

EUROCHAMP-2020 – ACTRIS TC technical workshop

Monday 12th October

Participants: Bénédicte Picquet-Varrault (CNRS), Matilde Oliveri (CNRS), Jean-François Doussin (CNRS), Paolo Laj (CNRS), Kristina Höhler (KIT), Ottmar Möhler (KIT), Alfred Wiedensohler (TROPOS), Amalia Muñoz (CEAM), David Bell (PSI), Dennis Niedermeier (TROPOS), Cathrine Lund Myhre (NILU), Markus Fiebig (NILU), Evelyn Freney (CNRS), Gordon McFiggans (UMAN), Hartmut Herrmann (TROPOS), Hendrik Fuchs (FZJ), Silvia Danelli (INFN), Iulia Patroescu Klotz (BUW), Falk Mothes (TROPOS), Iustinian Bejan (UAIC), Martin Brüggemann (TROPOS), Max McGillen (CNRS), Mila Rodenas (CEAM), Niklas Illmann (BUW), Rainer Steinbrecher (KIT), Rami Alfarra (UMAN), Romy Fösig (KIT), Stéphane Sauvage (IMT), Thérèse Salameh (IMT), Thorsten Hohaus (FZJ), Jan Kaiser (UEA), Romeo Olariu (UAIC).

An initial presentation is given to the plenary by Bénédicte Picquet-Varrault (CNRS) on the objectives of the meetings and the expected outcomes.

Trace gas measurements (Thérèse Salameh- IMT)

Thérèse Salameh presents the services offered by the Centre for Reactive Trace Gas In-Situ. Following the presentation, it is asked to better specify which services could be particularly tailored for simulation chambers. Those are:

- Travelling standards, as chambers will work on higher concentrations
- Standard operating procedures (SOP) should also be used by chambers
- Advocate tools: transferable to EUROCHAMP needs?
- Flagging: working with ambient level of concentrations. Thérèse S. wonders if this may be of relevance for chambers' needs.

Jean-François Doussin (CNRS) believes that, rather than the level of concentration, the plausibility check is the key aspect; in addition, the most complex aspect, which is not taken into account here, is the data submission process. Stéphane Sauvage (IMT) underlines that their validation process is experiment based and therefore suitable for chambers' data.

After several contributions, it results that there is a necessity to improve level of information, in order to improve the traceability of data. Markus Fiebig (NILU) also underlines that if the Ci-Gas centre is not collecting level 0 data, then it should be written in their data policy.

Paolo Laj (CNRS) asks whether it is clear who is responsible, in the different NFs and TCs, for setting up the instruments, since all instruments should follow some specific standards.

From the discussions, a clear need for an overview of the services provided by each instrument is currently missing. Bénédicte P.V. suggests to have a list of base instruments, for which SOP should be used. The final objective would be to improve the traceability of the data. If this is already available for Ci-Gas, then Thérèse S. can send it to Bénédicte P.V.

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For Ci-Gas, the offered services are reviewed one by one, to check which ones are already suitable for simulation chambers, and which other should be adapted. Among the list, the ones needing particular adaptation are the following:

- Measurement guidelines: the SOP proposed by Ci-Gas should be suitable for observational and exploratory platforms, but it would be necessary to double check this aspect.
- Innovation developments: this service can imply a strong collaboration with chambers, it is very suitable.
- Station performance: chambers could participate to this exercise through the validation of their instruments and as host platforms to run intercomparison campaigns. On this point, Paolo L. underlines the need to always consider how to fund such intercomparisons, which use a NF for a TC calibration exercise. Will they rely on EU funds, like ATMO-ACCESS? This needs to be kept in mind.
- Station audits: this service is linked to the NF labelling process and could be suitable and useful for chambers, for calibration issues or data validation. Paolo L. asks whether the TC staff has the expertise to evaluate chamber instruments linked to trace gas, considering that their expertise is mainly based on observational platforms. Stéphane S. believes that the team has very complementary expertise, which can fulfil this type of audit.
- Data review process: this service, in particular the quality check, needs to be adapted for chambers, as discussed before. Stéphane S. underlines that it is still not sure for him whether they have the full expertise needed to evaluate the quality of the data coming from all the different types of experiments performed. Jean-François D. explains that every day a different experiment can be performed, so going in such a level of detail is too complex for TCs. Probably, the whole data validation process needs to be adapted, it is not possible to use the same one as for observational platforms.

→ To work on this particular service, it is proposed to establish dedicated working groups to build data workflow per each instrument, composed of TC responsible and representatives of the chambers. The objective will be to provide a document with the dedicated services for each instrument. For Ci-Gas, after an internal discussion, the most suitable representative will be defined.

Aerosols measurements

European Centre for Aerosol Calibration and characterization (ECAC) Alfred Wiedensohler - TROPOS

Paolo L. asks to Alfred W. whether they already have an overview of the different MPSS operated in chambers. It is replied that currently the TC staff does not have a precise overview, they estimate that the instruments are mainly TSI, probably from relatively old versions, which sometimes have problems for converting data into the format of level 0 ACTRIS data. Currently an internal discussion is taking place at ECAC to decide to which models they will provide certifications.

Gordon McFiggans (UMAN) points out that their instruments are sometimes modified, to perform activities at very different concentrations, their activities differing a lot. Alfred W. specifies that they haven't set any criteria for chambers yet, but they surely will have to ensure that these instruments fulfil some minimum parameters to perform high quality measurements. If they have to work on

instrumentation with which they are not familiar, from unknown manufacturers, they have to perform a case-by-case analysis and ensure their high quality.

Jean-François D. asks about access to the script for analysis of SMPS data. Being able to analyze data with this script would be a significant improvement, as most chambers use TSI instruments, whose calculation system is very complicated and inaccessible. But he is not sure whether the provided code would work for a commercial non modified TSI SMPS.

Alfred W.: they will provide a tool to convert the data into the level 0 of ATRIS. Each NF can then send the data to NILU and it will be included. But this not for all TSI systems, this is why they are investigating which models should be considered as minimally reliable. The old versions have several problems, in general instruments should be updated, and for this the implementation phase will be crucial.

Jean-François D. continues on the comment made by Gordon M. underlying that sometimes at chambers, base instruments are modified for specific applications. So it should be decided whether these instruments should be considered as base or specific ones. Alfred W. replies that they are fully aware that many variables at chambers cannot be quality assured, they will provide such QA only for base instruments. Additional measurements won't be considered because they are not ACTRIS variables.

→ In any case an instruments can be modified, but it remains a base instrument when it measures a base parameter (or ACTRIS variable).

David Bell (PSI) asks about the recommended frequency of CPC calibrations and how long calibrations last. Alfred W. replies that it depends on how intensively the instrument is used, and at which concentration. Normally calibrations should be performed on a yearly basis, but if it is used at high concentrations, then a calibration would be necessary every half year. Concerning the duration, one days is necessary to perform the actual calibration, but together with the shipping and the cleaning, the whole process can last up to one week.

Recent advances in nanoparticle characterization and harmonization (Tuukka Petäjä – UHEL)

Gordon M. underlines that this is a very interesting contribution to the EUROCHAMP handbook and it can help to bridge a gap. Looking at the Nature article, what sort of recommendation is given to approach the problem of chamber wall losses?

Tuukka P. admits that there is gap in the protocol where this aspect is not tackled well enough. He suggest to work together on this particular aspect of measuring aerosols into chambers and of interpreting the concentrations of precursors. Surely there are influences from the chamber walls.

Paolo L. asks what the next steps are, considering that the service is not available yet, and how things will be put in place considering that at this stage, no nanometer information is provided by chambers in the DC. What is plan to implement this specific service? Tuukka P. replies that they are currently developing this SOP for particle size magnifier and, thanks to this meeting, they will be able to include the SOP for the chambers as well.

Bénédicte P.V. asks whether it is planned to involve the chamber community in the upcoming implementation phase. Tuukka P. believes that the chambers should participate, but rather in the part

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related to oxidized organics (coordinated by Tuija Jokinen – UHEL, who is in contact with the chambers' group).

→ The practical next step to surely work on is the Handbook, because the chambers' group knows which contribution they could mainly add.

Aerosol Chemical Monitor Calibration Centre ACMCC (Evelyn Freney – CNRS)

Jean-François D. underlines that indeed ACSM are probably not the most relevant instruments for chambers, AMS are more often used. He asks how the service can be adapted to include AMS and so benefit to chambers. Evelyn F. states that initially all AMS instruments should be calibrated for the mass calibration in the same way as the ACSM; for the size distribution calibration, this still needs to be implemented as part of the protocol they provide.

Jean-François D. is not sure that large intercomparisons, which seem to be the main service provided by AMCC, are suitable for chambers. What could be more of interest for chambers? Evelyn F. believes that such large intercomparisons could be interesting for AMS instruments associated to chambers to identify issues for different organic species by using the chamber environment.

Gordon M. asks for clarifications on what is actually meant in ACTRIS as level 0 data product for mass spectrometers and how the process to get to data products delivered from the ACSM or AMS is incorporated in the TC. Will derived products be considered as standardized products?

Evelyn F.: for now the submitted data from NFs is not level 0, it is already concentration of organic sulfates, nitrates, etc. They are not providing more advanced products, but this will surely evolve with this work together with chambers.

Organic tracers and aerosol constituents Calibration Centre OGTAC-CC (Falk Mothes – TROPOS)

Jean-François D. underlines that the focus of this service is to have instruments working in a classical mode and having people being trained on how to use, so the focus is on the parameters. Falk specifies that indeed the objective is to recommend a specific calibration procedure.

Jean-François D. suggests to better specify the list of target compounds and how it can evolve for needs of chambers and other NFs as well. Falk M. agrees that indeed this list has not been created yet, some work is currently being done on biogenic organic compounds, and a call will be published in the framework of EUROCHAMP-2020 for an inter-laboratory campaign on anthropogenic compounds.

Hartmut Herrmann (TROPOS) adds that they already had two other ILCs on particle phase products on POV oxidation. They can of course adapt these works to the needs of both communities.

Jean-François D. asks if, in the future, it is foreseen to have some sort of OGTAC certification for users, and which will need to be verified every year or so.

Falk M.: if at OGTAC we are able to set up some SOPs together with the different communities during the implementation phase, we will have a clear standard procedure that all users will be able to follow; this goes beyond simple training, which is an added value that we offer, but the SOP will allow everyone to

follow the recommended procedure for a given instrument. The current activity is more linked to training, but this will evolve to become more QA/QC provision.

Paolo L. asks to Alfred W. about the link with the unit in Italy for metals and dust, which should be part of the TC. For metals and dust. Alfred W. it is not sure that this is needed for the work performed in chambers. It is replied that yes, some experiments linked to dust and to fossil fuel and car emissions (so heavy metals) are performed in chambers. The Italian unit focuses more on elemental analysis, so relevant for car emissions, even though it is not sure if they can distinguish between fossil fuel and biomass fuel.

→ Evelyn F. asks if there is a way to see all the instruments operated at the different chambers. It is available, even if probably it is not fully updated, and can be asked to Matilde O. Anyway, the pages on the website are updated.

The possibility to organize an intercomparison of ACSM and AMS at chambers is raised by Evelyn F. It is of course possible, for example one is scheduled for organic nitrates in HELIOS (in the ACROSS project).

Conclusions:

While some TC units are already set up, some others are still building the experimental protocols, so the collaboration with chambers is fundamental should participate to develop them

→ Necessity to create specific working groups: for trace gas, for aerosols and for clouds. Everyone interested in participating should contact Bénédicte P.V.

Tuesday 13th October

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Topical Centre for Cloud In-Situ Measurements – CIS (Kristina Höhler – KIT)

Jean-François D. wonders if the technology and the science provided are mature enough to provide techniques and standard protocols; he also asks about the base and specific instrumentation in relation to chambers.

Kristina agrees that the instruments are very new, but there is some common base science on how to measure INP and on how to treat the data; even if there no historic work, the community is present and willing to create SOPs. The implementation phase will be fundamental. Ottmar Möhler (KIT) reinforces the reply, stressing that scientific importance of ice nucleating particles in the climate system. They are not starting from zero, many intercomparisons were done in the past.

Jean-François D. doubts that a significant number of chambers will work on ice nuclei in the future; this may change if the PINE instrument becomes more reliable, but so far it does not seem realistic. The

chambers which are currently measuring ice nuclei are already expert in the subject, and are already part of the TC.

Ottmar M.: the objective of today is indeed to address those who already measure ice nuclei to increase the collaboration, if others are interested for example to complement aerosol studies with INP measurements, this can be some form of new collaboration.

Hartmut H. underlines that the work done in the TC can be relevant, for example, for measuring sulfate, which is cloud produced. Another good link with EUROCHAMP work is the need to analyze cloud droplets. Another example again is the modelling work being done in E2020, which could be extended to ecosystems.

→ Kristina H. asks to receive the list of instruments operated in chambers.

Jean-François D. does not question the expertise and their research, he doubts about the interest of this service and its costs: France is reluctant to connect the CESAM chamber to CIS, because of its high costs and because its interest is not clear. Ottmar M.: they already have one customer for INP, which is starting now, assembling and offline analysis are already reliable and accurate. The IMP part is indeed the moment to write SOPs, get feedback and contribution from the rest of the community.

Bénédicte P.V. believes that the service provided can be useful. She rather questions the expected number of users (necessary to reduce the costs): it is not sure that the number can really increase, as very few chambers can generate clouds. Many are Teflon made, and can generate SOA and then study the capability of these particles to serve as ice nuclei. The service proposed here is different than providing SOP for calibrating cloud nuclei instruments, those instruments will be bought by few chambers, because of their specific design. This aspect has implications on the cost of the service. But this can be a subject for the TC dedicated working group.

Kristina H.: at this stage it is not necessary to establish a chambers working group, but rather invite chamber representatives to join the NF workshop, which will take place next February. In addition, some countries have not defined their NFs yet, so it is possible that more chambers will be interested in the end.

Bénédicte P.V.: either we consider that this instrumentation is not mature enough to have SOP, and in this case it ends in the specific instrumentation, leaving more flexibility for the data workflow; or if we decide that it is mature enough, in that case we need to create our data workflow, and this is the specific objective of the working groups. The group is fundamental, and participating in one workshop would not be enough. Kristina H. agrees but, in order to avoid a too complex and parallel structure, she wants to stress the need that this groups is part of the overall discussion with all the other NFs.

Chamber operations and experimental protocols (Astrid Kiendler-Scharr – FZJ)

Bénédicte P.V. asks whether it is relevant to propose standard protocols for experiments in chambers. Hendrik Fuchs (FZJ) believes that the experimental protocol highly depends on the scientific objective of each experiment, so in his opinion it is difficult to generate standard protocols to be followed in any situation. But he suggests to add a category of experiments in the Data Center called “chamber characterization experiments”, where such experiments could be added. Bénédicte P.V. agrees with that.

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Rami Alfarra (UMAN) asks for more clarifications on the difference between original and classical protocols. He agrees with Hendrik F. that some standard guidelines (general procedures to follow like how to clean, etc.) could be defined, but not precise protocols, since they would be too specific for each chamber.

Ottmar M.: a protocol does not necessarily need to include all these details, it is rather an overview of you performed the experiment, the instruments used, etc.

Astrid K.S.: it depends on the goal of such protocols: are they meant to be used for the harmonization and intercomparability of chambers or are they specific for each chamber?

In conclusion, from the discussions it seems that the two proposed branches (original protocols and classical protocols) are not relevant. Classical protocols for which standard protocols should be followed, are too difficult to define. It would rather be better to work on a single branch, or type of protocols. The next steps are:

- 1) to provide guidelines to run experiments. Could this be done through the Handbook or should we go more in detail?
- 2) to create a new type of experiments (“characterization experiments”) in the DC.

Rami A. suggests to first define the purpose of these protocols. Once this is defined, it will help shaping the next steps. Jean-François D. considers that the level of information needed is the one necessary for an external user to download the experimental data and to be able to re-use it.

Astrid K. S. proposes to have a shared understanding of the level of details, and once it is agreed, to make sure these details are written. It is also necessary to decide how these procedures are provided to users: through a simple document? How should the current lab books be made available for external users? And how to define the linking characterization experiments?

Bénédicte P.V. proposes to organize another working group to decide the minimum information that should be provided by NFs for data submission to the DC (lab notebook, level of details of the auxiliary mechanism, calibration plots ...). Jean-François D. asks to the others to share solutions found by the other groups: in CESAM, for example, there is a standardized lab note book, in a written form, when submitting data it is necessary to put everything in an electronic format.

Rami A.: in MAC-MICC they use One Note, so that any operator of any instrument can input data, finally a PDF can be exported and archived. But more in general, as suggested by Astrid K.S., it is necessary to agree on a time log of any chemical or physical change made to the experiment, just noting the time and the action, plus qualifying the action when possible. Then it can be adapted to different software.

→ A specific working group for simulation chambers will be set. The topics will be defined by the group itself.

- The lab note book and its complementarity with the current PDF files
- Goal of characterization experiments and of auxiliary mechanism parameters

In conclusion, Bénédicte P.V. will ask by email to participants in which working group they want to participate.