset is prepared following metadata standards and guidelines for ACSM field measurements, which will enhance interoperability with other datasets and platforms once the EBAS submission process is completed.

Reusability: The dataset includes detailed mass profiles and temporal variations of the identified OM factors, along with necessary metadata and error estimations. This comprehensive documentation ensures that the data will be reusable for various research purposes and analyses.

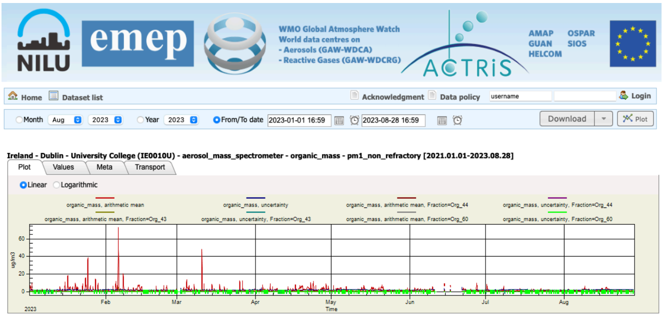

Fig. 1: Screenshots showing uploaded OM data on EBAS website.

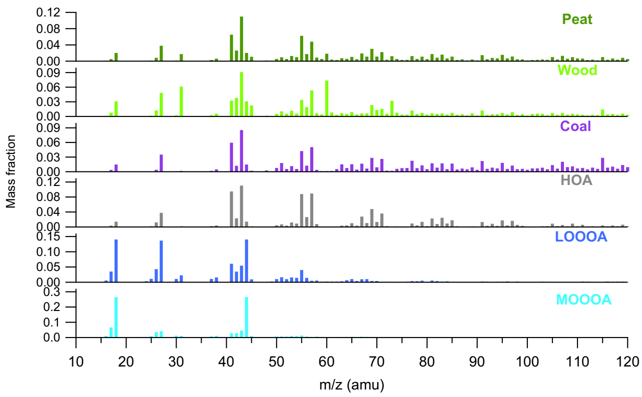

Fig. 2: Mass profiles of six OM factors identified by rolling-PMF in Dublin in 2023

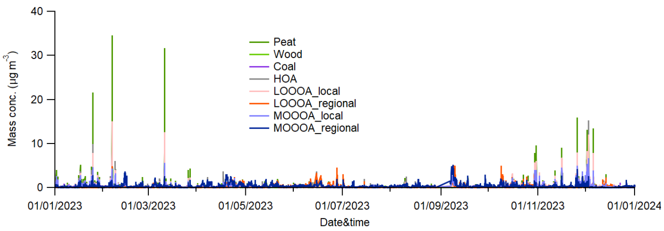

Fig. 3: Time series of OM factors identified by rolling PMF and machine learning approach, including primary OM factors from peat, wood, coal burning and traffic/oil burning (HOA), and two oxidized OM factors, i.e., LOOOA and MOOOA from local sources and regional transport.

4.4 Data description

The validated OM data from Dublin in 2023 has been submitted to the EBAS database, publicly accessible by specifying the country (Ireland), station, and component (organic_mass) on the EBAS website (Fig. 1, https://ebas-data.nilu.no/).

The advanced rolling-PMF was performed for the source apportionment of OM dataset obtained from Dublin in 2023, deconvolving six OM factors. These included four primary organic aerosols originating from peat, wood, and coal burning, as well as hydrocarbon-like organic aerosols (HOA) from traffic and domestic oil burning. Additionally, two types of oxygenated organic aerosols (OOA) were identified: less oxidized OOA (LOOOA) and more oxidized OOA (MOOOA). Fig. 2 depicts the mass profiles of the six OM factors identified by rolling-PMF.

Based on the PMF-redrived OM factors, a machine learning approach was developed to enhance the OOA source apportionment by further separating OOA into locally emitted OOA (LOOOA_local and MOOOA_local) and regional transported OOA (LOOOA_regional and MOOOA_regional). Fig. 3 presents the time series of all OM factors from Dublin in 2023.

The source apportionment data will be submitted to the EBAS database after the relevant procedure is developed within EBAS. The University of Galway has initiated the process to establish this procedure in collaboration with the EU infrastructure project ACTRIS.

4.4 Conclusion and possible impact

The advanced source apportionment of organic matter (OM) in submicron aerosols (PM_1) conducted in Dublin throughout 2023 has yielded significant insights into the sources and dynamics of OM. Using high-resolution data from the Quadrupole Aerosol Chemical Speciation Monitor (Q-ACSM) and advanced rolling Positive Matrix Factorization (rolling-PMF) combined with machine learning techniques, six distinct OM factors were identified. These factors include primary organic aerosols (peat, wood, and coal burning; hydrocarbon-like organic aerosols from traffic and domestic oil burning) and two types of oxygenated organic aerosols (less oxidized OOA and more oxidized OOA). The dataset, although not yet available on EBAS, has been well-documented with detailed metadata, mass profiles, and temporal variations, and is available through temporary solutions until the EBAS submission process is finalized.

The detailed source apportionment provides valuable insights into the sources and relative contributions of different OM factors, thereby enhancing our understanding of urban air pollution. This information is crucial for evaluating and improving model predictions, which in turn enhances the accuracy of regional aerosol models. The comprehensive data and methodologies developed in this milestone support the development of evidence-based strategies for air quality management and environmental protection. The availability of high-quality OM source apportionment data, once the EBAS submission process is complete, will benefit researchers and policymakers across Europe by facilitating further studies and policy development. Specifically, the detailed OM source apportionment results from Dublin in 2023 are particularly valuable for identifying sector-specific emissions. By quantifying contributions from different sources such as biomass burning, traffic, and domestic heating, the project supports targeted emission control measures. Additionally, OM acts as a short-lived climate forcer, influencing regional and global climate patterns. The detailed apportionment of OM sources provides crucial information for assessing their impact on climate dynamics, aiding in the development of mitigation strategies for climate change.

A significant outcome of this milestone is the development of a new source apportionment method that combines rolling PMF with machine learning techniques. This innovative technique can be applied to other locations across the EU, making it a valuable tool for regional studies. Implementing this methodology in various EU regions will enhance the comprehensive understanding of OM sources and dynamics. Furthermore, the methodologies and results from this milestone foster interdisciplinary collaboration among consortium members, promoting innovation and the exchange of knowledge. The data and insights gained can inform EU-wide policies on air quality and climate change, contributing to the broader goals of environmental protection and sustainable development.

In conclusion, the successful completion of M27 not only advances our scientific understanding of OM sources but also provides practical tools and data for improving air quality management and addressing climate change at both regional and global levels. This milestone represents a significant step forward in enhancing our capacity to tackle environmental and public health challenges associated with atmospheric aerosols.

4.5 References

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5. History of the document

Version	Author(s)	Date	Changes
Version 1	L. Lei, J. Ovadnevaite	27/06/2024	New document
	S. Walter	12/07/2024	Final formatting and upload