

# Deliverable D8.1: Intermediate report on trans-national access to EUROCHAMP-2020 calibration facilities

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This report is based on the intermediate assessment of EUROCHAMP-2020 calibration services and access provision (MS8.3). It comprises the number and quality of access provided so far as well as the actual status of the four calibration facilities, an evaluation of user feedback, and a definition of potential measures to improve the number of access.

#### 1. Numbers and quality of access provided and actual status of the calibration facilities

The overall objective of work package 8 is the provision of access to four calibration facilities complementing the existing calibration opportunities in atmospheric sciences, employing the specific capabilities of atmospheric simulation chamber facilities for calibration purposes. Three of the calibration facilities are candidates to be integrated in the ACTRIS-RI activities in a sustainable manner, e.g. within the Topical centers 'Cloud in situ' and 'Aerosol in situ' as Central Facilities. Within the first three months of the EUROCHAMP-2020 project, the User Selection Panel for the transnational access proposals was established and immediately started to review the first applications. For access to calibration facilities, a specific application form and review protocol were developed. The new, unique, and cost efficient calibration and training opportunities were immediately announced on the website homepage and on websites of the EUOCHAMP-2020 partners, as well as within the ACTRIS community, through the social networks and during several international conferences and workshops. Information about the new calibration opportunities was also distributed during user meetings, to explain possibilities of training and participating to calibration workshops.

In parallel to these activities, calibration protocols were developed and traceability chains were established. Finally, the provision of access to the four calibration facilities has progressively been increasing, especially during the second year of the EUROCHAMP-2020 project. The following table provides an overview of the current usage status und the expected total usage.

Calibration facilities	Unit	Usage		
		expected	so far	
AIDA Calibration Centre for Cloud Physics (ACcloud)	1 DAY	20	-	
Calibration Centre for Soot Measurements (CCSM)	1 DAY	20	6	
World Calibration Centre for Aerosol Physics (WCCAP)	1 RWD	120	9	
Organic Tracers and Aerosol Constituents Calibration Centre	1 DAY (ILC)	100	25	
(OGTAC CC)	1 DAY (Training)	100	25	
Sum (units)		360	65	
Sum (%)		100%	18%	

#### Table 1: Overview of status and total usage



Table 1 shows that at midterm, only 18% of the total expected usage has been spent. This is explained mainly by an induction period lasting for the first year until the information about the new calibration opportunities had been spread and trans-national access activities could be planned and applied for. With the access activities planned for ACcloud, CCSM, and OGTAC CC there is a very good chance that all expected access units will be used during the project (cf. Table 2). However, more advertisements, with a special focus on WCCAP, seems to be necessary in order to spend all user units allocated within the four years.



#### Table 2: Overview of actual and planned trans-national access activities

## **User statistics**

Of the 29 individual users of calibration facilities the majority were females and from groups outside the EUROCHAMP-2020 consortium (cf. Figure 1).









Figure 2: Access to calibration centres by new users

Almost 80% of the users had never before used the EUROCHAMP-2020 calibration facilities.

The progress achieved in the individual calibration facilities as well as the details of the Trans National Access activities are outlined in the following.

#### AIDA Calibration Centre for Cloud Physics (ACcloud)

Based on a previous collaboration with the German national institute of standards, **KIT** developed dedicated protocols for the calibration of a broad range of atmospheric hygrometers like radiosondes, dew point mirrors, photoacoustic hygrometers, and various spectroscopic methods at or within the AIDA chamber. This included the validation of the traceability of the reference hygrometer to national standards and procedures for the connection or inclusion of the instruments to be calibrated to the AIDA chamber.



Figure 3: The water vapour pressure measured inside the AIDA simulation chamber in presence of dense ice clouds (red circles) agrees well with the water vapour pressure calculated according to the equation by Murphy & Koop (2005).

To validate the intrinsic AIDA reference by

generating dense clouds which provide saturated conditions (~ 100% RH), a series of new cloud experiments were done. As one example, Figure shows the excellent agreement of the water vapour pressure measured inside dense ice clouds with the water vapour pressure calculated with the temperature dependent parameterization given by Murphy & Koop (2005). The in situ (inside the cloud) measurements by a tuneable diode laser hygrometer was, within uncertainty limits, also in agreement with a reference frost point mirror hygrometer (traceable to national standards). An international hygrometer calibration workshop is planned for February 2020.



KIT published first results of the Fifth International Ice Nucleation Workshop (FIN) hosted at the AIDA facility (DeMott et al., 2018) providing a basis for further developing ACcloud.



Figure 4: Comparison of various ice nuclei counters during the Fifth International Ice Nucleation Workshop (FIN) at ACcloud.

Furthermore, KIT the University of Leeds and Bilfinger Noell GmbH developed and validated a new Portable Ice Nucleation Experiment (PINE) at ACcloud. This new instrument will be the first instrument of its kind for fully-automated long term INP measurements at high sensitivity and time resolution. A commercial version of PINE is developed together with Bilfinger Noell GmbH and will be available from early 2019. Protocols for calibrating mobile INP instruments are currently finalized.

A first INP intercomparison and calibration activity at ACcloud is planned for May 2019. The ACcloud is part of the proposal for the ACTRIS topical center "Cloud in situ".

## Calibration Centre for Soot Measurements (CCSM)

**PSI** established the Calibration Centre for Soot Measurements (CCSM) and developed requirements and approaches to achieve traceability and harmonization of *refractory Black Carbon* (rBC) mass measurements. Black Carbon (BC) mass measurements are common across the whole atmospheric chemistry community. Yet each technique has its own characteristics and caveats that are often overlooked. The simulation chamber can provide a platform to characterize the different techniques. In order to better relate the different techniques, quantitatively, and traceably, there are requirements for the harmonization and traceability across the methods. The harmonization and standardization of calibrations and general measurement will go some way to reconcile the different techniques. Figure shows an example time series of measurements of "black carbon mass" from 5 different instruments based on 3 commonplace methods: 1) Equivalent black carbon (eBC) mass inferred from light absorption coefficient, 2) Thermal-optical elemental carbon (EC), 3) Laser-induced incandescence (LII) resulting in refractory black carbon (rBC) mass. Whilst the qualitative agreement is good, in



absolute terms the choice of instrument will determine the "measured" BC mass and thus influence subsequent scientific interpretation.



The strategy of the CCSM is to provide the platform for the harmonization and traceability across the methods, with a focus on rBC mass measurement. The suite of instrumentation combined with excellent scientific and technical knowledge at the CCSM is extremely useful in providing the tools required to make accurate and traceable measurements of rBC. For example, *the ideal calibration approach* for the single particle soot photometer (SP2) is to reference against a particle mass classifier (PMC) on a single particle level specifically for the BC type under investigation (PMC mass selection to be cross-checked with traceable PSL size standards). This requires availability of the BC type of interest in pure form such that classified particle mass equates BC mass. Figure 4a shows the setup for this ideal calibration approach. It is further required to establish traceability of number concentration measurements (either a referenced and traceable CPC, or an electrometer). *Only the combination of traceable BC mass concentration.* 





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In practice it is not always possible to perform "ideal" experiments for a number of reasons. BC properties vary between sources and combustion conditions, and the BC types of interest are not always available in pure form. Therefore *the primary goal of the LII harmonization activities at PSI facilities is to ensure proper instrument performance and harmonization using a suitable reference BC aerosol* following the setup shown in Figure 4b. However, PSI and the CCSM appreciate that it may be desirable for expert users to independently perform *BC-type specific calibrations*. Figure 4c shows the proposed setup for such a calibration, whereby the BC-type aerosol of interest is thermally denuded (to remove any non-BC components), mass classified,



Figure 7: Calibration curves of the SP2 differ with BC type. High EC mass fraction CAST soot is an additional artificial BC type used at the CCSM as the sensitivity of the SP2 to CAST soot is comparable to its sensitivity to typical ambient BC.

and then measured by an SP2 (e.g. Broda et al., 2018). As shown in Figure 5 the SP2 proportionality constant (derived from raw signals) is known to depend on BC type (Moteki et al. 2010, Baumgardner et al., 2012, Laborde et al., 2012), and thus ideally all instruments SP2 would be calibrated and then backreferenced to a "standard" BC material such as Aquadag. The role of the CCSM would be to provide its expertise to the wider SP2 community such that ambient rBC measurements from SP2s around the world, in different environments and on different be traced back and compared with far higher certainty than is

currently offered from the factory. Further to continuous wave LII, the CCSM aims to include the original pulsed-shot LII technique in the general CCSM activities. Although traceability for pulsed-shot LII can in principle be independently established, the main goal of the CCSM within the EUROCHAMP-2020 activities is to achieve harmonization (and quantification of related uncertainties) of the pulsed-shot LII approach with the SP2 measurements.

So far, PSI has organized one **TNA activity** at the CCSM and the next, a major calibration workshop, is planned for spring 2019:

1. **CCSM-001-2017**: The Institute of Atmospheric Sciences and Climate (CNR-ISAC) participated in a calibration and training activity for single particle soot photometer related to deploying SP2 instruments during the ACTRIS-JRA1 campaign at Mt. Cimone



and Bologna in 2017 and a field experiment in Bolivia at the Chacaltaya GAW station (TNA PI: A. Marinoni).

2. Provisionally planned for spring 2019: an SP2 calibration workshop at PSI facilities focusing on instrument best practices for a consistent and harmonized SP2 calibration with the specific goal of instruments being prepared for the Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAIC) deployment in 2019/2020. The aim is a joint pre-deployment calibration and to train users how to consistently process the raw data. SP2 manufacturer Droplet Measurement Technologies (DMT) has confirmed their attendance and will supply the new SP2-XR instrument, MOSAIC participants will attend where possible, and remaining slots will be open to other interested parties.

## Organic Tracers and Aerosol Constituents Calibration Centre (OGTAC CC)

**TROPOS** established within the framework of EUROCHAMP-2020 a calibration centre for the analysis for organic tracer and aerosol constituents (OGTAC CC). This new calibration center is focused on the most up-to-date techniques for the molecular analysis of the organic composition of the atmospheric aerosol and include among its target key organic for tracer which are extremely useful for both sources and processes apportionment. For this reason, its service is extremely valuable to harmonize the practices among the chamber community with respect to organic analytical chemistry and to provide references for the field and observation community. OGTAC CC provides training of users with advanced analytical techniques and inter-laboratory comparison (ILC).

For the first OGTAC CC activity (**OGTAC CC-Training-001-2017 and 002-2017**) the topic of Liquid Chromatography coupled with Mass Spectrometry (LC/MS) was selected as this is the most dominating technique for the target analysis of atmospheric relevant tracer compounds. The analytical training course focused on the target analysis of atmospheric relevant particle-phase constituents. The training offered the possibility to all applicants to get practical training at state of the art instruments, discussions with experts, and to strengthen their network.

Within two weeks (10 Access days) 11 international users from France, Spain, Poland, Ireland, Romania and Denmark and 7 national users from Germany were trained. The training conducted focused on the application of LC/MS for the analysis of atmospherically relevant particulate products. In particular High-Performance Liquid Chromatography Electrospray Ionization coupled to Time-of-Flight Mass Spectrometry (HPLC/(-)ESI-TOFMS), Ultra-Performance Liquid Chromatography Electrospray Ionization a Time-of-Flight Mass Spectrometer (UPLC/ESI-IMS-QTOFMS).

The course covered:

- Training at the HPLC/ESI-TOFMS and UPLC/ESI-IMS-QTOFMS;
- Lectures in atmospheric particle related chemical analysis;



- Practical training for filter collection, extraction, analysis and quantification of target compounds;
- Derivatisation and enrichment procedures.

Thus, within one week the participants learned each step from sample collection to quantitative data analysis, with special emphasis for a high level of QA/QC during each phase of sample treatment. Due to the high number of proposals received, a few had to be rejected because of capacity limitations. However, most of them applied for the upcoming training course on LC/MS, which is therefore already booked out.

Seven of the users of the analytical training course participated afterwards also in an interlaboratory comparison (**OGTAC-CC-ILC-001-2018**) organized by the OGTAC CC. In total 13 laboratories from Europe (France, Spain, Germany, Poland, Denmark, Switzerland, Slovenia and UK) and the US participated. The ILC comprises the distribution of filter samples collected in the TROPOS ACD aerosol chamber LEAK and at the TROPOS research station Melpitz (Germany) with subsequent chemical analysis at the participating laboratories. This activity was finished at the end of August 2018.

FirstName/Name	Gender	Institution	Institution	User	New
			country	status	user
Elena Gómez Alvarez	F	University College Cork	Ireland	PDOC	Yes
Niall P. O'Sullivan	М	University College Cork	Ireland	PGR	Yes
Aline Gratien	F	CNRS-LISA	France	ACA	Yes
Cecile Mirande-Bret	F	CNRS-LISA	France	EXP	Yes
Cornelia Amarandei	F	Alexandru Ioan Cuza University of Iasi	Romania	PGR	Yes
Georgiana Balusescu	F	Alexandru Ioan Cuza University of Iasi,	Romania	PGR	Yes
Nathalie Hayeck	F	CNRS- IRCELYON	France	PDOC	Yes
Teresa Vera	F	Fundacion CEAM	Spain	PDOC	yes
Agata Kołodziejczyk	F	Institute of Physical Chemistry Polish Academy of Sciences	Poland	PGR	yes
Kumar Sarang	М	Institute of Physical Chemistry Polish Academy of Sciences	Poland	PGR	yes
Shamjad Moosakutty	М	Aarhus University	Denmark	PDOC	Yes

## Table 3: List of international participants at OGTAC CC ILC (TNA granted)

In addition to the TNA users also 7 national (German) users participated in the activities at OGTAC CC. This shows the attractiveness of the calibration facility and led to intensified knowledge exchange and networking during the TNA activities.

In October 2018, a third TNA Training activity (**OGTAC-CC-Training-003-2018**) was performed at the CC, focusing on detailed molecular characterization of organic aerosols from Domestic Solid



Fuel burning (DSF). The user group (University of Cork) aimed to identify and quantify well-known combustion markers in ambient and fuel-burning samples of PM, but also new combustion markers for different fuel types to support apportioning potential contributions of coal, peat and wood burning to ambient levels of PM. The training focused on HPLC/ESI-TOFMS, HPAEC-PAD, and CPP-GC/MS.

## World Calibration Centre for Aerosol Physics (WCCAP)

TROPOS established the WCCAP in 2002 to serve as a competence center for in-situ physical and optical aerosol measurements as part of the worldwide GAW-program of the WMO. This WCCAP is worldwide unique for the quality assurance of physical and optical in-situ aerosol measurements and station audits to improve infrastructures. As part of the European Centre for Aerosol Calibration (ECAC, <u>www.actris-ecac.eu</u>), the WCCAP provides Calibration and Intercomparison Workshops especially for the ACTRIS community with focus on the following instruments:

- Condensation Particle Counter CPC
- Mobility Particle Size Spectrometer MPSS
- Aerodynamic Particle Size Spectrometer APSS
- Optical Particle Size Spectrometer OPSS
- Integrating Nephelometer IN
- Absorption Photometer AP
- Extinction Monitor EM
- Cloud Condensation Nuclei Counter CCNC
- On-Site Intercomparisons & Audit OSIA (only for MPSS)

Since May 2015 more than 563 instruments have been calibrated.

In EUROCHAMP-2020 the WCCAP has two main objectives: increasing the quality of aerosol measurements within EUROCHAMP-2020, and providing external users with more access to the WCCAP. A EUROCHAMP-2020 internal survey evaluated in 2018 the amount and diversity of physical aerosol instrumentation suitable for WCCAP services.

A first calibration workshop especially for the EUROCHAMP community with focus on Condensation Particle Counter and Mobility Particle Size Spectrometer has been organized in June 2018 (TNA projects of **WCCAP-001-2018** and **002-2018**). Further calibration workshops are scheduled for 2019.

The WCCAP is part of the proposal for the ACTRIS topical center "Aerosol in situ".

## 2. Evaluation of user feedback

So far, no user feedback is available for the AIDA Calibration Centre for Cloud Physics (ACcloud). However, ACcloud received several positive comments on previous



intercomparison and calibration activities at the facility as well as expressions of interest to participate in future intercomparison and calibration activities.

User feedback on the first calibration activity at the Calibration Centre for Soot Measurements **(CCSM)** in February 2018 was very positive for both training and calibration activities.

"The facility was very useful both in providing training for evaluating previous measurements (including calibrations) and in optimizing and calibrating the SP2 instrument for the following field campaign in Bolivia. PSI laboratories were very well equipped for our purpose and people extremely available to help to collaborate to reach the goal of the SouMount Project."

User feedback on the first calibration activity at the World Calibration Centre for Aerosol Physics **(WCCAP)** was very positive on the high quality of service provided compared to the costs.

"It is extremely useful to have the opportunity to get aerosol instruments like CPCs calibrated at the WCCAP. It is not only much cheaper than calibrations e.g. by the major manufacturers but the WCCAP gives also very useful advices for instrument operation and applies adjustments to the instruments. The complete calibration procedure is done in a very professional manner."

The Organic Tracers and Aerosol Constituents Calibration Centre **(OGTAC CC)** conducted two training sessions with 20 participants from France, Spain, Poland, Ireland, Romania and Denmark and Germany. All users were asked to answer a feedback questionnaire including the following points: overall impression, organisation, balance between theory and practical work, structure of the course, content, oral presentations, and practical part. Everybody could rate between 1 (excellent), 2 (very good), 3 (good), 4 (fair) and 5 (poor). All participants filled the questionnaire. Analysis of these questionnaires resulted in an average rating of 1.7, which can be counted as very good. Finally, the participants were asked if they would recommend this course. In this case a unanimously result was obtained as all participants recommended the course.

The majority of the users highlighted the importance of the possibility to learn and train all necessary basics. All of them joined the discussion during the lectures and during the handson sessions. Few users also made suggestions for improvements and these will be taken into account for up-coming sessions. They include an extension of the practical part and a dedicated session on method development.

## 3. Potential measures to improve the access to the calibration facilities

In order to better disseminate the possibilities offered by the EUROCHAMP-2020 calibration facilities, the respective calls will be advertised using the ACTRIS mailing list and on their meetings. If possible, a link to the calibration facilities will be added at the ACTRIS homepage and a survey among ACTRIS partners for suitable instruments will be made. Furthermore, the calls for



calibration workshops will be advertised at universities known to use respective instruments and via the European aerosol societies (e.g. WCCAP). Companies like instrument manufacturers will be invited to participate in calibration workshops to increase the attractiveness for all users. To improve the attractiveness also for students they should receive credit points for training activities wherever this is possible. The calibration opportunities will be featured stronger at conferences e.g. at the EUROCHAMP-2020 booth or in suitable presentations. Contacts to national institutes of standard will be used to identify and address further potential users.

#### 4. Intermediate assessment summary

After an induction period of one year, the usage of the EUROCHAMP-2020 calibration facilities has increased significantly. A poll among the EUROCHAMP-2020 partners regarding aerosol instrument calibration allowed to quantify the short- and mid-term needs. Still some more advertisement about the new calibration opportunities is needed especially also outside the EUROCHAMP-2020 community. Measures to achieve this have been defined and are under way. However, most of the calibration opportunities are used as expected. The majority of users are females from groups outside the EUROCHAMP-2020 consortium which have not been at the calibration facilities before.

By the end of the project and in the perspective of building ACTRIS-ERIC, all participating EUROCHAMP-2020 groups will set up a QA/QC plan that includes their participation in the calibration activities. Three of the four EUROCHAMP-2020 calibration activities are included in proposals to become part of the topical centers 'Aerosol in situ' and 'Cloud in situ' in the ACTRIS-ERIC.

All user feedback was generally very positive with special emphasis on the personal engagement of the people at the calibration facilities. Some of the feedback can be used to improve the service offered.

#### **References:**

- Baumgardner, D., Popovicheva, O., Allan, J., Bernardoni, V., Cao, J., Cavalli, F., ... Gonzalez, C. (2012). Soot reference materials for instrument calibration and intercomparisons: a workshop summary with recommendations. Atmos. Meas. Tech, 5, 1869–1887.
- Broda, K. N., Olfert, J. S., Irwin, M., Schill, G. P., Mcmeeking, G. R., Schnitzler, E. G., ... Jiang, J. (2018). A novel inversion method to determine the mass distribution of non-refractory coatings on refractory black carbon using a centrifugal particle mass analyzer and single particle soot photometer.
- Cavalli, F., Viana, M., Yttri, K. E., Genberg, J., & Putaud, J.-P. (2010). Toward a standardised thermal-optical protocol for measuring atmospheric organic and elemental carbon: the EUSAAR protocol. Atmos. Meas. Tech, 3, 79–89.
- Kanaya, Y., Taketani, F., Komazaki, Y., Liu, X., Kondo, Y., Sahu, L. K., ... Takashima, H. (2013). Comparison of Black Carbon Mass Concentrations Observed by Multi-Angle Absorption Photometer (MAAP) and Continuous Soot-Monitoring System (COSMOS) on Fukue Island and in Tokyo, Japan. Aerosol Science and Technology, 47(1), 1–10.
- Kondo, Y., Sahu, L., Kuwata, M., Miyazaki, Y., Takegawa, N., Moteki, N., ... Kita, K. (2009). Stabilization of the Mass Absorption Cross Section of Black Carbon for Filter-Based Absorption Photometry by the use of a Heated Inlet.



Aerosol Science and Technology, 43(8), 741–756.

- Kondo, Y., Sahu, L., Moteki, N., Khan, F., Takegawa, N., Liu, X., ... Miyakawa, T. (2011). Consistency and Traceability of Black Carbon Measurements Made by Laser-Induced Incandescence, Thermal-Optical Transmittance, and Filter-Based Photo-Absorption Techniques. Aerosol Science and Technology, 45(2), 295–312.
- Laborde, M., Mertes, P., Zieger, P., Dommen, J., Baltensperger, U., & Gysel, M. (2012). Sensitivity of the Single Particle Soot Photometer to different black carbon types. Atmospheric Measurement Techniques, 5(5), 1031–1043.
- Miyazaki, Y., Kondo, Y., Sahu, L. K., Imaru, J., Fukushima, N., & Kano, M. (2008). Performance of a newly designed continuous soot monitoring system (COSMOS). Journal of Environmental Monitoring, 10(10), 1195.
- Moteki, N., & Kondo, Y. (2010). Dependence of Laser-Induced Incandescence on Physical Properties of Black Carbon Aerosols: Measurements and Theoretical Interpretation. Aerosol Science and Technology, 448(44).
- Murphy, D., M., Koop, T. (2005) Review of the vapour pressures of ice and supercooled water for atmospheric applications, Q. J. R. Meteorol. Soc., 131, pp. 1539–1565.