



TNA User Report

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Project title	Heterogeneous formation of organosulfates : towards a parameterisation of the kinetics - Part 2 : off-line aerosol chemical characterisation
Name of the accessed chamber	OGTAC CC/ LEAK-LACIS
Number of users in the project	1
Project objectives (max 100 words)	The aim of the visit to the calibration centre for organic tracer and particulate aerosol constituents (OGTAC CC) of the Atmospheric Chemistry Department (ACD) at TROPOS was to gain insight and training in the detection and quantification of organosulfates and biogenic SOA marker compounds in chamber-generated SOA with LC/MS techniques.
Description of work (max 100 words):	As part of the training, sample preparation and separation technique (LC/MS) were described and explained in great details. Sample preparation (extraction) was completed under expert supervision. OS and marker quantification measurements on approximately 50 filter samples were prepared, analysed and interpreted. Marker compounds were quantified with authentic standards while OS were interpreted according to their integrated peak area due to the lack of standards.

Principal Investigator's and group's information	
First name	Emilie
Family name	Perraudin
Nationality	French
Activity domain ¹	Chemistry, Earth Sciences & Environment
Home institution	University of Bordeaux
Institution legal status ²	University
Email	emilie.perraudin@u-bordeaux.fr
Gender	Female
User status ³	Academic
New user	Yes

¹ Physics; Chemistry, Earth Sciences & Environment; Engineering & Technology; Mathematics; Information & Communication Technologies; Material Sciences; Energy; Social sciences; Humanities.

² UNI= University and Other Higher Education Organisation;

RES= Public Research Organisation (including international research organisations and private research organisations controlled by public authority);

SME= Small and Medium Enterprise;

PRV= Other Industrial and/or Profit Private Organisation;

OTH= Other type of organization.

³ UND= Undergraduate; PGR= Post graduate; PDOC= Post-doctoral researcher; RES= Researcher EXP= Engineer; ACA= Academic; TEC= Technician.

Trans-National Access (TNA) Scientific Report

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Instructions

Please limit the report to max 5 pages, you can include tables and figures. Please make sure to address any comments made by the reviewers at the moment of the project evaluation (if applicable, in this case you were informed beforehand). Please do not alter the layout of the document and keep it in Word version. The report will be made available on the eurochamp.org website. Should any information be confidential or not be made public, please inform us accordingly (in this case it will only be accessible by the European Commission, the EUROCHAMP-2020 project partners, and the reviewers). Please include:

- Introduction and motivation
- Scientific objectives
- Reason for choosing the simulation chamber/ calibration facility
- Method and experimental set-up
- Data description
- Preliminary results and conclusions
- Outcome and future studies
- References

Name of the PI: Emilie Perraudin

Chamber name and location: OGTAC CC at TROPOS ACD

Campaign name and period: Heterogeneous formation of organosulfates: towards a parameterisation of the kinetics - Part 2 : off-line aerosol chemical characterisation

Introduction and Motivation

Organic compounds make up a large fraction of aerosol particles and vary in composition depending on the meteorological conditions, the location as well as the stage of processing. Thus, aerosol particles contain hundreds of different compounds that may affect the chemical and physical properties and further impacting human health and climate change. Due to the different nature of the particulate organic compounds, a huge ensemble of instruments is necessary to detect and quantify them. The typical set-up for each kind of groups includes a sample preparation, a separation step of the target compounds, the detection of the separated compounds and their quantification using authentic standard molecules. Each step depends on the target compounds and the used technique. Even that many groups are working on the detection and quantification of marker compounds, general guideline and standard operation procedures missing largely. Thus OGTAC CC as first CC worldwide for organic marker compounds provides an enormous benefit for the aerosol community as it harmonizes the analytic of organic particle-phase constituents and builds up a strong network of all groups in Europe working on this area. This OGTAC CC activity was focused on the Liquid Chromatography coupled with

Mass Spectrometry (LC/MS) as it was most suitable for the targets to be addressed in the present project. Targets to be quantified were BSOA marker compounds and organosulfates.

Organosulfates (OSs) are part of the highly complex organic fraction of atmospheric aerosols and have been measured in ambient aerosols, rain and fogwater, in a wide diversity of environments. These compounds have been shown to be of secondary origin and some of them are used as markers for biogenic secondary organic aerosols (BSOAs), enhanced in the presence of air masses from anthropogenic sources. OSs formation pathways have been investigated in laboratory experiments from the oxidation of biogenic volatile organic compounds (BVOCs) and the reactive uptake on acidic sulfate particles of various oxygenated products, amongst them epoxides (such as isoprene epoxydiols or alpha-pinene oxide (aPO)) are the most efficient precursors. However, the debate is still open on whether the OSs found in atmospheric aerosols are also produced by ionic or radical mechanisms.

Scientific objectives

The aims of this TNA visit were i) to gain insight and receive training in the analytical technique of LC/MS, which was developed and is routinely employed by researchers at the host facility, ii) to determine the concentration of BSOA marker compounds iii) to interpret the data obtained for organosulfates. Based on this data and in strong cooperation with the parallel TNA at the ACD chamber insights were gained about the kinetics of OS formation and involved organic species.

Reason for choosing the simulation chamber/ calibration facility

The OGTAC CC was the ideal location to perform this offline chemical analysis as it has the required instrumentation and necessary protocols, as well as the expertise to train and guide visitors. Following training, sample preparation, analysis and quantification was completed under expert guidance and supervision, thus a very valuable data set was generated in an efficient and reliable manner.

Method and experimental set-up

The filter samples were generated in the aerosol chamber at TROPOS ACD (see report for details) by oxidizing alpha-pinene oxide under various conditions. Time-resolved filters were collected every 15 minutes throughout experiments. Two types of filters were used, i.e. PTFE and Fluoropore. By collecting onto two completely different filter materials, information about their applicability for targets can be provided. After collection, half of the filters was extracted and analysed according to Mutzel et al., 2016. The quantification was done with dedicated software (Bruker Quant Analysis) using authentic standard compounds, including terebic acid, terpenylic acid, pinonic acid, pinic acid, MBTCA, and DTAA. For organosulfates, trend analysis was performed by interpreting integrated peak areas.

Outcome and future studies

The main objectives of the proposed TNA activity were successfully completed. A high level of training was received and each of the samples were analysed, generating a reliable data set. The findings of this project will provide new quantitative insights into organosulfate formation. The results obtained during this TNA project in combination with parallel TNA project at the aerosol chamber, will solve few questions about the kinetics of OS formation. More time and work are needed to evaluate the findings

of this project in combination with the huge online data set obtained during the respective TNA project at the aerosol chamber.