EUROCHAMP 2020

TNA User Report

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Project title	The effects of Phase state on Secondary organic aerosol (SOA) Gas-particle Partitioning
Name of the accessed chamber	The atmospheric simulation chamber SAPHIR
Number of users in the project	1
Project objectives (max 100 words)	The scientific objectives of the current project are to characterize the phase state of SOA generated in the SAPHIR chamber and to understand its effect on gas-particle partitioning of semi-volatile organic materials.
Description of work (max 100 words):	An extensive range of instrumentation for characterising the gaseous and particle composition and the physical properties of the particles will be deployed to ensure broad characterisation of the systems and allow interpretation of the observed phase state behaviour and gaining insight into the roles of aerosol phase state in gas-particle partitioning.

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New user	

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[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.
[4] Reproduce the table for each user who accessed the infrastructure

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:

Chamber name and location: SAPHIR, Juelich, Germany

Campaign name and period:, 10th July –5thSep, 2019

Text:

Introduction and motivation

The understanding of gas/particle partitioning of oxidized semi-volatile organic compounds(SVOCs) is of great importance to clarify the integral process in the formation of secondary organic aerosol(SOA), which plays a key role in air quality and climate. At present, there is little data that characterizes the total gas/particle partitioning of ambient SOA due to the highly complex character of SOA. Some smog chamber experiments have been conducted to examine the partitioning of SOA generated from individual volatile organic compound(VOC) or VOC mixture. Evidences from chamber experiments found a higher contribution of SVOCs to the aerosols than that predicted by equilibrium partitioning theory, which suspected the significant role of phase state in SOA gas-particle partitioning (J Gkatzelis, Georgios I.; Hohaus, Thorsten et al,.2018, ACP). It is therefore driving us to understand how the phase state influences the SOA gas-particle partitioning. Recent studies performed in the laboratory, field campaign and model simulations have further emphasized the importance of aerosol phase state to the SOA formation (Shiraiwa et al., 2012, GRL; Ye et al., PNAS, 2016; Shiraiwa et al., 2011, PNAS), for example, phase state can directly affect the mass transfer process of organic molecules. The equilibrium time between highly volatile organic compounds and liquid aerosols can be from seconds to minutes, and the gas-particle equilibrium time of semi-solid, low volatile and large particles can increased from hours to days.

Scientific objectives

The scientific objectives of the current project are to characterize the phase state of SOA generated in the SAPHIR chamber and to understand its effect on gas-particle partitioning of semi-volatile organic materials. An extensive range of instrumentation for characterising the gaseous and particle composition and the physical properties of the particles will be deployed to ensure broad characterisation of the systems and allow interpretation of the observed phase state behaviour and gaining insight into the roles of aerosol phase state in gas-particle partitioning.

Reason for choosing the simulation chamber / calibration facility

The SAPHIR chamber provides either artificial trace gas mixtures or emissions from plants that are housed in a separate plant chamber, which could form SOA from a range of precursors.Therefore, it is suitable for the investigation of systems with ranging complexity when associated with appropriate instrumentation.

Method and experimental set-up

For the measurement, the chemical composition of the aerosols were detected by AMS, molecular markers with TAG, a partitioning measurement of SVOCs using an Aerosol Collection Module (ACM) in combination with a PTR and SOA phase state measurement with a three-arm impactor combined with a condensation particle counter (CPC) (TSI 3772), which was described in detail in Liu et al. (2017) deployed from PKU group. The rebound fraction (BF) of the selected mono-disperse organic aerosols generated from different precursors with seed aerosols in SAPHIR chamber were detected under various relative humidity condition. The BF of SOA, as well as its linkage with chemical information, such as oxidation state will provide insight into the phase state and phase transition of SOA.

A series of experiments were focused on the formation of SOA in iso-reactivity mixtures aiming to produce particles including oxidation products of a variety of precursors. To enhance uptake of SVOCs seed aerosol can be add to the chamber. Five different VOCs will be introduced in SAPHIR. Precursor concentration and relative humidity will be varied to influence the phase state of the SOA.

Data description

The schematic diagram of the three-arm impactor is shown in Fig 1, detailed description of instrumentation information can be found in *Liu et al.* [2017]. Generally, the whole system consist of the particle selected part using DMA with an X-ray, one RH djuestment system using the Nafion tube and the impaction part with three special designed impactors operated in parallel in the system which combined with one CPC. Thus, the size-resolved particle rebound fraction(BF) under different RH level can be obtained.

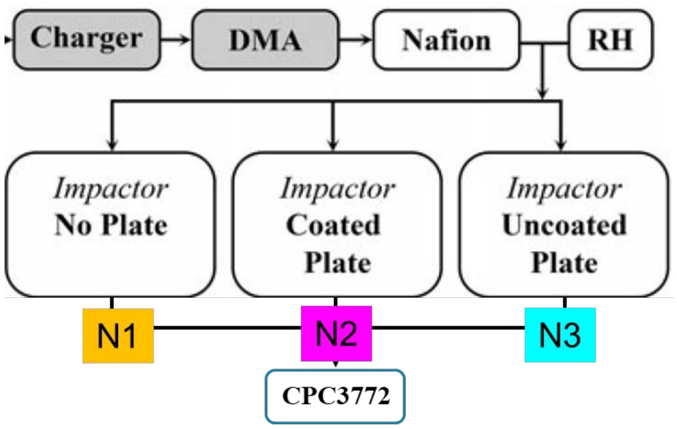

Fig 1. Schematic of the three-arm impactor

The test sample will go seperately into the three channels. The first channel have not equipped with the impactor plate which means all the particles can go through the first channel, representing whole particle population(N1). The second channel have equipped with a grease-coated plate which provided an sticky surface that all the particles striking on the plate are stuck. The particles that smaller than cutpoint size(95nm) don't strike on the plate that are counted by the cpc(N2). The third channel have equipped an uncoated plate which provides a solid surface and allows particles rebounding from impactors. The particle population measured after the third channel represents the sum of particles that don't strike the impactor and that strike but rebound from the impactor(N3). Finally, the rebound fraction *BF* is defined in equation [1].

$$BF = \frac{N_3 - N_2}{N_1 - N_2} \qquad [1]$$

Preliminary results and conclusions

6 experiments were conducted which including the photooxidation of Methyl salicylate in the presence of $(NH4)_2SO_4$ seed aerosols under 70%RH and 75%RH, the photooxidation of β-pinene in the presence of $(NH4)_2SO_4$ seed aerosols under 40%RH, the photooxidation of α-pinene, o-cresol and mixed system with α-pinene and o-cresol in the presence of $(NH4)_2SO_4$ seed aerosols under 70%RH(Fig2,3,4). Here, parts of the preliminary results were showed. The following figures are the results of BF as a function of RH. The size-resolved BF was compared using the different size points. The photooxidation time was listed by the colorbar.

The BF tendency of α-pinene reaction system is presented in figure 2. The BF tendency of o-cresol reaction system is presented in figure 3. For the mixture of α-pinene and o-cresol system, the BF behavior change seems to be dominated by o-cresol (Figure 4).For all these three experiments, the initial RH setup is 70%, but the actual RH inside the SAPHIR is changing based on the temperature and reaction inside, that means the seed particles of ammonia sulfate exist at liquid state at the beginning. And the photooxidation is provided by the sunlight. 100nm and 200nm particles are selected for the measurement.

The results show that the rebound behaviour tends to be weaker firstly then becomes stronger with the increasing photooxidation time. Particles remain rebounding when the RH was under 30% (BF>0.8), but changed to adhere when the RH increased (BF<0.1), suggesting a transition from solid or semi-solid to liquid state. The phase transition RH change from 40%RH to 80%RH which means that the surface of the particles become more viscous with the oxidation. The size-resolved differences show that 100nm particles tend to be more 'liquid' even the RH is low(RH≤30%) when comparing to 200nm particles(Figure 2). The BF of o-cresol system show that particles keep at solid or semisolid when the RH is below 70%. And there are no obvious differences between 100nm and 200nm particles(Figure 3).

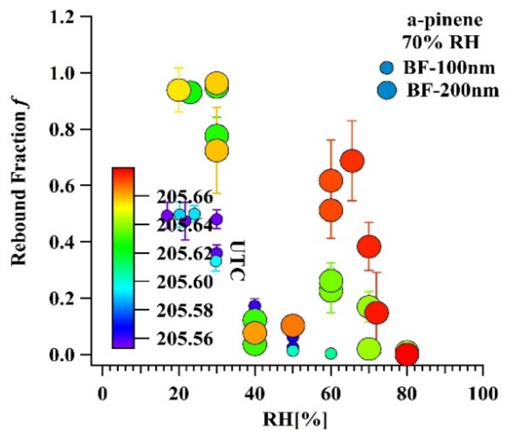

Fig2. The result of α-pinene system

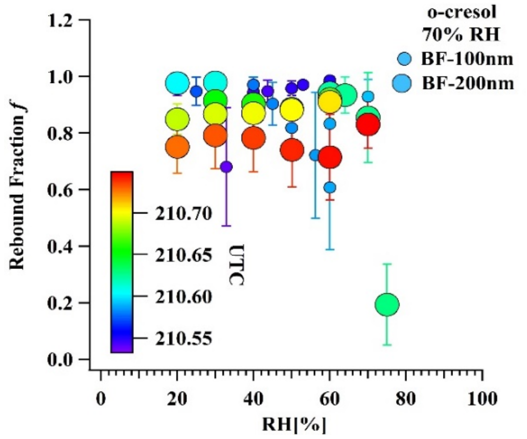

Fig3. The result of o-cresol system

For the mixture of o-cresol and α-pinene system, the BF behavior shows silimar to o-cresol system. The BF keep at 0.9~1.0 when the RH is below 70% which indicate that the formation particles exist as solid or semisolid state. The oxidation time doesn't show significant difference on the rebound behaviour of mix system(Figure 4).

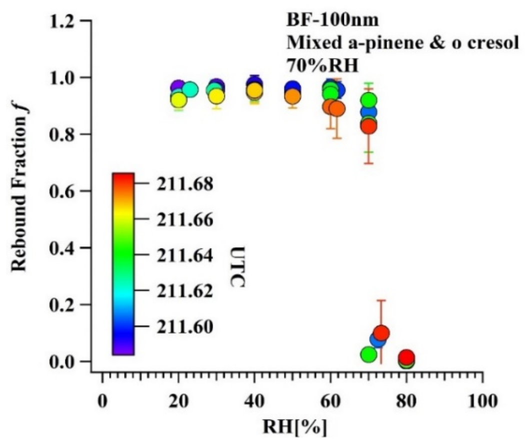

Fig4. The result of binary system with α-pinene and o-cresol

Here, some preliminary conclusions can be conducted. At the beginning of the photooxidation, the rebound ability of α-pinene derived SOA particles becomes weaker due to the sticky SOA layer on the surface of particles. If the SOA formation is sufficient, the particles tend to mix internally with lower liquid water content, which lead particles tend to be more solid.

Outcome and future studies

The chemical information of particels and other trace gases are collected and still being analysed. The results of three-arm impactor look encouraging. For the next step, more data will be combined which include chemical composition and gas-particle partitioning to prove some speculations.