Deliverable D6.8: Final scientific highlights from EUROCHAMP-2020

Authors: David Bell, Christian George, Gordon McFiggans, Amalia Muñoz, Bénédicte Picquet-Varrault, Harald Saathoff, Peter Wiesen.

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Content

Foreword

This document presents some selected highlights of the EUROCHAMP-2020 project, and therefore does not aim at providing a comprehensive overview of all achievements. The reader is then referred to final technical report, which provide further details on all work packages.

1. General objectives

Predicting the behavior of the atmosphere over all time scales (hours to decades) is not only a very exciting scientific challenge, it also brings great benefits to society and the European economy. Examples include short-term public warnings of hazardous air quality and the long-term evaluation of climate change and consequent policy effectiveness. Atmospheric predictions use complex models that are underpinned by observations and a sound understanding of the underlying processes and interactions between atmospheric components and the environment. Atmospheric simulation chambers are among the most advanced tools for studying and quantifying atmospheric processes and are used to provide many of the parameters incorporated in air quality and climate models. Without chamber-derived parameters to constrain predictive models, any forecasts of the atmosphere are highly unreliable, both in the short- and long-term.

The atmosphere is very complex, providing a significant challenge for the scientific community. Emissions of pollutants alter the composition of the atmosphere thereby contributing to poor air quality and climate change, while, at the same time, climate change influences atmospheric composition through a series of feedback processes including variations in temperature, dynamics, hydrological cycle, atmospheric stability, emission intensity of biogenic compounds and transformation processes in the troposphere. The number of drivers of change is very large and the various systems are strongly coupled, making it extremely difficult to quantify climate-induced feedback mechanisms on atmospheric composition.

Due to this complexity, the level of scientific understanding of the climate drivers, the health impacts of complex mixtures of air pollutants, and the interaction between the two is still very low. In order to support the development of effective policies in this area, the scientific community needs to address the following key questions:

- How is the atmospheric composition changing as a result of anthropogenic pressures and climate-induced stress on the Earth System?
- What are the health impacts of exposure to complex pollutant mixtures, especially in urban environments?
- Are there critical thresholds beyond which interactions in the atmospheric system will lead to disproportionate impacts on climate?

- How is it possible to develop and implement robust policies at the local, national and international level to address both climate and air quality to make society more resilient to the impacts of global change?

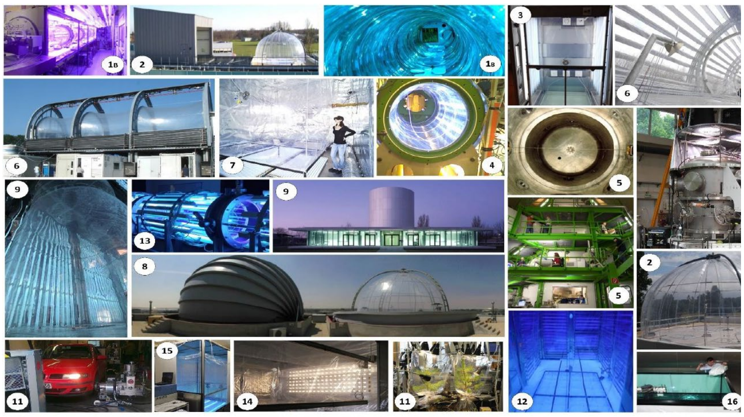
EUROCHAMP-2020 was aiming to play a central role in enabling European researchers to tackle these grand challenges by providing a sustainable, integrated, distributed infrastructure of atmospheric simulation chambers to support detailed studies of the atmospheric processes that govern both air quality and climate, as well as their impacts on the environment and society.

2. Atmospheric simulation chamber characterization and interoperability

The European atmospheric simulation chambers show strong diversity (size, shape, material, light source, range of concentrations achievable, suitability to study certain types of compounds or processes, etc). This diversity allows complementary studies but may also influence the raw chamber results. Characterizing and understanding how the properties of each chamber influence their results is mandatory in order to achieve a better interpretation of experiments and data inter-comparability among different chambers.

Chamber-dependent sets of parameters to achieve better comparability and then to derive chamber-independent process parameters have been quantitatively documented.

Overview of chamber-dependent parameters affecting chemistry



Strong diversity: Size, shape, material, light source, range of concentrations, suitability to study certain types of compounds or processes, etc

Within this task a comprehensive sets of key parameters allowing a full description of all the EUROCHAMP-2020 chambers and their specific characteristics have been collected, validated, organized and disseminated. Also, chamber-dependent specific boundary conditions and parameters affecting radical chemistry and SOA formation have been quantified. Main outcomes are:

- **Directory of each chamber's detailed characteristics**. A web page (http://www.eurochamp.org/chambers/) listing characteristics and technical details of the different chambers, including size, shape, light source, main type of experiments to be carried out, analytical techniques, species that can be analyzed, etc has been released. This directory serves as a knowledge base for the building of add-ons to the Database of

Atmospheric Simulation Chamber Studies (DASCS), which are necessary to improve the usefulness of records for modellers and is useful for TNA users.

- **Photolysis frequencies** used in each chamber both using natural and artificial light for photolysis and photo-oxidation studies have been determined and reported in the webpage to make results from experiments comparable. For this purpose, actinic radiation measurements and dedicated chemical actinometry experiments have been done.
- An **auxiliary mechanism** (i.e. a background chemistry description) and additional proper parameters to define the chamber behavior in photo-oxidation background conditions have been developed and documented for each chamber, and have been linked to the DASCS and can be obtained from the webpage. Wall loss rates for a selection of VOCs and OVOCs have been also reported. These auxiliary mechanisms allow to add chamber-specific properties to physical or chemical models, (e.g. MCM/GECKO-A) allowing separation of the chamber-specific chemical processes from the underlying processes that are being studied in experiments.
- **Chamber dependent parameters affecting SOA formation.** Given that aerosol wall deposition rates are affected by electrostatic sources, turbulence, gravity, etc., and depend on the chamber material, flows inside the chamber and other parameters such as size, shape, and charge of particles, chamber dependent parameters affecting SOA formation have been determined to characterize size dependent particle physical loss rate, which has been summarized in a report. Devoted experiments using reference aerosols have been carried out in each chamber (e.g., ammonium sulfate and sodium chloride of different particle sizes), allowing results in different chambers comparable, and to quantify aerosol processes.

Multi-chamber studies and model tools: radical chemistry, VOC oxidation and SOA Formation.

Using the parameters determined in the previous tasks, the same selected well-known and relevant chemical systems have been investigated in different chambers, i.e. with different sizes, materials, light sources, etc. The results provide a comprehensive intercomparison, characterize experimental differences among chambers and the information that can be obtained, and provide more structured and integrated constraints for modelling studies constituting the basis for the assessment of the interoperability of the chambers. Main outcomes are:

Multi-chamber studies assessing the simulation of photo-oxidation systems and production of SOA from VOC oxidation. Experiments using different propene/NOx ratios, as well-known mechanisms, have been carried out in different chambers and have been modelled providing a common evaluation of the sensitivity and performance of the auxiliary mechanisms calculated previously. On the other hand, a comprehensive set of experiments for α-pinene and toluene under different chemical conditions (ozonolysis and photo-oxidation under different NOx and VOC-limited conditions, different relative humidity and presence or lack of seeds) have been performed to characterize experimental differences among chambers, considering their type of walls, source of light used, etc., providing more structured and linked constraints for modelling studies. SOA and gas-phase products including precursors, products and intermediate species have been monitored, and yields of selected products have been calculated. Results of the experiments have been evaluated form the point of view of: (i) the impact of light source, (ii) the impact of chamber wall material, (iii) evaluation of reaction mechanisms. Results demonstrate that there are still gaps related to the different pathways of oxidation and gas-phase and secondary organic aerosol formation. Therefore, a key conclusion is that it is important that characterization experiments are carried out on a regular basis in order to keep the chamber specific auxiliary mechanisms updated. This characterization has to consider a broad range of experimental and operational conditions (i.e. different VOC/NOx ratios, relative humidity, light and dark conditions) to better understand and model the results and make them comparable among the different chambers.

3. Trans-national access to EUROCHAMP-2020 calibration facilities

It was the aim to provide access to four EUROCHAMP calibration facilities to achieve special benefit for users of atmospheric simulation chambers, ACTRIS-2 facilities, airborne platforms for atmospheric studies, and SMEs improving and validating existing or new instruments. These facilities should complement existing calibration opportunities in atmospheric sciences and demonstrate the specific usefulness of atmospheric simulation chamber facilities for calibration purposes. Finally, the calibration facilities should be integrated in the ACTRIS-ERIC activities in a sustainable manner (e.g. as topical centers).

All calibration centers of EUROCHAMP 2020: for Cloud Physics (ACcloud), for Soot Measurements (CCSM), for Aerosol Physics (WCCAP), and for Organic Tracers and Aerosol Constituents (OGTAC CC), developed dedicated calibration and training protocols and established suitable traceability chains. In intensive interactions with users, relevant SMEs, international advisory boards, and national institutes of standards, the corresponding protocols were refined and adapted to ensure highest usefulness and applicability. These activities lead to the following results:

- Protocols for calibrating ice nucleating particle (INP) instruments and for the calibration of a broad range of atmospheric hygrometers.
- Protocols for calibrations with black carbon (BC) standards (fullerene soot, Aquadag) and real-world BC aerosols (diesel soot coated with secondary organic aerosol, BC mixed with magnetite dust).
- Protocols on training quantitative sampling and chemical analysis of major secondary organic aerosol constituents of biogenic and anthropogenic origin.

- ➢ Standard operation procedures (SOPs) for inter laboratory comparisons for the chemical analysis of marker compounds of secondary organic aerosol of biogenic and anthropogenic origin.
- ➢ Protocols for the calibration of instruments to measure aerosol particle number, size, light scattering, extinction, and cloud nuclei concentrations as well as recommendations for quantitative aerosol sampling.

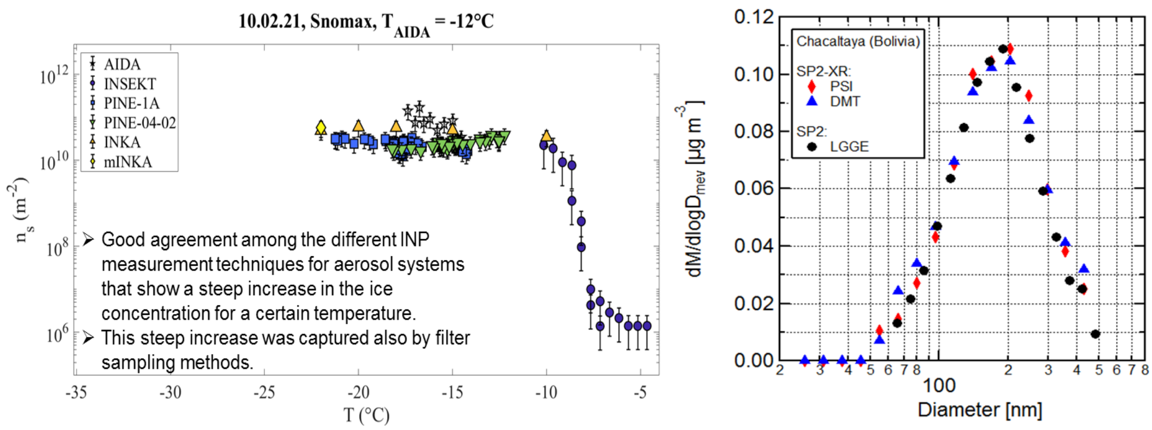


Figure 1. (Left) Example of methods developed at ACcloud for calibrating ice nucleating particles (INP) measurements. (Right) Example of excellent agreement of independent refractory black carbon (rBC) measurements achieved in a field study following calibration at CCSM.

Throughout the project the new, unique, and cost efficient calibration and training opportunities became more and more popular so that 360 calibration units (days) were used including 125 training days. Finally, the EUROCHAMP 2020 calibration facilities are integrated in ACTRIS-ERIC as central facilities having a leading role in the topical centers ‘Cloud in situ’ and ‘Aerosol in situ’. Thus, they will continue to provide recommendations not only for chamber studies but will support all national facilities in ACTRIS in consequently ensuring highest data quality.

4. EUROCHAMP Data Centre

The overall goal of the EUROCHAMP Data Centre is to increase the use of simulation chamber data and data products by a large community of users in atmospheric science research and related areas, as well as the private sector. It offers free and open access to high quality scientific data and data products as well as tools to improve services to users (visualization, handling and valorization of data).

The original database developed during previous EUROCHAMP projects was hosted by CEAM (http://eurochampdatabase.es/) and was based on a decentralized concept where all data were physically stored on institution’s servers. It included two pillars:

- The *Database of Atmospheric Simulation Chamber Studies* (DASCS) which provides access to experimental data (level 2 data), typically time-series of measured parameters during an experiment in a simulation chamber.

- The *Library of Analytical Resources* (LAR) which provides quantitative analytical resources that include infrared spectra and mass spectra of molecules and derivatives (level 3 data).

A new EUROCHAMP Data Centre

A new architecture has been defined and the original database has been transferred to the "Atmosphere and Service Data Pole" AERIS (CNRS, France) in order to make EUROCHAMP Data Centre more operative, secured and sustainable. In addition, EUROCHAMP Data Centre has been upgraded and fully redesigned to make it more user-friendly, operative, secured and sustainable (see D9.2).

Numerous tools and services have also been developed by AERIS in order to facilitate and enhance data provision and usage (see D9.5 and D9.9):

- A new user-friendly web interface has been developed and all data have been transferred to a unique server (AERIS, CNRS) to ensure sustainable data curation and access,
- Online tools have been developed for data providers in order to allow standardized submission of data and metadata and therefore enhance the quality and completeness of data. In particular, a program has been developed to help in the generation of EDF[1] files which is the standard format for providing data in the DASCS. Tools have also been developed to allow duplication of metadata sheets and the provision of data in "private" or "public" access modes.
- In order to comply with the FAIR[2] principles, a new tool has been developed to automatically generate a DOI[3] when a new metadata sheet is created in public access. The creation of DOI for each dataset is crucial to rationalize the data citation and provide traceability of the data usage.
- Tools have been developed for data users to allow for very easy and intuitive search, visualization and handling of data,
- Tools for real-time monitoring provision and usage statistics have been developed and made available for EUROCHAMP partners.

Creation of a new database: The Library of Advanced Data Product (LADP)

A major output of the work performed is the creation of a third pillar, the *Library of Advanced Data Products* (LADP), which provides access to different types of level 3 data products obtained from level 2 data processing. They include rate constants of gas phase reactions, quantum yields and photolysis frequencies of trace gas compounds, secondary organic aerosol (SOA) yields, mass extinction/absorption/scattering coefficients and complex

[1] Eurochamp Data Format
[2] Findable, Accessible, Interoperable, Reusable
[3] Digital Object Identifier

refractive index of aerosols, growth factors of aerosols and modelling tools (see D9.6). These advanced products are especially useful for researchers working on atmospheric observations, as well as atmospheric model development and validation. They include products for the development of chemical mechanisms in atmospheric models (e.g. rate coefficients, photolysis frequencies, SOA yields), products for the retrieval of satellite data and for radiative transfer modelling (e.g. aerosol optical and hygroscopic properties), and modelling tools to interpret field measurements as well as laboratory studies.

Data provision during E-2020

Thanks to a strong partnership involvement throughout the project and to the various tools developed by AERIS to facilitate the data provision, the number of data in the DASCS has doubled in four years (in comparison to the number of data provided within EUROCHAMP-1&2). More than 1700 experiments are now offered to the end users in the DASCS. New infrared and mass spectra have also been added in the LAR and more than 300 advanced products have been provided to the LADP.

Visibility of EUROCHAMP DC

Usage statistics are monitored since EUROCHAMP DC website has been developed. As shown in Figure 1, the number of visits of the website has regularly increased since statistics are monitored, indicating that the visibility of the data center has greatly increased. Since June 2018, the total number of visits is more than 11 200. From the geographic distribution of visitors, it can be observed that they are distributed worldwide demonstrating that EUROCHAMP Data Centre is highly visible within the entire scientific community and far beyond Europe.

The number of data views and downloads are also monitored since May 2018 for DASC and LAR and since June 2019 for LADP. These statistics are presented in Table 1. In total, between May 2018 and June 2021, data and metadata have been viewed more than 35 000 times and more than 2 300 downloads have been performed by users. These numbers are very high and demonstrate the visibility and usefulness of this database. They also show that despite LADP has been developed recently (2019), many views and downloads have been made by the users, demonstrating that these advanced products generate high interest in the scientific community.

Figure 2. Number and geographic distribution of visitors of EUROCHAMP-2020 Data Centre website from June 2018 to June 2021.

Table 1: Number of unique views, total views and downloads of data since statistics are monitored (May 2018 for DASCS and LAR and since June 2019 for LADP).

Database	Unique views[4]	Total views	Downloads
DASCS	6 279	9 426	766
LAR	2 731	3 486	692
LADP	6 327	22 330	896
Total	**15 337**	**35 242**	**2 354**

5. Evolution of atmospheric simulation chamber infrastructure to address broader scientific and societal needs – Highlights

Here, the main subtasks were broken down to cover 1) to better enable the study of climate change drivers, 2) studies of the impact of air quality of health and cultural heritage, 3) process studies of increasing realism and complexity, and 4) strengthening of instrumental capabilities. Within each of these subtasks there were significant advances addressing the associated milestones and deliverables, and a few will be highlighted here.

[4] Number of views by unique users

Developing instrumentation and procedures to better quantify aerosol-radiation and aerosol-cloud interactions

Figure 3. The new dynamic cloud simulation chamber AIDAd for studying aerosol-cloud interactions

Black carbon makes up a large contribution, though not well quantified, contribution to the warming of the atmosphere. Further complicating light absorption by black carbon, organic coatings present on black carbon particles can enhance light absorption through refracting and reflecting light to the black carbon core. Previously in literature, the lensing effect was estimated to be between 5 – 140%. Measurements presented in Liu et al. (2017) demonstrate for the first time that the lensing effect is strongly depending upon the mass fraction of the coating relative to the black carbon "core". Particles with a ratio of non-black carbon: black carbon below 1.5 possessed no significant absorption enhancement. These results suggested that vehicular emissions should be treated as effectively bare black carbon, while primary organic aerosol emissions from biomass burning should be treated as an internally mixed particle with an absorption enhancement.

Evolution of atmospheric simulation chamber infrastructure to enable the studies of the impact of air quality on health and cultural heritage

Aerosol particles (also known as particulate matter, PM) play a critical role on the climate and human health, with PM globally representing the 5th highest mortality risk factor. Despite the evidence of PM playing a large deleterious role on health, there are still uncertainties about the nature of this effect and quantifying the biological response. These uncertainties come from the complexity of the mixtures found in atmosphere where both PM and reactive trace gases are present in large quantities. The CESAM chamber was utilized as an innovative platform to perform feasibility experiments to demonstrate exposure to animals is possible using the chamber,

Figure 4. Atmospheric Chemistry Department – Chamber (ACD-C) allowing the investigation of toxicological effect of aerosols

which included a day-night cycle by turning the lights on and off (COLL et al., 2018). Preliminary results showed that mice exposed to the simulated environment had typical responses of oxidative stress and xenobiotics, while the control group largely did not. This preliminary study was used as a solid justification for a larger Horizon-2020 project.

Evolution of atmospheric simulation chamber infrastructure to enable process studies of increasing realism and complexity

Figure 5. Chambers deployed to investigate vehicule emissions, eventually mixed with biogenic compounds

Many chambers involved in Task 10.3 developed methods to couple complex emission sources (e.g. biomass burning, vehicles, etc…) to the atmospheric simulation chamber. However, coupling these sources to a chamber alone does not fully capture the complexity in the atmosphere where emissions from biogenic sources will mix with anthropogenic emissions. Kari et al. (2019) studied mixtures of α-pinene with vehicular emissions from a gasoline direct injection engine. This study found that SOA production from α-pinene was inhibited by both NO_x emissions and the interaction with volatile organic compounds (VOCs) emitted by the engine. It is hypothesized that gas-phase reactions resulted in products with higher saturation vapor concentrations, which did not condense. Overall, the yield of α -pinene SOA was ~50% lower in the presence of GDI emissions.

Strengthening of the instrumental capability of atmospheric simulation chambers to investigate atmospheric oxidation processes

Within this task there were many instruments were developed and applied to measurements in the atmospheric simulation chambers, including a series of different instrumental intercomparison campaigns. Measurement of OH reactivity, though, represents an important atmospheric measurement that requires good interoperability and understanding of measurement artefacts. A campaign was performed in the Julich SAPHIR chamber using a series of OH reactivity measurements applying various methods (Fuchs et al., 2017). This quality assurance effort demonstrated the capability of all instrument to accurately measure OH reactivity in atmospheric simulation experiments. As expected, the

Figure 6. Development of CEAS for detection of Glyoxal, m-glyoxal and NO_2

precision of Comparative Reactivity Method (CRM) instruments were reduced compared to the methods applying direct detection of the OH decay. One down side found was that systematic errors could arise, and although correction factors are determined in laboratory characterization measurements that may not be able to cover all atmospheric conditions adequately.

6. Development of models to aid interpretation and exploitation of chamber experiments – Highlights

The overall goal of the modelling activities within EUROCHAMP was to further integrate and improve the capabilities of Europe’s atmospheric simulation chambers to address a broad spectrum of scientific questions related to the understanding and mitigation of air pollution, its health effects and impact on climate change.

The modelling activities were organized to enable the optimisation of the process by which chamber experiments are exploited and utilised. Once a process is well characterised through a combination of aerosol chamber experiments and model simulations, it can be incorporated into larger-scale 3-dimensional models to allow predictions of their effect on air quality and climate.

Most importantly, to enable broadest possible exploitation of our chamber results, a compilation of the modelling tools has been made available through a link from the EUROCHAMP Library of Advanced Data Products at: [https: //data.eurochamp.org/modelling-tools/](https://data.eurochamp.org/modelling-tools/).

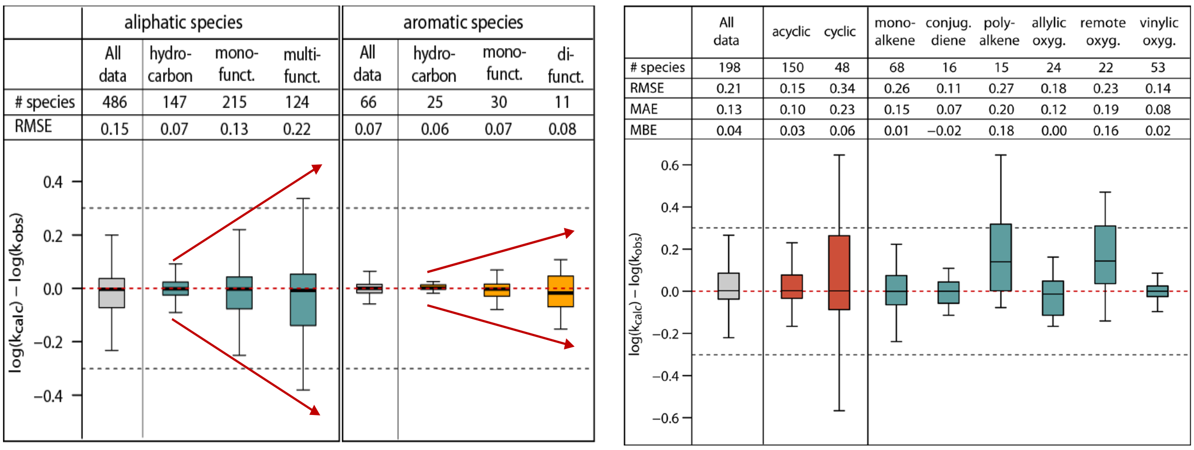


Figure 7: Root mean square error, mean absolute error, mean bias error and box plots for the error distribution in the estimation of k_{298K} values for OH (left) and ozone (right) reactions for a full set and subsets of the aliphatic (Jenkin et al., (2018a)), aromatic (Jenkin et al., (2018b)) and alkene (Jenkin et al., (2020)) species in the respective databases.

An emphasis on continued chemical mechanism development in both gaseous and condensed phases has enabled substantial advances in our understanding of chemical processes in simulation chambers. Many EUROCHAMP partners have participated in these developments. For example, the recent maturation and adoption of automatic mechanism generation has required significant effort in protocol and structure-activity relationship (SAR) development. The development and coding of modular protocols using these SARs into the MCM / GECKO-A framework enables the testing and application near-explicit models of gas phase chemistry for comparison with chamber results. Figure 7 illustrates the performance of SAR predictions for OH and ozone reactions of a range of VOC classes.

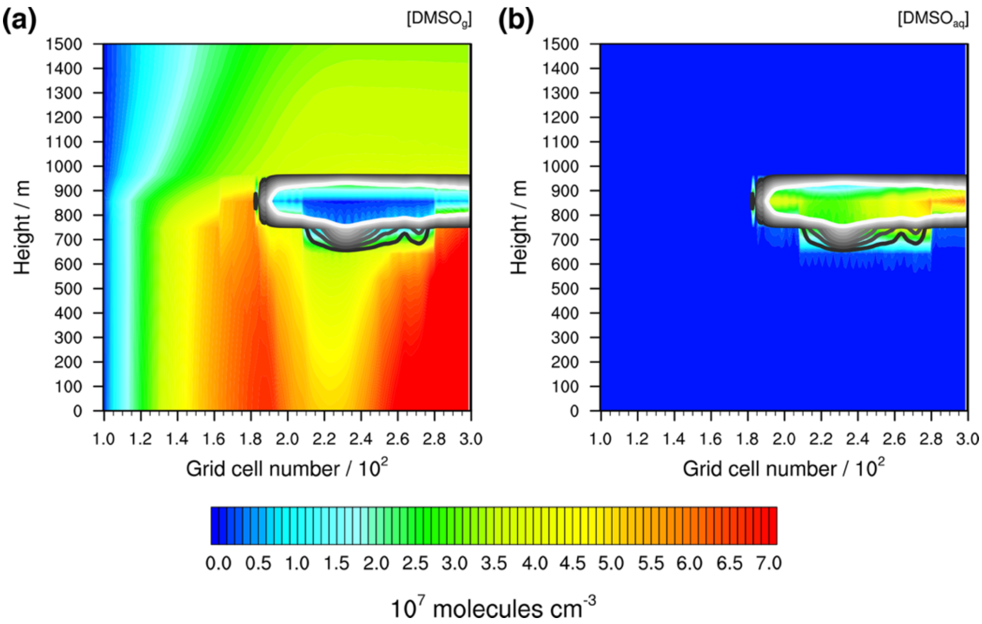


Figure 8: Simulated concentrations of DMSO (a) in the gas phase and (b) in the aqueous phase under stratiform cloud condition after 12 h of modelling time. The x axis represents the innermost horizontal grid cells divided by 100. The black contour lines represent the simulated clouds. The black line indicates a LWC of 0.01 g m^{-3} and the white line to 0.1 g m^{-3}. The area framed by the white line includes LWC above 0.1 g m^{-3}.

As a second example, a condensed multiphase halogen and dimethyl sulfide (DMS) chemistry mechanism was developed by substantially reducing the CAPRAM DMS module 1.0 (CAPRAM-DM1.0) and the CAPRAM halogen module 3.0 (CAPRAM-HM3.0) and implemented in the COSMO-MUSCAT CTM. 2D simulations were used to investigate the effect of stratiform and convective cloud conditions on the marine multiphase chemistry (Hoffmann et al., 2020) as shown in Fig. 8. A direct photochemical effect of clouds results from the high rate of in-cloud dimethyl sulfoxide (DMSO) oxidation rates, enhancing the formation of methane sulfonic acid compared to aerosol chemistry. An indirect photochemical effect results from cloud shading, particularly from stratiform clouds, reducing photolysis rates and e.g. Br activation, BrO formation and consequently, DMS oxidation by up to 30 % under optically thick optical clouds.

Beyond the development of chemical models, there has been development of a wide range of tools for interpretation of physical processes in chambers. Computational fluid dynamics (CFD) models have been used to simulate mixing and cloud processes in the AIDA and LACIS-T chambers. There has additionally been substantial development and delivery of open-source model tools for interpreting chamber studies of i) coupled gas phase photochemistry and aerosol microphysics and ii) warm, mixed-phase and cold cloud microphysics.

The CHemistry with Aerosol Microphysics in Python (PyCHAM; O'Meara et al., 2020, 2021) is an open-access, zero-dimensional, user-friendly model developed for the testing, evaluation and quantification of processes occurring in chamber experiments of coupled gaseous photochemical and aerosol systems. The PyCHAM graphical user interface (GUI) enables model control, running and output plotting and a manual documents the files required for input conditions, gas-phase chemistry scheme and conversion to the required SMILE strings. Alternatively the open-source Python code can be accessed to enable command line control. Windows, Mac and Linux versions are available on: https//github.com/simonom/PyCHAM

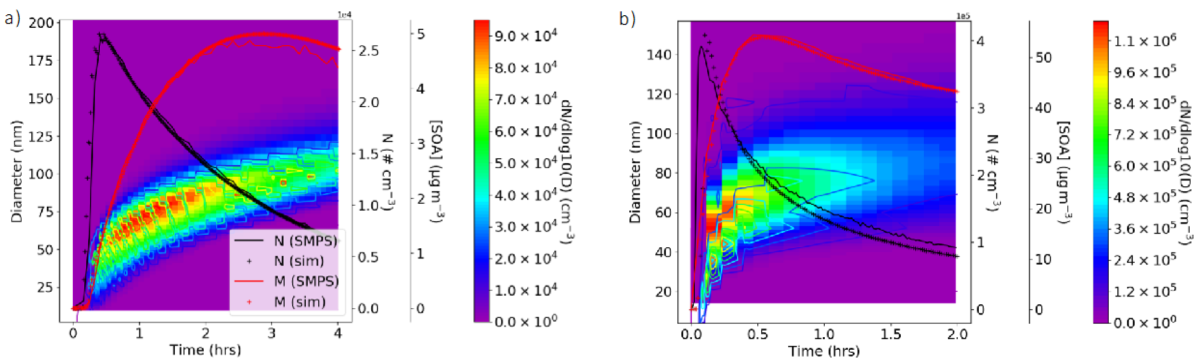


Figure 9: Simulated α-pinene ozonolysis in MAC and AIDA using an extension appended to the MCM in PyCHAM, with only wall loss (with effective absorptive wall mass for vapours) tuned for each chamber. Measured and modelled number size distributions shown by filled and line contours respectively.

Fig. 9 compares PyCHAM-simulated and measured aerosol size distributions from unseeded α-pinene ozonolysis experiments in MAC and AIDA using the MCM plus an extension to consider the production of highly oxidised organic molecules (HOM) in the first-generation oxidation of α-pinene. Such multi-chamber constraints have the potential to provide greater confidence in model process parameters.

PyACPIM is an an open-access Python cloud microphysics model with Windows, Mac and Linux versions available at: https://github.com/emmasimp/py-cloud-parcel-model/tree/GUI-with-semi-vols

The GUI includes of co-condensation of semi-volatile components to investigate their impacts on warm droplet activation in chamber experiments. Example simulations of such experiments are shown in Fig. 10. PyACPIM can be used to simulate warm, cold and mixed-phase cloud conditions and can be driven by an updraught for ambient simulations and by a prescribed cooling rate for chamber simulations. In chamber studies, Frey et al. (2018) used PyACPIM to interpret the effectiveness of secondary organic aerosol (SOA) as ice nucleating particles (INP), and Simpson et al. (2018) to evaluate the effects of the competition between INP and CCN in MICC.

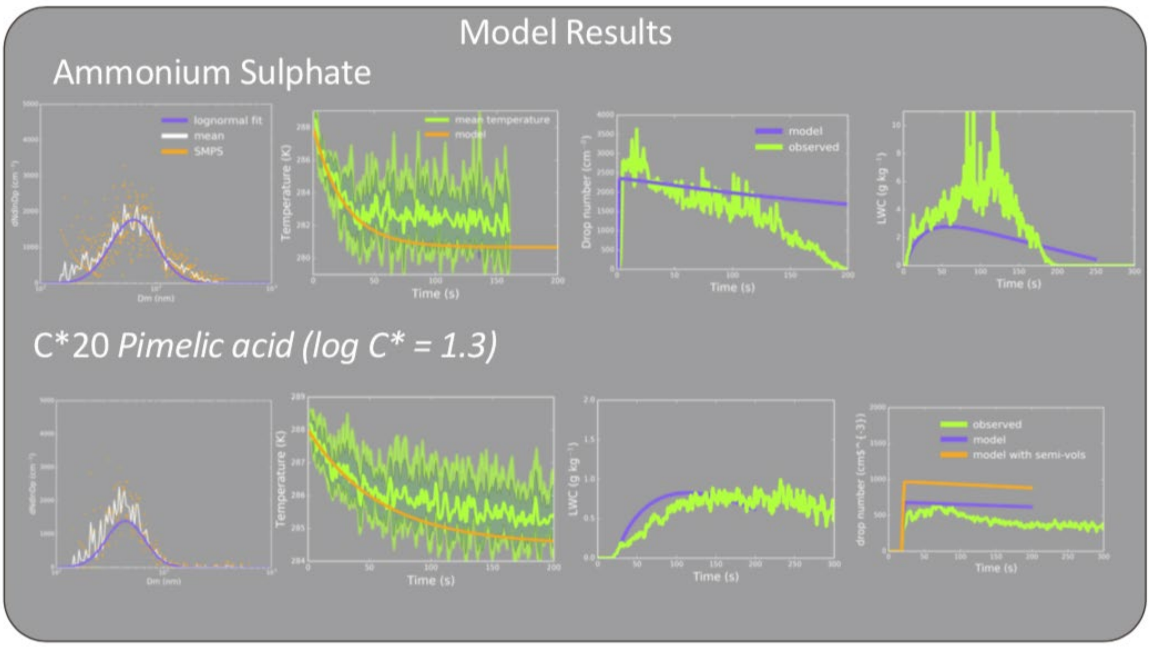


Figure 10: PyACPIM GUI snapshot showing warm cloud activation on ammonium sulphate and semi-volatile organic particles, comparing simulated with experimental data.

Several partners have participated in the development of tools to retrieve SOA particle volatility from chamber measurements for constraint of volatility basis set (VBS) representation in CTMs. PSI have applied the VBS to attribute the contributions of compound classes in wood burning emissions and the UEF group have developed a method to define VBS as well as viscosity. The FORTH group has developed an algorithm to estimate parameters such as volatility product distribution, effective vaporization enthalpy and accommodation coefficient combining SOA yield measurements with thermograms (from thermodenuders) and areograms (from isothermal dilution chambers) from different experiments and laboratories. Following evaluation of the algorithm with “pseudo-data” it has been used to estimate the uncertainty of the resulting parameterization for different atmospheric conditions (temperature, concentration levels, etc.) as shown in Fig. 11 and reported in Uruci et al., 2021.

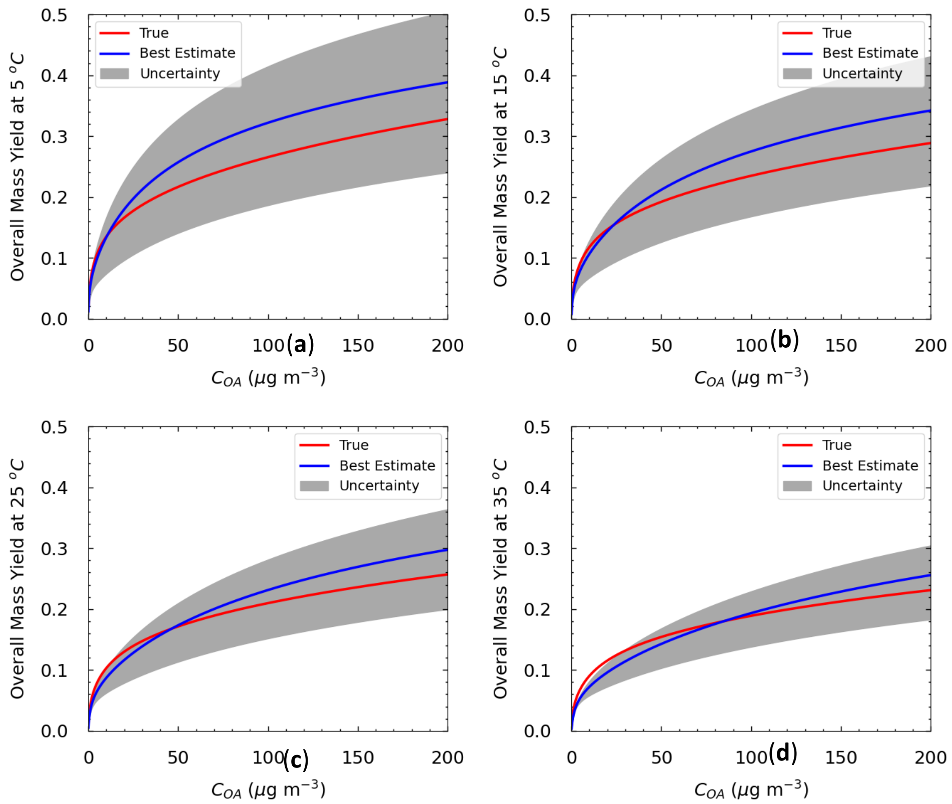


Figure 11: Yields calculated by the true (red) and estimated (blue) stoichiometric coefficients of a typical test of the algorithm at: (a) 5 °C, (b) 15 °C, 25 °C, and (d) 35 °C. The grey area represents the uncertainty range of the best fits.

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