SCIENTIFIC REPORT 2018–2020

Max Planck Institute for Chemistry
(Otto Hahn Institute)

MAX PLANCK INSTITUTE
FOR CHEMISTRY

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FOR CHEMISTRY

Atmospheric Chemistry · Climate Geochemistry · Multiphase Chemistry · Particle Chemistry

SCIENTIFIC REPORT 2018–2020

CONTENT

Cover picture:
Fog rising above the Amazon rainforest near the ATTO research site. The picture was taken by Andrew Cozier, standing on the ATTO tower.

PREFACE

BETWEEN CONTINUITY AND CHANGE

"Change BEFORE continuity" – this principle of the Max Planck Society was formulated by its President Martin Stratmann at the "25 Years of Science and Reunification" event five years ago.

At the Max Planck Institute for Chemistry, the period from 2018 to 2020 has been characterized by scientific continuity as well as change. With four departments, four independent research groups, and around 350 employees, our Institute operates proficiently and productively. The Atmospheric Chemistry, Climate Geochemistry, Multiphase Chemistry, and Particle Chemistry Departments collaborate closely in many projects and initiatives. One example was the successful cross-departmental CAFE-AFRICA campaign in summer 2018. In this aircraft-based measurement campaign, MPIC scientists investigated the combined influence of natural, anthropogenic, and biomass burning emissions on the aerosol and oxidation chemistry of the tropical atmosphere.

Our Institute performs Earth system research. In addition to the interactions between the lithosphere, hydrosphere, biosphere, and atmosphere, the influence of humans, which has become a significant geological force, has come to the fore. Paul Crutzen's statement "We are no longer in the Holocene, we are in the Anthropocene", captures, in a nutshell, the impact of human activity on planet Earth. Today, more than two decades after Paul coined the term at a meeting in Mexico, more than 5,000 peer-reviewed scientific articles indexed in the Web of Science and Scopus have addressed the Anthropocene concept. There is no other fundamental concept in the history of science that has spread across disciplines as quickly as that of the Anthropocene.

Many of our research groups study themes that involve identifying or quantifying the impacts of humans on the Earth system. This includes, for example, research into the influence of fossil fuel and biomass combustion on the composition of the atmosphere, air quality, and climate. Public health-related aspects of air pollution are also increasingly the subject of investigation at our Institute, in line with the concept of "planetary health".

To tackle some of the fundamental research questions, we make use of infrastructure that was established within the Earth System Partnership by several Max Planck Institutes: The German Climate Computing Center (DKRZ), the High Altitude and LOng Range Research Aircraft (HALO), three long-term observational stations – the Amazon Tall Tower Observatory (ATTO), the Zotino Tall Tower Observatory Facility (ZOTTO) and the Barbados Cloud Observatory (BCO). In 2019, the research yacht *S/Y Eugen Seibold* became part of this infrastructure in support of climate geochemistry research.

Our research in the year 2020 was strongly influenced by the COVID-19 pandemic. Scientifically, there are nonetheless several successes to report. While large parts of Europe were put into lockdown during spring, we performed the BLUESKY cross-departmental aircraft measurement campaign to document atmospheric chemistry in the near-absence of air traffic. During the summer, the *S/Y Eugen Seibold* carried out important analyses across the North Atlantic Ocean. Furthermore, new research projects emerged, including a practical one in which aerosol measurement devices were used to test the quality of filter materials of face masks. Some of these projects are described in more detail in the departmental reports.

Without doubt, the pandemic and the associated lockdowns have left and will continue to leave marks. International research campaigns that involved extensive preparations had to be postponed, laboratory and service work had to be reduced or organized in shifts, and numerous planned experiments were delayed or cancelled. It also affected the work at the ATTO station in Brazil. Since many measurements are automated, however, the station continues to provide valuable meteorological, chemical, and biological data, including the concentrations of greenhouse gases.

The COVID-19 pandemic represented a great challenge for many employees, and especially for young scientists; early-career researchers are at our Institute for only a limited period of time during which career progress is critical. But then again the pandemic also triggered interesting adjustments. We learned that research is still possible, with one particularly fruitful strategy being analysis of the rich datasets that have been collected in preceding years: teams organized and met online, conferences took place via web platforms, and seminars were run virtually. It makes me proud to see how quickly our Institute has mastered this digital change.

Another notable development in 2020 has been that Gerald Haug became the President of the German National Academy of Science, Leopoldina, being a great honor for him and the institute.

Continuity in research, and maintaining our status as a leading institution in Earth system science also means coping with leadership change. Two of our directors will retire in 2024 and 2025. Plans for a generational change, associated with scientific and directional revitalization, have been initiated early on, both to secure the future of the Institute and to ensure smooth transitions. Our exemplary handling of the COVID-19 situation, in which colleagues have developed innovations in response to restrictions, shows our resilience. Hence, I am confident that we are well equipped to foster the next generation of excellent Earth system scientists in the years ahead.

Jos Lelieveld
Managing Director
December 2020

From the left: Christening of the research yacht *S/Y Eugen Seibold* in 2018, group picture of the Anthropocene Working Group meeting at the MPIC in 2019, research aircraft HALO on the runway during the CAFE-AFRICA campaign 2018.

From the left: A donation to the Institute - the painting "Fein(d)staub" by Udo Lindenberg, a Fridays for Future message sent from the ATTO site, and researchers onboard the HALO aircraft during the BLUESKY campaign in 2020.

ADDENDUM

Professor Dr. Dr. h.c. mult..
PAUL J. CRUTZEN
*3.12.1933 †28.1.2021

The board of directors and the staff of the Max Planck Institute for Chemistry are mourning the loss of the long-time director and Nobel laureate in Chemistry, Paul J. Crutzen. He passed away on January 28, 2021, at the age of 87—three weeks after this report was printed.

The Dutchman was Director of the Air Chemistry Department at our Institute from 1980 to 2000. Together with Mario J. Molina and F. Sherwood Rowland he was awarded the Nobel Prize in Chemistry 1995 for identifying how nitrogen oxides deplete the Earth's ozone layer and discovering chemical processes that cause the ozone hole.

Paul's scientific work focused on the human influence on the atmosphere, the climate, and the earth system. He coined the term 'Anthropocene', which he used to describe the current era in which human activity is profoundly influencing global atmospheric, biological, and geological processes on our planet.

In numerous publications and public lectures, Paul discussed the extent to which mankind exploits the natural resources of planet Earth. He typically ended presentations with a picture of himself and his grandson calling on the audience to preserve the Earth for future generations.

Paul's limitless scientific curiosity, his creative ideas, and his charismatic personality have shaped the institute and many generations of scientists worldwide. We have been very honored to know and work with Paul, and is death is an irreplaceable loss for us all. He will be dearly missed.

Jos Lelieveld
on behalf of the Board of Directors

Max Planck Institute for Chemistry
February 1, 2021

Condolences www.mpic.de/4677594/trauer-um-paul-crutzen

GENERAL INFORMATION

Our goal: a comprehensive scientific understanding of chemical processes in the Earth System. Our methods: ground-based, ship, aircraft and satellite measurements, laboratory investigations, numerical models.

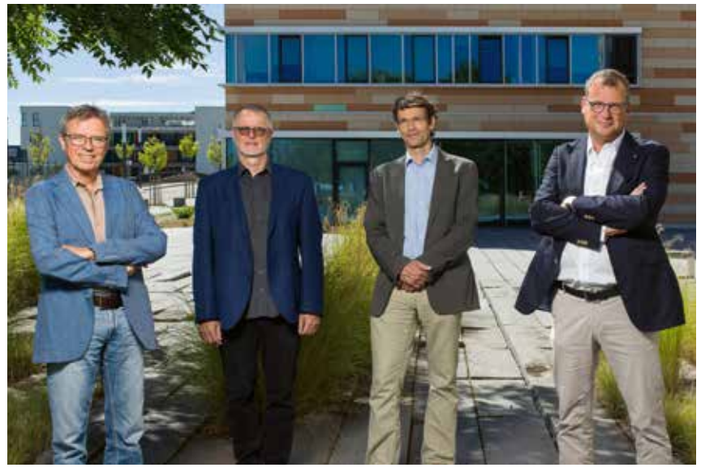
OBJECTIVES AND ORGANIZATION

THE INSTITUTE

The Max Planck Institute for Chemistry has a long tradition of multidisciplinary research at the interfaces between chemistry, physics, biology, and the geosciences. Current research at the MPIC focuses on a comprehensive understanding of chemical processes in the Earth system, including the atmosphere, biosphere, and oceans. Investigations address a wide range of interactions between air, water, soil, life, and climate over the course of Earth history up to the Anthropocene – today's human-driven epoch.

Scientists conduct laboratory experiments and use ground-based observatories, vehicles, ships, airplanes, and satellite instruments to obtain measurement data and collect samples during long-term observations and expeditions. Mathematical models that simulate chemical, physical, and biological processes from molecular to global scales complement the experimental studies. One of the common themes of research at MPIC is to determine how air pollutants, including reactive trace gases and aerosols, affect the atmosphere, biosphere, climate, and public health. Other key topics are the air-sea exchange and biogeochemical cycling of greenhouse gases, oceanic nutrients, and related substances.

At present, the Institute employs some 350 staff in four departments and four additional research groups. Each department is led by a director who is a scientific member of the Max Planck Society and has the responsibility of defining the scientific objectives and guiding the research of the department. The directors jointly guide the Institute's development and take turns in serving as the spokes-person of the board of directors and managing director of the Institute. Gerald Haug has been serving in this position in 2019. Due to his election as President of the German National Academy of Science Leopoldina he handed the office over to Jos Lelieveld in 2020.



Jos Lelieveld, Stephan Borrmann, Ulrich Pöschl and Gerald H. Haug (from left to right).

DEPARTMENTS

The **Atmospheric Chemistry Department** directed by Jos Lelieveld studies ozone chemistry and radical reaction mechanisms, and their role in atmospheric oxidation pathways and the global cycles of trace compounds. These processes, which are important for the self-cleaning capacity of the atmosphere, are studied through laboratory investigations and field measurement campaigns, in particular with aircraft. Computer models that simulate meteorological and chemical interactions are used to support and analyze the field measurements. Models are also applied to assess the impacts of natural and anthropogenic emissions of gases and particles on air quality and climate. Jos Lelieveld holds also a part-time professorship at the Cyprus Institute in Nicosia, Cyprus.

The **Climate Geochemistry Department** directed by Gerald H. Haug addresses climate-ocean-atmosphere processes and large-scale dynamics in global biogeochemical cycles as revealed by sedimentary and fossil records. To quantify the mechanisms and causes of major changes in Earth's environmental conditions the department employs a diverse geochemical toolbox that includes light stable isotopes of foraminifera shells and organic matter, biomarkers, and trace metals, as well as high-resolution non-destructive analytical techniques. Gerald Haug is also President of the German National Academy of Sciences Leopoldina, since March 2020.

The **Multiphase Chemistry Department** directed by Ulrich Pöschl investigates chemical reactions, transport processes, and transformations between solid matter, liquids, and gases. These processes are essential for the interplay of the Earth system, climate, life, and public health. Among the focal points are gas-particle interactions in aerosols and clouds as well as the health effects of fine particulate matter. The applied methods include laboratory experiments, field measurements, and model studies using physical, chemical, and biological techniques.

The **Particle Chemistry Department** is directed by Stephan Borrmann who is also a full professor at the Johannes Gutenberg University of Mainz. Its research focuses on the composition and physical properties of micro- and nanoparticles in Earth's environment, and on interactions between atmospheric aerosols, clouds and climate. Methodologies employed include single and multiple particle mass spectrometry in the laboratory and in field measurement campaigns, mostly using aircraft.

FURTHER RESEARCH GROUPS

The **Aerosols, Air Quality and Climate** group led by Yafang Cheng and supported by the Minerva program of the Max Planck Society addresses central questions of environmental research and Earth system science, such as the influence of soot particles and other aerosols on air quality and climate.

The **High Pressure Chemistry and Physics** group led by Mikhail Eremets studies matter at extremely high pressures aiming at superconductivity. This research has been supported by an Advanced Grant from the European Research Council and central funds of the Max Planck Society.

The **Terrestrial Palaeoclimates** group led by Kathryn Fitzsimmons and supported by the Max Planck Research Group program of the Max Planck Society studies loess deposits in Eurasia to gather information on past climates.

The **Satellite Remote Sensing** group led by Thomas Wagner analyzes spectral data obtained from satellite instruments that measure the atmospheric absorption of solar radiation, with the goal of retrieving and studying the global distributions of trace gases, aerosols, and clouds.

External Scientific Members
For scientific collaboration and networking, the Max Planck Society also appoints renowned scientists as external scientific members. The two external scientific members currently affiliated with the Max Planck Institute for Chemistry are Stuart A. Penkett from the University of East Anglia, United Kingdom, and Ulrich Platt from the University of Heidelberg, Germany.

SCIENTIFIC ADVISORY BOARD

An international Scientific Advisory Board that reports to the President of the Max Planck Society evaluates the Institute's research every three years. The Scientific Advisory Board consists of internationally renowned scientists and their evaluation serves to ensure the appropriate and effective use of the Institute´s resources. The members are:

Edouard Bard, Climate and Ocean Evolution, Collège de France, France

Lucy Carpenter, Department of Chemistry, University of York, York, United Kingdom

Maria Kanakidou, Department of Chemistry, University of Crete, Herkalion, Greece

Markku Kulmala, Institute for Atmospheric and Earth System Research, University of Helsinki, Helsinki, Finland

Kimberly Prather, Scripps Institution of Oceanography, University of California San Diego, La Jolla, CA, USA

Akkihebbal Ravishankara, Department of Chemistry, Colorado State University, Fort Collins, CO, USA (Chair of the Scientific Advisory Board)

Paul Wennberg, California Institute of Technology, Pasadena, CA, USA

James Zachos, PBSci-Earth & Planetary Science Department, Institute of Marine Sciences, University of California, Santa Cruz, USA

ORGANIZATION CHART

Atmospheric chemistry

Jos Lelieveld
Managing Director

Kinetics and photochemistry
J. Crowley

Optical spectroscopy
H. Fischer

Radical measurements
H. Harder

Atmospheric modeling
A.Pozzer

Organic reactive species
J. Williams

Climate geochemistry

Gerald H. Haug

Isotope biogeochemistry
S. Galer

Paleoclimate research
K. Jochum

Organic isotope geochemistry
A. Martínez-García

Geoscientific databases
B. Sarbas

Micropaleontology
R. Schiebel

Inorganic gas isotope geochemistry
H. Vonhof

Multiphase chemistry

Ulrich Pöschl

Chemical kinetics and reaction mechanisms
T. Berkemeier

Biomolecular analyses and interactions
J. Fröhlich

Organic pollutants and exposure
G. Lammel

Inflammatory processes
K. Lucas

Aerosol analysis and microscopy
C. Pöhlker

Aerosol, cloud and surface interactions
H. Su

Particle chemistry

Stephan Borrmann

Instrumental aerosol analytics
F. Drewnick

Nano and micro-particle research
P. Hoppe

Aerosol and cloud chemistry
J. Schneider

Atmospherical hydrometeors
M. Szakáll, K. Diehl, (JGU Mainz)

Aerosol and cloud physics
R. Weigel, (JGU Mainz)

Further research groups

Aerosols, air quality and climate
Y. Cheng

High pressure chemistry and physics
M. Eremets

Terrestrial palaeoclimates
K. Fitzsimmons

Satellite remote sensing
T. Wagner

Joint services

Communications
S. Benner

Administration & technical services
–

IT
T. Disper

Administration
I. Lemm

Instrument development & electronics
F. Helleis

Facility management & operational technology
C. Pallien

Junior scientist support
K. Sulsky

Workshops
R. Wittkowski

December 2020

Group picture during the Institute meeting in 2018.

MAJOR COLLABORATIONS AND PROJECTS

The research departments and groups of the Institute collaborate with a large number of international partners in the framework of numerous projects. Major collaborations involving multiple departments and groups are listed below. Further projects are described in the departmental and group reports.

EARTH AND SOLAR SYSTEM RESEARCH PARTNERSHIP

To foster scientific collaboration between the thematically related Max Planck Institutes and associated partners, the Earth System Research Partnership (ESRP; www.earthsystem.de) was established in 2003 between the MPI for Chemistry in Mainz, the MPI for Meteorology in Hamburg, and the MPI for Biogeochemistry in Jena. The partnership was renamed the Earth and Solar System Research Partnership in 2017 when the MPI for Solar System Research joined. Among the associated partners are the MPI for Dynamics and Self Organization (Göttingen), the MPI for Marine Microbiology (Bremen), the MPI for Terrestrial Microbiology (Marburg), and the Institute for Advanced Sustainability Studies (Potsdam).

The objective of the ESRP is to understand how planet Earth functions as a complex system and to improve the predictability of the effects of human actions. Over the last century, there have been marked changes in climate, air quality, biodiversity, and water availability. Additional, and potentially more rapid, changes are predicted. To find solutions to the challenges posed by these changes, the ESRP studies the complex interactions and feedbacks between land, ocean, atmosphere, biosphere, and humans in the field, in the lab, and through numerical models. For this purpose, the ESRP develops, maintains, and utilizes joint research infrastructures, e.g., the German Climate Computing Center (DKRZ) for computing for Earth system science, airborne in-situ measurements (HALO research aircraft), and ground-based long-term observations such as the Amazon Tall Tower Observatory (ATTO), the Barbados Cloud Observatory (BCO), and the Zotino Tall Tower Observatory (ZOTTO) in the Siberian taiga.

ESRP meeting in Göttingen in 2018.

HALO AIRCRAFT

To optimize atmospheric research and Earth observations, the Institute uses the HALO aircraft, a research aircraft stationed at the German Aerospace Center (DLR). The aircraft has a maximum range of 12,000 km, and is able to operate at an altitude of up to 15.5 km. HALO was approved for scientific missions in 2012 after eight years of construction and testing. Since then, the MPIC has been involved primarily in the scientific missions described below.

2014 – Mid-Latitude-Cirrus (ML-CIRRUS)
The objectives of this mission over Europe and the North Atlantic included investigation of the indirect effects of aerosol on cirrus clouds, the quantification of the contribution of aerosol particles from ground-level sources and air traffic pollution, as well as the clarification of processes in the formation of cirrus clouds.

2014 – Aerosol, Cloud, Precipitation, and Radiation Interactions and Dynamics of Convective Cloud Systems (ACRIDICON-CHUVA)
This mission over the Amazon rainforest in Brazil aimed at elucidating aerosol-cloud interactions and their effects on atmospheric dynamics, radiation, and precipitation. In particular, the differences between unpolluted air and polluted air as well as the impact of biomass burning and other anthropogenic aerosols on the formation and evolution of clouds were studied and quantified.

2015 – Oxidation Mechanism Observation (OMO)
The mission addressed the "self-cleaning capacity" of the atmosphere and how natural and anthropogenic compounds are chemically transformed in the upper troposphere. The OMO aircraft measurement campaign focused on oxidation processes and air pollution chemistry downwind of South Asia during the summer monsoon.

2017+2018 – Effect of Megacities on the Transport and Transformation of Pollutants on the Regional to Global Scales (EMeRGe)
This mission addressed the impact emissions from major population centers have on air pollution at local, regional, and hemispheric scales. EMeRGe

conducted dedicated airborne measurement campaigns, as well as coupled interpretation and modeling studies primarily of short-lived climate pollutants (i.e., reactive gases, temporary reservoirs, and aerosol particles). The first part of the campaign was conducted in summer 2017 with flights over Europe. The second part operated flights over Asia and was conducted in 2018.

2018 – Chemistry of the Atmosphere: Field Experiment in Africa (CAFE-AFRICA)
The main objective of the CAFE-AFRICA mission, conducted in August and September 2018, was to study the influence of the massive biomass burning emissions from southern Africa, combined with growing industrial, urban and desert dust emissions, on the atmospheric oxidation capacity over the tropical and South Atlantic Ocean.

2020 – BLUESKY
The aim of the research mission BLUESKY was to investigate how reduced emissions from industry and transport during the COVID-19 lockdown are changing atmospheric chemistry and physics. Together with scientists from the DLR and the Goethe University Frankfurt, the MPIC measured concentrations of trace gases and pollutants in the air over European urban areas and in the flight corridor to North America.

Further missions of the HALO aircraft in which the MPIC is involved as a leading or contributing institution are planned:

2021 – Formation, Lifetime, Properties and Radiative Impact of High-Latitude Cirrus Clouds (CIRRUS-HL).

2022 – Chemistry of the Atmosphere: Field Experiment in Brazil (CAFE-BRAZIL)
Operating the HALO aircraft from Manaus, this mission will study tropospheric oxidant photochemistry in combination with particle formation and growth mechanisms under pristine conditions found over the Amazon rainforest. Originally, this mission was planned for spring 2020 but had to be postponed due to the COVID-19 pandemic.

AMAZON TALL TOWER OBSERVATORY (ATTO)

The Amazon Basin plays a key role in the carbon and water cycles, climate change, atmospheric chemistry, and biodiversity. It is affected by human activities, and more pervasive change is expected to occur in the future. Thus, it is essential to establish long-term measurements that provide a baseline record of present-day climatic, biogeochemical, and atmospheric conditions and to continue to monitor changes in the Amazon region related to global change and the Anthropocene, the current era of globally pervasive and steeply increasing human influence on planet Earth. The Amazon Tall Tower Observatory (ATTO) has been set up in a pristine rainforest region in the central Amazon Basin, about 150 km northeast of the city of Manaus, Brazil. Two 80-m towers have been operated at the site since 2012, and a 325-m-tall tower was completed in 2015. The ATTO project is a Brazilian-German collaboration between the Instituto Nacional de Pesquisas da Amazonia (INPA), the Universidade do Estado do Amazonas (UEA), the Max Planck Society (MPG), and further research partners. On the German side, the project was initiated and established by the MPIC, and it continues to be coordinated in collaboration between the MPI for Biogeochemistry and the MPIC.

S/Y EUGEN SEIBOLD

The *S/Y Eugen Seibold* is a modern research yacht that has been operated by the MPI for Chemistry since 2018. It aims at sampling and analyzing seawater, plankton, and air samples in order to better understand the interactions between the ocean and the atmosphere. The *S/Y Eugen Seibold* team successfully carried out 16 scientific expeditions in spring and summer 2019. In 2020, a north-to-south transect was probed in the eastern North Atlantic starting from the polar circle and reaching as far south as the equator, comprising a wide range of marine provinces and environmental conditions. The yacht was financed by the Werner Siemens Foundation, Switzerland.

EMME-CARE

The Eastern Mediterranean Middle East – Climate and Atmosphere Research Center (EMME-CARE) project was established with the goal of creating a regional center of excellence for climate and atmospheric research in the Eastern Mediterranean and Middle East (EMME) region, which has been identified as a global climate change hotspot. Opened in 2019 and affiliated with the Cyprus Institute in Nicosia, it focusses on the causes and effects of climate change in the area, and developing regional research networks, and mitigation and adaptation solutions.

The Climate and Atmosphere Research Center (CARE-C) of the Cyprus Institute, which has been established in this long-term project, is steered by the MPI for Chemistry, which together with the French Commissariat à l'Energie Atomique (CEA) and the University of Helsinki, Finland, constitute the Advanced Partners in the EMME-CARE project.

FIELD MEASUREMENTS AND EXPEDITIONS 2015–2020

SCIENTIFIC PUBLICATIONS

PUBLICATION STATISTICS

The results of the fundamental scientific research conducted at the Institute are mainly published in peer-reviewed scientific journals. From 2009 to 2019, 2,270 peer-reviewed journal articles and reviews were published at the MPIC; on average, 206 publications per annum. According to Web of Science, nearly 65 % of the total set are Open Access papers.

Through the end of 2019, MPIC-authored publications from 2009 to 2017 were cited 72,553 times. This is an average of 40.4 citations per paper, an increase of about 20 % compared to an average of 33.7 citations per paper in the years 2006 to 2016.*

Between 2009 and 2017, the Institute published papers that belong, on average, to the top fourth (27.3 %) most cited papers within their subject categories. A value of 50 % represents the median and thus an average citation impact compared to all publications from the same subject areas and publication years. Thus, the MPIC citation impact is far above the average of the relevant scientific community.

Approximately one quarter (23.6 %) of the MPIC papers belong to the 10 % most cited papers within their subject categories. In 21 out of 28 relevant subject categories, the Institute has achieved a subject-based observed-to-expected citation ratio far above the international standard of the corresponding field (>1.5). The MPIC citation impact is significantly higher than the country averages of Germany and the United States of America, and also higher than the average of the Chemistry, Physics and Technology Section (CPTS) of the Max Planck Society.

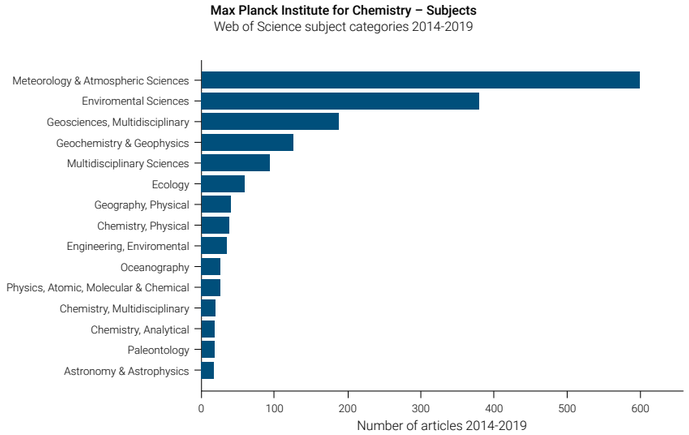


Figure 1: Most frequent Web of Science (WoS) subject categories of the journals in which the MPI for Chemistry published during the time span from 2014 – 2019.

In summary, the metrics used to measure normalized citation impact show that the MPIC has a very high impact. Moreover, individual Institute members have been ranked repeatedly as "Highly Cited Researchers". A comprehensive listing of scientific publications during the past decades is available on Institute's web pages (http://www.mpic.de/en/research/publications.html), further information and citation statistics are provided on the web pages of individual researchers (Researcher ID, Google Scholar, etc.), and selected highlight studies have also been advertised in press releases (https://www.mpic.de/3538502/press-releases).

OPEN ACCESS

The Max Planck Society and the Max Planck Institute for Chemistry are among the leading proponents of open access to scientific publications and scholarly knowledge. Since the year 2003, the Max Planck Society is hosting and supporting a series of international meetings, the "Berlin Open Access Conferences", which are dedicated to the promotion of open access and yielded some of the key statements and developments in the global move to open access. From the beginning, MPIC scientists have been actively involved in this development and continue to play a leading role.

The "Berlin Declaration on Open Access to Knowledge in the Sciences and Humanities" (https://openaccess.mpg.de/Berlin-Declaration) was issued in 2003, has been signed by over 650 leading scholarly organizations around the world, and continues to attract further signatories.

The international initiative „Open Access 2020" (OA2020) aims to transform existing scholarly journals from subscription to open access publishing in a smooth, swift and scholarly oriented way.

Since its release in 2016, the OA2020 Expression of Interest in the „Large-scale Implementation of Open Access to Scholarly Journals" has been signed by over 140 scholarly organizations – including the Alliance of Science Organizations in Germany, the European University Association representing more than 800 universities in 47 countries and other major organizations in Europe, Asia, and the Americas. Through transformative agreements with traditional publishers as well as support for new and improved open access publishing platforms, the MPG, other institutions, and several countries have managed to establish open access to large fractions of their publication output (up to ~80 %).**

Already before the Berlin Declaration on Open Access, the MPIC and its researchers were pioneers in the foundation and successful development of innovative forms of open access publishing. Since the year 2001, scientists from the MPIC have led the way in the conception, development, and application of interactive open access publishing with public peer review, which is now also spreading across other fields in the sciences and humanities.

In fact, some of the very first and most successful international open access journals have been founded and grown to top visibility and scientific reputation under the aegis of researchers at the MPIC engaged in the European Geosciences Union (EGU): Atmospheric Chemistry and Physics (ACP) since 2001; Biogeosciences (BG) since 2004; and Atmospheric Measurement Techniques (AMT) as well as Geoscientific Model Development (GMD) since 2008.**

Through these and related activities, the Institute indeed continues to serve as a pace-maker for open science for the benefit of scientific and societal progress.

The publication list of the Institute is available at https://www.mpic.de/Publikationen

** The bibliometric data are taken from the report "A bibliometric analysis of the MPI for Chemistry, in the publication period 2009–2019" by Thomas Scheidsteger and Robin Haunschild, Max Planck Society, Information Retrieval Services.*

*** For more information see www.mpic.de/4123205/open-access.*

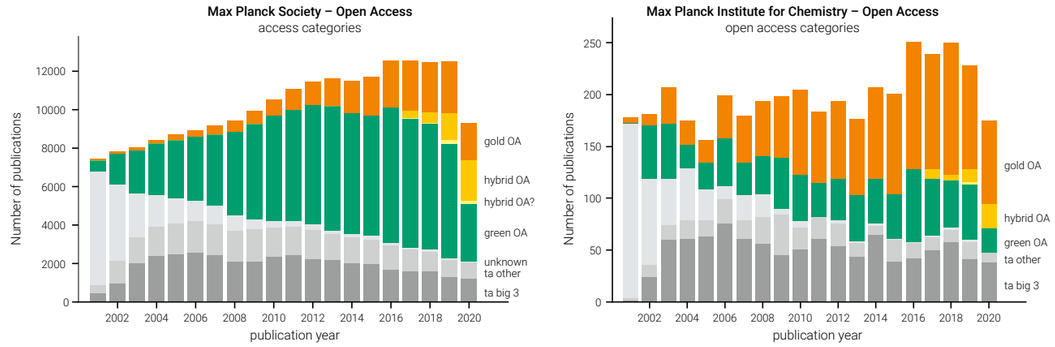


Figure 2: Publication output by open access (OA) categories for the entire Max Planck Society (left) and for the MPIC (right). Orange: gold OA, yellow: hybrid OA, green: green OA, light gray: toll access publications by various publishers, dark gray: toll access publications by one of the "big 3" publishers Elsevier, Springer Nature, and Wiley.

JUNIOR SCIENTIST SUPPORT: GRADUATE SCHOOLS AND POSTDOCTORAL PROGRAM

The support of junior scientists is of major importance for the MPIC. Besides two graduate schools for PhD students – the Paul Crutzen Graduate School (PCGS) and the Max Planck Graduate Center (MPGC) – a postdoctoral program was established in 2018.

PAUL CRUTZEN GRADUATE SCHOOL (PCGS)

To give them the best possible support during their stay at the Institute, all PhD students affiliated with the MPIC are automatically members of the Paul Crutzen Graduate School (PCGS).

Each PhD student has an individual PhD Advisory Committee (PAC) with experts from the Institute as well as from outside institutions such as the Johannes Gutenberg University Mainz (JGU). The committee monitors the progress of the dissertation project and gives not only scientific support but also recommendations on further skills that should be acquired for graduation and a successful career.

Within the graduate school, various lectures in atmospheric environmental and climate sciences, soft skill courses, language classes, and extracurricular and social activities are offered. The curriculum is adapted to the individual needs of each doctoral student. A course in atmospheric chemistry as a core research topic of the Institute is mandatory as well as a course on good scientific practice.

PhD students are supported in organizing their own seminars and conferences, such as the Paul Crutzen Days – an annual conference organized by and for the PhD students.

The Graduate School coordinator can be addressed at any time on any issue, and as an impartial and trustworthy partner, is ready to support the PhD students and help pursue their interests.

Currently, 62 students, 29 of them female and 33 male from 13 countries, are enrolled in the PCGS.*

MAX PLANCK GRADUATE CENTER (MPGC)

The MPGC is a cross-institutional graduate school of the MPIC, the Max Planck Institute for Polymer Research, and four departments of the JGU in Mainz: Chemistry, Pharmaceutical Sciences, Geography and Geosciences; Physics, Mathematics and Computer Science; Biology; and University Medicine. Since 2019, the former Graduate School of Excellence Material Science in Mainz of the JGU is affiliated with the MPGC.

The MPGC is especially pertinent for PhD students with an interdisciplinary research project and supervisors from different institutions and faculties. To make it more accessible for international PhD students with diverse scientific backgrounds, the MPGC has its own doctoral regulations to overcome the limitations imposed by traditional faculty rules of the university. International PhD students are welcome to invite experts from their home university to become a member of the supervision committee, thereby further fostering international cooperation.

The monitoring system of the MPGC and the curriculum is analogous to the PCGS. 11 PhD students from the MPIC are currently members of the MPGC. (In total, 74 PhD students belong to the MPGC; 29 are female, 45 are male and 12 different nationalities are represented)*.

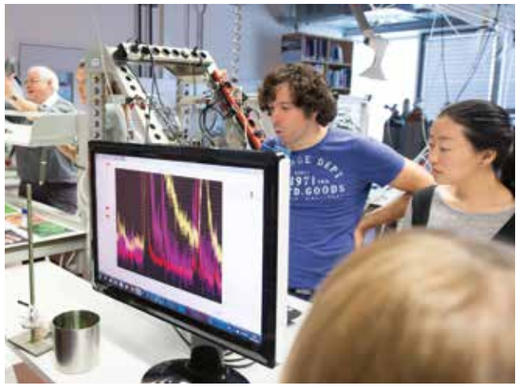
POSTDOCTORAL PROGRAM

The postdoctoral period is a very challenging time for every young scientist, not least because of the effort required to handle professional and private lives. Thus, a postdoctoral program comparable to the PhD program was established to give these scientists the best possible support during their stay at the Institute and to prepare them for their future careers, either within or outside academia. The postdoctoral program provides soft skill courses, career counselling and career training, and individual coaching and fosters networking within and outside the Institute. The program is coordinated by a central contact person who protects the confidentiality of the postdocs. Furthermore, the Institute also provides support with child/family care.

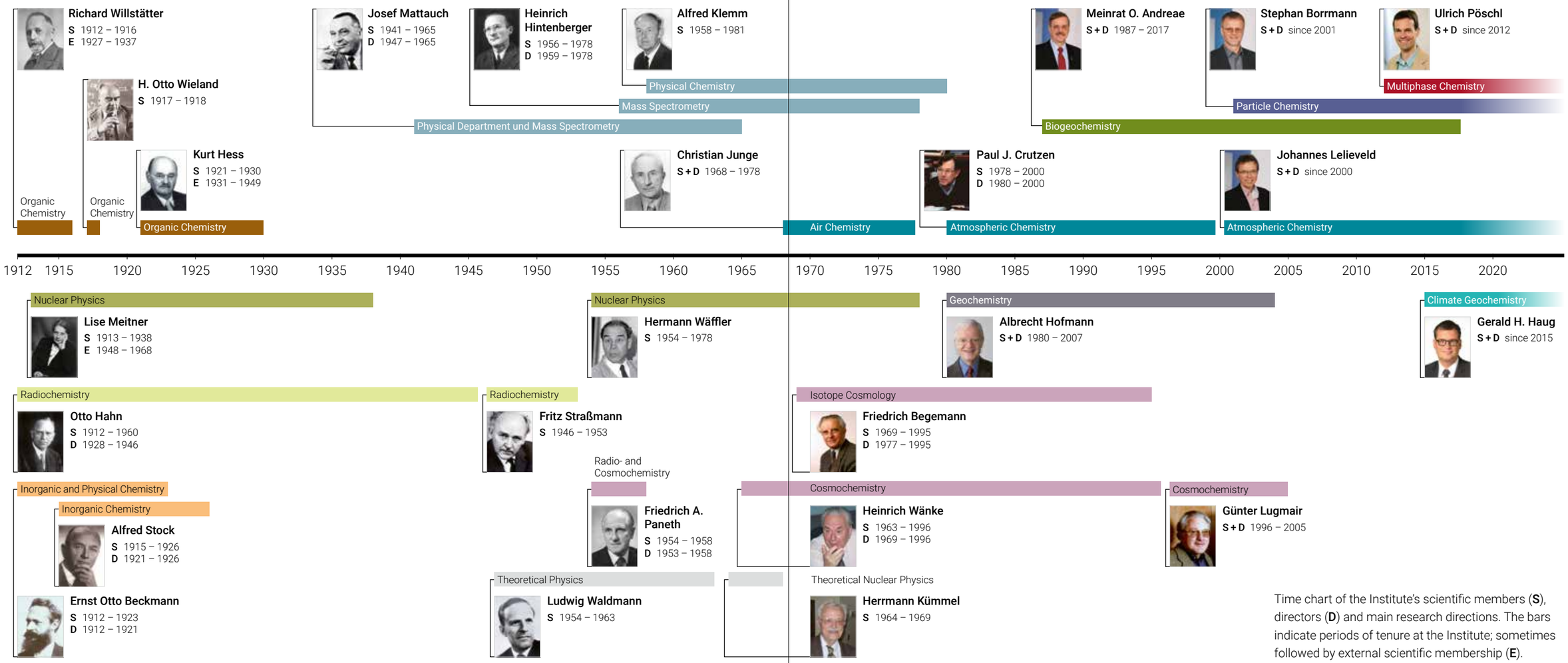
GUEST PROGRAM AT THE MPIC

The Guest Program represents a straightforward tool for granting scholarships to scientists who visit the Institute for a limited period of time (PhD students up to six months; postdocs up to two years), either to engage in ongoing research projects of the MPIC or to use the infrastructure and expertise for their own research projects. The uncomplicated application and admission process of the Guest Program is an important, flexible tool to enhance scientific exchange and to expand collaborations. Participants of the Guest Program are included in the regular PhD or Postdoc procedures and receive the same support as all other MPIC members.

* December 2020



HISTORY



Time chart of the Institute's scientific members (**S**), directors (**D**) and main research directions. The bars indicate periods of tenure at the Institute; sometimes followed by external scientific membership (**E**).

Research at the Max Planck Institute for Chemistry has been at the forefront of science throughout its existence. Since the Institute's foundation in 1912, three of its directors were awarded with the Nobel Prize for Chemistry: Richard Willstätter in 1915 for the revelation of the structure of chlorophyll and other plant pigments, Otto Hahn in 1944 for the discovery of nuclear fission, and Paul Crutzen in 1995 for the elucidation of atmospheric ozone chemistry.

The research departments and focal points of the Institute have gone through a history of change and scientific evolution as illustrated in the time chart above. What began in 1912 with classical organic, inorganic and physical chemistry at the Kaiser Wilhelm Institute for Chemistry in Berlin evolved into radiochemistry and nuclear physics in the 1930s, leading to the discovery of nuclear fission by Otto Hahn, Lise Meitner and Fritz Strassmann.

As the Institute was severely damaged towards the end of World War II it was moved to the Swabian Alp in today's Baden-Wuerttemberg. There the chemists worked provisionally from 1944 to 1949 until the Institute moved a second time to the campus of the newly founded Johannes Gutenberg University in Mainz. At the same time it was integrated into the Max Planck Society, the successor of the Kaiser Wilhelm Society, and reopened as the Max Planck Institute for Chemistry. Since 1959 the Institute also carries the name "Otto Hahn Institute" in honor of its previous director and the first president of the Max Planck Society.

In the 1960s and 1970s the Institute's research portfolio was extended from Physical Chemistry, Nuclear Physics and Mass Spectrometry to Cosmochemistry, Isotope Cosmology and Air Chemistry. Meteorites and moon dust samples were studied and the interplay of atmospheric gases, particles and meteorology were investigated. In the 1980s new departments for Geochemistry and Biogeochemistry were founded, in 2001 the Particle Chemistry Department was established jointly with the Institute for Atmospheric Physics at the Johannes Gutenberg University of Mainz, in 2012 the Multiphase Chemistry Department, and in 2015 the Climate Geochemistry Department was founded.

Nowadays, the research focus of the Max Planck Institute for Chemistry is on Earth System science, in particular on the chemical processes occurring in the atmosphere and their interactions with the biosphere and oceans. It also includes the influence of humans, as unprecedented urbanization and industrialization in the past centuries have changed the course of natural processes on our planet, in an epoch now known as the Anthropocene.

ATMOSPHERIC CHEMISTRY

Self-cleaning capacity of the atmosphere. Photochemistry, oxidation mechanisms, transport processes and climate effects of trace gases and aerosol particles.

ATMOSPHERIC CHEMISTRY DEPARTMENT

"PHOTOCHEMICAL PROCESSING OF THE AIR"
OXIDATION REACTIONS CLEANSE THE ATMOSPHERE FROM NATURAL AND ANTHROPOGENIC POLLUTANTS

The atmosphere removes millions of tons of natural and anthropogenic pollutant emissions each year through oxidation reactions. This self-cleansing mechanism profoundly changes the characteristics of the emitted species such as reduced and partly oxidized gases. Most gases react with radicals, predominantly hydroxyl (OH), which results in less volatile and more soluble products that can be removed by precipitation and deposition onto the Earth's surface. During oxidation reactions, secondary pollutants can be formed, which diminish air quality and contribute to climate change. Fine particulate matter and ozone, for example, have atmospheric lifetimes of up to several weeks and can be transported over large distances. Thus, air pollution is not merely a local phenomenon. Our department studies the chemical mechanisms that "process" the emissions from local to global scales.

The department employs instrumented mobile platforms such as aircraft and ships, as well as ground-based stations, to gain insights into interdependencies between emissions, chemical transformations, and atmospheric transport. Our custom-built instrumentation measures many reactive species and their reaction products, and the wealth of data obtained helps improve computer models that simulate air quality and climate.

The group led by Hartwig Harder uses laser-based fluorescence techniques to measure highly reactive gases, including radicals. The group of Horst Fischer uses optical detection and wet-chemical methods to measure primary emissions and atmospheric reaction intermediates, such as aldehydes and peroxides. The group led by John Crowley uses laser-cavity methods and chemical ionization mass spectrometry to study the chemistry of nitrogen oxides, for example. Jonathan Williams's group uses mass spectrometric techniques to measure organic compounds and their reaction products. The group led by Andrea Pozzer develops local-to-regional and global models to analyse the measurement data.

Results show how the atmosphere regulates concentrations of OH and other oxidants and reveal to what extent reactive gases alter the properties of other species, including aerosols such as dust, organic and sea spray particles. The chemical "processing" of aerosols affects their lifetime and, in turn, the properties of clouds, climate, nutrient cycles, and public health. The latter is an emerging area of focus in our department on which we collaborate with groups in epidemiological and biomedical sciences.

The department studies natural volatile organic compounds (VOCs) that are released in vast amounts by vegetation. We compare tropical with boreal environments, two settings in which VOCs can have very different characteristics. The VOC isoprene, released by the canopy, dominates tropical rainforest emissions, while monoterpenes are more typical for the boreal environment. Isoprene and monoterpenes can react with ozone, forming particles, and also generate radicals that contribute to the reactivity of the forest air. Among various reaction products, Criegee intermediates, predicted by laboratory and modeling studies, have long been enigmatic. We have now measured these intermediates in boreal ecosystems and evaluated their role in atmospheric chemistry. In the tropics, we uncovered a hitherto unknown, large source of sesquiterpenes from soils.

In the past years, we instrumented the High Altitude and LOng Range Research Aircraft (HALO), which was first deployed on a mission that measured the outflow of deep convective clouds during the wet season in South Asia. The data revealed that the summer monsoon sustains an effective cleansing mechanism that removes pollutants. However, some species remain and are lofted above the clouds to reach the stratosphere. HALO missions that started in 2018 under the name "Chemistry of the Atmosphere – Field Experiment" (CAFE) aim to chemically characterize the tropical atmosphere over Africa, South America, and the Atlantic and Pacific Oceans. In spring 2020, during the COVID-19 lockdowns, we performed an additional HALO mission over Europe to study the impacts of the major declines in emissions from land and air traffic on atmospheric chemistry and the climate.

Figure 1: In many cities air quality is poor, but via chemical and transport processes anthropogenic emissions influence the atmosphere on a much larger scale, being documented by our measurements. The department investigates how pollutants interact with natural emissions, and to what extent they change the global atmosphere and climate.

JOS LELIEVELD

25 July 1955 Born in The Hague, The Netherlands

1984 Study of natural sciences at Leiden University

1984 – 1987 Research associate at Geosens B.V.

1987 – 1993 Research scientist at the Max Planck Institute for Chemistry

1990 PhD in Physics and Astronomy Utrecht University

1993 – 2000 Professor of Atmospheric Physics and Chemistry University of Wageningen and Utrecht

since 2000 Director at the Max Planck Institute for Chemistry and Scientific Member of the Max Planck Society

Professor in Atmospheric Physics, University of Mainz, and Professor at the Cyprus Institute, Nicosia

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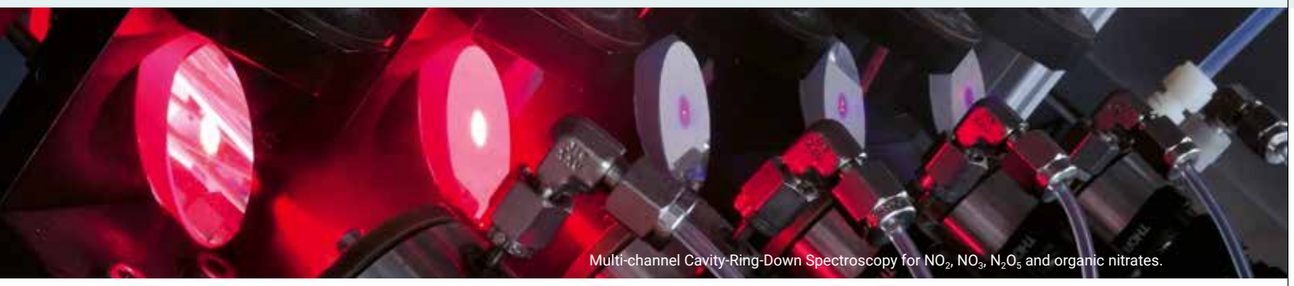
LIFETIME OF NO_x: CHEMICAL PROCESSES INVOLVING NO_3 AND OH

JOHN CROWLEY



Multi-channel Cavity-Ring-Down Spectroscopy for NO_2, NO_3, N_2O_5 and organic nitrates.

INTRODUCTION

The rate and nature of the chemical processing of pollutant emissions of NO into the atmosphere has a strong influence on, e.g., photochemical ozone and particle formation and the atmospheric oxidation capacity. NO, formed by bacterial activity in soils, lightning and in combustive systems related to biomass burning and anthropogenic activity, is oxidized to NO_2, which together with NO forms the NO_X family ($NO_X \equiv NO + NO_2$). The loss of NO_X to generate NO_Y (total reactive nitrogen) proceeds mainly by the sequential oxidation of NO_2 throughout the diel cycle, which is initiated by reactions involving OH radicals (mainly during daytime) and NO_3 radicals (mainly at night). The difference between NO_Y and NO_X is defined as NO_Z ($NO_Z \equiv NO_Y - NO_X$). Two major contributors to NO_Z are HNO_3 (especially in the lower stratosphere) and both organic (RNO_X) and particulate nitrate (NO_3^-) in the boundary layer, the latter formed, e.g., by the uptake of N_2O_5 into aqueous particles (Figure 1).

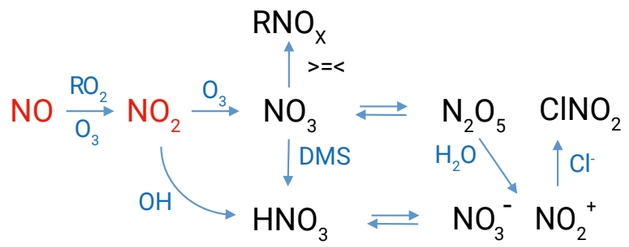


Figure 1: Day and nighttime routes from NO_X (red) to selected NO_Z (black).

RESULTS

The reaction of NO_2 with OH is the most important process by which NO_X is lost on a global scale, yet different expert evaluation panels have reported divergent parameters for the rate coefficient. We have re-examined the rate coefficient for this pressure-, temperature-, and bath gas-dependent reaction using the pulsed laser photolysis technique combined with two-fold absorption spectroscopy (broadband and 365nm) for measurement of NO_2 and laser-induced fluorescence for OH. Our data, which cover a substantial fraction of the fall-off regime (10–700 Torr), are highly precise and enable the third-body quenching efficiency of H_2O to be established for the first time. The influence of H_2O on the rate coefficient is illustrated in Figure 2 A and indicates that the contribution of collisional quenching by H_2O to the rate coefficient in humid, tropical regions is approximately equal to that of O_2 and decreases the lifetime of NO_2 by about 10%. A parameterization of the rate coefficient based on our data was incorporated into a global chemical transport model to show, e.g., that use of the IUPAC recommendation results in underestimation of the HNO_3/NO_2 ratio by as much as a factor of 1.3 in the lower stratosphere (Figure 2 B).

During the "Air Quality and climate change in the Arabian Basin" (AQABA) project we deployed three instruments on a ship to investigate the (inter)conversion of NO_X to NO_Y along a route through the Mediterranean Sea, the Suez Canal, the Red Sea, the Arabian Sea, and the Arabian Gulf. Combining results from a newly built thermal dissociation cavity ring-down spectrometer (TD-CRDS) for NO_X and NO_Y with those from a five-channel TD-CRDS instrument set up to measure NO_2, NO_3, N_2O_5, and organic nitrates, we examined the NO_X/NO_Y ratio and the composition of NO_Y throughout the two-month journey. The results for the Mediterranean Sea are illustrated in Figure 3 A. For most regions we found that, on average, NO_X (40–50%) and HNO_3 (30–40%) accounted for the majority of NO_Y with smaller contributions from particle nitrate and organic nitrates. This is related to the high temperatures encountered during the journey, which partitioned HNO_3 to the gas-phase and shortened the lifetime of PAN. Our measurements of NO_3, N_2O_5, and $ClNO_2$ (the latter using a chemical ionization mass-spectrometer) also indicated that, at night, the heterogeneous loss of NO_X via the formation and uptake into aqueous aerosol of N_2O_5 was less important than routes involving gas-phase reactions of NO_3 (e.g. with DMS or trace gases associated with ship emissions and/or oil-related activities) so that formation of $ClNO_2$ was suppressed. The regional variation in the $ClNO_2$ production efficiency (per NO_3 formed) is illustrated in Figure 3 B. The very low yields of $ClNO_2$ observed in the Arabian Gulf are a result of very high nighttime temperatures (~30°C) that result in short lifetimes for N_2O_5 and large concentrations of reactive organics (from on- and off-shore oil-related activities) that react with NO_3. Indeed, the short lifetime of NO_3 throughout much of AQABA resulted in nocturnal losses of NO_X that competed with the daytime reaction of OH with NO_2.

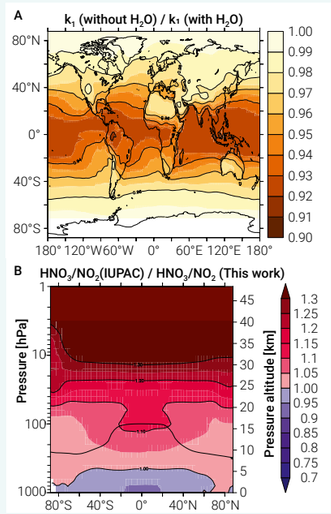


Figure 2: A) Relative change in the rate coefficient for the reaction between OH + NO_2 when neglecting the effect of water vapor. B) Relative change in the HNO_3/NO_2 ratio with the new parameterization compared to IUPAC. The black line is the tropopause.

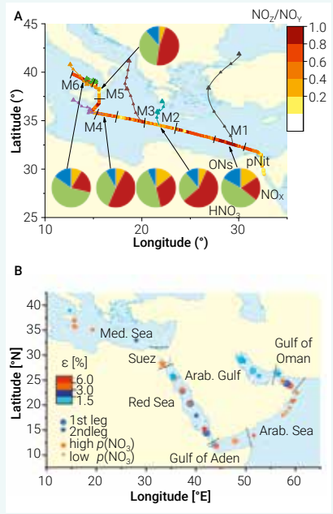


Figure 3: A) NO_2/NO_Y ratio and composition of NO_Y at various locations along the shipping route (ONs = organic nitrates, pNit = particle nitrate). HNO_3 was calculated via: $HNO_3 = NO_Z - (ONs + pNit + NO_X)$. B) Efficiency (ε) of $ClNO_2$ formation per NO_3 formed in the reaction between NO_2 and O_3.

"*In situ* observation combined with laboratory studies provide insight into the chemical processes that define atmospheric composition from the boundary layer to the lower stratosphere."

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NITROGEN OXIDES AND THEIR INFLUENCE ON THE OXIDATION CAPACITY OF THE TROPOSPHERE

HORST FISCHER

The HALO research aircraft.

INTRODUCTION

Nitrogen oxides ($NO_X \equiv NO + NO_2$) play a pivotal catalytic role in the oxidation capacity of the troposphere, influencing the generation of the three dominant oxidants in the lowest layer of the Earth's atmosphere. NO_X catalyze the photochemical production of ozone (O_3), contribute to recycling of OH from the hydroperoxy radical (HO_2), and form nitrate radicals during the night (NO_3). The concentration of O_3 is central to the primary formation rates of the OH and NO_3 radicals, with the net ozone production rate (NOPR) exhibiting a non-linear dependence on NO and volatile organic compound reactivity (VOCR) towards OH (Figure 1).

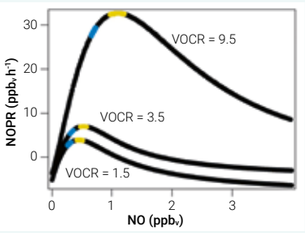


Figure 1: NOPR as a function of NO for different VOCR levels. Blue and yellow bars indicate the change from NO_x to VOC limitation (adapted from Schroeder et al., 2017).

RESULTS

In the years 2017 to 2020 we participated in three major field campaigns with high-precision ship-based (AQABA) and airborne (CAFE-AFRICA; BLUESKY) NO_X measurements. Based on *in situ* observations of NO, NO_2, O_3, OH, HO_2, and photolysis rates, the NOPR was calculated from the difference between ozone production (reaction of NO with HO_2 and organic peroxy radicals) and loss (photolysis of O_3 and reaction with either OH or HO_2). During AQABA, which probed the marine boundary layer around the Arabian Peninsula, median NO_X mixing ratios varied between 0.2 ppbv over the Arabian Sea and 2.7 ppbv over the Arabian Gulf, with a range from about 0.06 ppbv to 10 ppbv. This allowed us to study the non-linearity of NOPR over three orders of magnitude of NO as shown in Figure 1. Calculated median NOPR values based on observations indicate a tendency towards ozone destruction over the Mediterranean Sea (-1 ppbv day^{-1}) and the Southern Red Sea (-4 ppbv day^{-1}), while substantial ozone production was deduced for the Northern Red Sea, the Oman Gulf (16 ppbv day^{-1}) and the Arabian Gulf (32 ppbv day^{-1}). The ratio between formaldehyde (HCHO) and NO_2 is a measure of the OH reactivity towards either volatile organic compounds or NO_X. It can be used to indicate whether O_3 formation is VOC- or NO_X-limited. For AQABA, the HCHO/NO_2 ratios indicated NO_X limitation for all regions except the Northern Red Sea and the Oman Gulf, which are in a transition zone. The accurate simulation of NOPR with the ECHAM/MESSy global circulation model (EMAC) is a demanding task, since it relies on a correct description of the underlying non-linear chemistry and an accurate representation of the involved species and their sources. For AQABA, EMAC tends to predict slightly higher NOPR values than those that are actually observed due to an overestimation of NO_X.

In the upper troposphere, NO produced from lightning dominates the NOPR as shown for observations over West Africa during CAFE-AFRICA (Figure 2). At altitudes higher than 12 km, NO enhancements caused by lightning were observed in deep convection over land and the Intertropical Convergence Zone (ITCZ) off the coast of Africa. The highest values are found over land (0.4 ppbv compared to 0.2–0.3 ppbv at the ITCZ). Interestingly, tropical storm Florence, which developed into hurricane Florence, and which was probed twice as it moved across the Atlantic, showed no sign of electrification when distant from the coast. In general, the NOPR closely follows the upper tropospheric distribution of NO. Values varied from 0.1 ppbv day^{-1} off the coast, to up to 0.3 ppbv day^{-1} over land. In the middle troposphere, O_3 destruction prevails at low NO concentrations.

OUTLOOK

During the COVID-19 induced lockdowns in spring 2020 air traffic over Europe and the Atlantic was approximately 85% reduced compared to 2019. This provided the unique opportunity to study the impact of reduced air traffic on NO levels in the UTLS. In the LS we measured an NO reduction of about 30% (0.04 to 0.06 ppbv) over Europe relative to the series of SPURT campaigns in early 2000. In addition, we found a strong decrease of carbon monoxide (CO) mixing ratios in the boundary layer during fly-bys at Frankfurt Airport of approx. 30 ppbv (~15%) relative to long-term observations obtained from MOZAIC/IAGOS measurement flights. Further modeling studies will show whether these reductions can be unambiguously attributed to the lockdown.

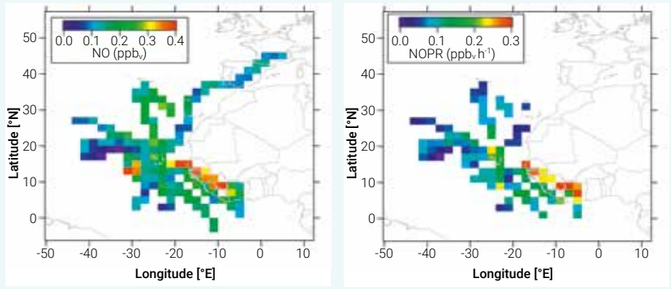
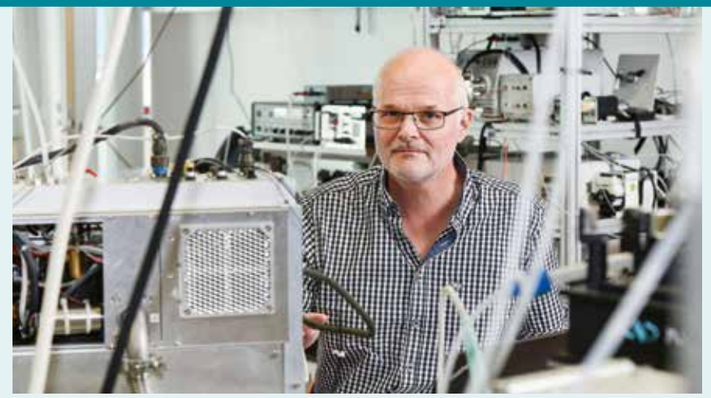


Figure 2: NO (left) and NOPR (right) at altitudes above 12 km measured during CAFE-AFRICA.



"The Optical Spectroscopy Group combines *in situ* observations of NO_X, HCHO, and H_2O_2 with modeling to study oxidation processes in the troposphere."

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OH AND HO_2 AFFECTING THE SELF CLEANING CAPABILITY OF THE ATMOSPHERE

HARTWIG HARDER

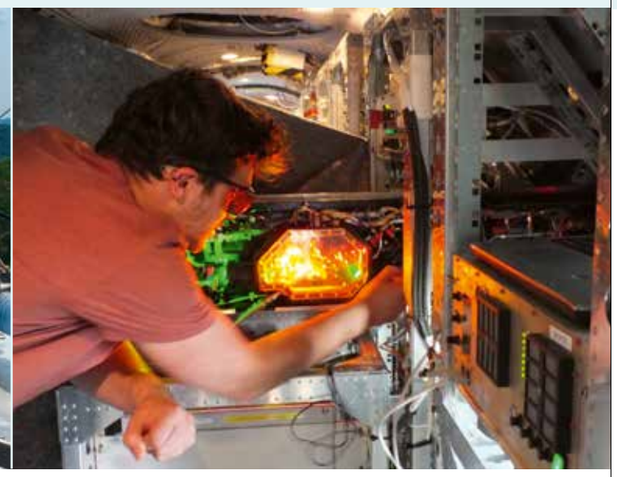


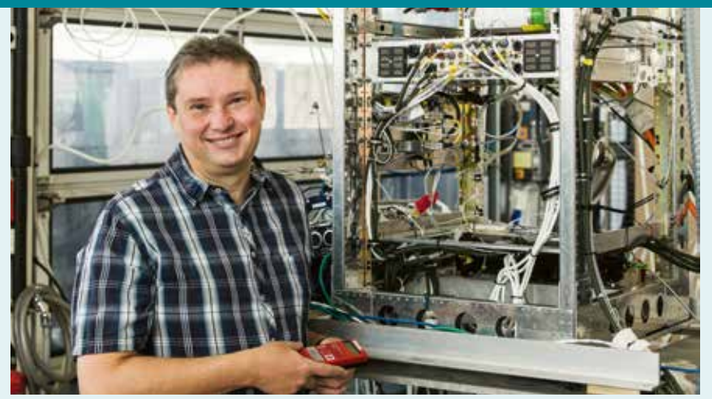
Figure 1: OH and HO_2 measurements above the canopy in Brazil (left), calibrating the OH and HO_2 measuring device onboard the HALO research aircraft.(right).

MONSOON INFLUENCE OF THE UPPER TROPOSPHERE

We have identified efficient chemical processing of Asian pollution in the upper troposphere. The polluted air is uplifted by convection during the summer monsoon. These air masses can be retained in the Asian Monsoon Anticyclone (AMA) above 10 km altitude for several weeks. Our measurements of the major oxidizing agents OH and HO_2 onboard the HALO research aircraft show that mixing ratios are up to 30 % and 70 % higher, respectively, inside compared to outside the AMA. Our chemical budget analysis demonstrated that reactions with NO result in efficient recycling of OH after reaction with CO or VOC to produce HO_2 and organic peroxy radicals (RO_2). NO formed by anthropogenic processes in the boundary layer, and in particular also by lightning, is recurrently injected into the AMA through convection.
In addition to the recycling of OH, the reactions of NO with HO_2 and RO_2 result in a rate of O_3 formation that is nearly a factor of two greater inside than outside the AMA, at a net ozone production rate of 0.2 ppb/h. Over the course of the retention period, this leads to significantly enhanced ozone concentrations of up to 90 ppb in the AMA, which in turn contribute to a larger primary source for OH. The enhanced ozone concentrations help maintain the OH recycling also in NO-depleted regions of the AMA that are unaffected by direct convective input of NO. Preliminary results from the CAFE-AFRICA campaign with the HALO aircraft similarly show enhanced concentrations of OH and HO_2 in the outflow of electrified systems. This is due to the uplift of boundary layer air, mixed with NO from lightning. In non-electrified convective systems, we observed an increase in HO_2 only, indicating that precursor gases like aldehydes and hydroperoxides, which contribute to radical production, are transported from the boundary layer, while OH recycling is inefficient. Further analysis of the data from CAFE-AFRICA is underway.

RAINFOREST INFLUENCE IN THE LOWER TROPOSPHERE

We are studying the OH radical recycling at the atmosphere-biosphere interface in the tropical rainforest at the ATTO site. The immense Amazon rainforest ecosystem is a significant source of reactive hydrocarbons. The rainforest environment is characterized by strong convection, especially in the wet season, which transports boundary layer air into the upper troposphere. Oxidation of uplifted trace gases by OH can lead to new particle formation and growth in the upper troposphere, one scientific focus of the upcoming CAFE-BRAZIL campaign with HALO. The fraction of emitted hydrocarbons that is uplifted is strongly affected by the oxidation capacity in the boundary layer, since hydrocarbon oxidation products such as aldehydes and organic hydroperoxides



"*In situ* measurements of OH and HO_2 on aircraft, ships and tall towers spanning the vertical profile of troposphere allow to investigate the impact of anthropogenic and biogenic emissions on the self cleaning capability of the atmosphere."

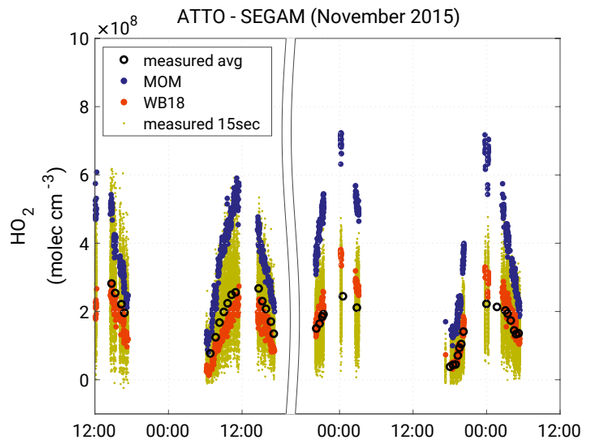


Figure 2: Comparison of measured HO_2 with CAABA / MECCA (Chemistry As A Boxmodel Application / Module Efficiently Calculating the Chemistry of the Atmosphere) model simulations using different chemical mechanisms: MOM (Mainz Organic Mechanism) based on Taraborrelli, D., et al. (2009, 2012) and WB18 based on Wennberg, P.O., et al. (2018).

are more water-soluble and therefore more prone to be washed out before release in the convective outflow into the upper troposphere. We analyzed our radical measurements in the boundary layer at ATTO by data-constrained model simulations using two different chemical degradation schemes for isoprene and terpenes as shown in the figure below. This comparison is indicative of our understanding of the self-cleaning potential and the hydrocarbon degradation mechanism. For the conditions typical at ATTO, we find that the computed radical concentrations in the two degradation schemes differ by a factor of two. The cause of this discrepancy is part of ongoing research in preparation of the CAFE-BRAZIL campaign.

OUTLOOK

We have enhanced our instrumentation by developing a low-pressure flow tube system, APACHE, for the calibration of the aircraft-based OH and HO_2 measurements, aimed at reducing uncertainties. Also, we are building an instrument for HALO that will allow detection of SO_2 with a detection limit of less than 5 ppt in one second. The new SO_2 instrument is based on previous work by colleagues at NOAA (USA) who detected the fluorescence of SO_2 between 240–400 nm after excitation at 216.9 nm. The photons used for excitation are produced by a fiber laser system at 1084.5 nm, followed by the fifth harmonic generation at 216.9 nm. We plan to deploy the new SO_2 instrument on HALO in the CAFE-BRAZIL campaign.

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NUMERICAL MODELING OF ATMOSPHERIC CHEMISTRY

ANDREA POZZER

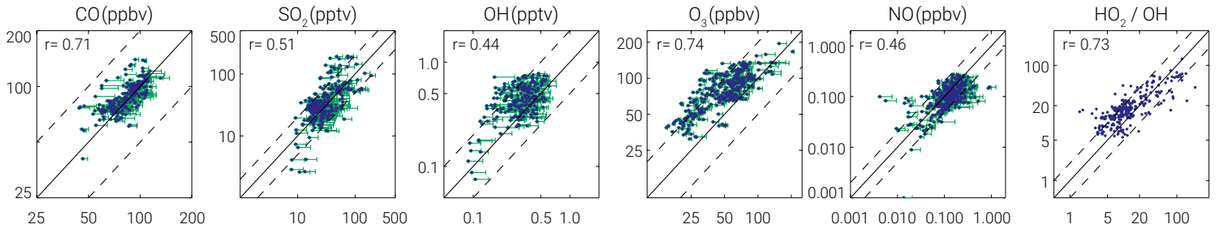

Figure 1: Selection of trace species measured during the OMO aircraft campaign at 300 to 120 hPa (9 to 15 km altitude), with error bars in green, compared with EMAC modeling results (correlation coefficients r). The solid lines indicate ideal agreement, and the dashed lines indicate agreement within a factor of two.

INTRODUCTION

Concentrations of pollutants in the atmosphere are influenced by many factors, such as emissions, transport, chemical transformations, and wet and dry deposition. Moreover, the products of chemical transformation can be in the form of gases (e.g. ozone) or aerosols and these can also interact with each other. It is therefore essential to develop computer models that account for these complex interactions and that can be used to study and predict concentrations of compounds that affect air quality and climate and quantify their role in the Earth system and planetary health.

RESULTS

Over the past few years, our group has advanced the EMAC numerical global model (ECHAM5/MESSy for Atmospheric Chemistry). One major development was the significant expansion and improvement of the chemistry module with respect to the representation of Volatile Organic Compounds (VOCs). Roughly 700 organic species are now explicitly included, with an oxidation mechanism with more than 1,500 reactions, describing the chemical transformations of 43 primarily emitted representative organic species (Sander et al., 2019). Due to this exhaustive account of VOCs, the EMAC version deployed at the MPIC now contains the largest chemical mechanism in global atmospheric chemistry–climate models. In addition, a module for tagging different species has been included in the chemical mechanism; the production rates from specific reactions can be monitored, thereby allowing a complete budgeting and source attribution of selected species. This is mostly used in combination with OH production and loss, so that comprehensive studies of OH formation and recycling can be performed.

In addition to gas-phase chemistry, a large effort has been devoted to model aerosol processes. For example, the step-by-step restructuring of the EMAC code involved implementation of new aerosol nucleation routines. The model does not only include state-of-the-art particle nucleation algorithms but also novel parametrizations of VOC nucleation and effects of ions from cosmic rays and radon decay (Ehrhart et al., 2018). The large chemical VOC mechanism and the possibility of modeling organic nucleation are enabling the group to break new ground in atmospheric chemistry research, specifically allowing us to implement and test the most recent results from the advanced experiments on nucleation performed at the CLOUD (Cosmic Leaving Outdoor Droplets) experimental facility at CERN.

Supported by these developments in modeling, our group has cooperated with experimental groups in the department to help interpret laboratory and field experimental observations. For example, comparing the EMAC model results for the same time period and location with the measurements taken during the OMO (Oxidation Mechanism Observations) aircraft measurement campaign (Lelieveld et al., 2018) showed good agreement between numerical results and observations (Figure 1). Subsequently, the model calculations were used to estimate the influence of the South Asian summer monsoon on air pollution emissions; this analysis indicated that these emissions are the dominant pollutants of the upper troposphere, whereas previously influences from Africa and West Asia had been hypothesized. This is significant as the lofting by deep convective clouds in the monsoon forms a major gateway for pollutants to enter the stratosphere. The EMAC tagging capability allowed a complete budgeting of the OH chemistry, which led to the conclusion that the South Asian monsoon does not only represent an important transport pathway for pollutants; it also sustains active OH chemistry, by which many pollutants are rapidly oxidized and removed.

The EMAC model was also used in "impact studies", where the effects of particular processes are investigated and quantified, thereby facilitating an estimation of their influence on atmospheric composition, air quality, and climate. For example, we showed that fossil fuel-related pollutant aerosols have masked 0.51 °C of the global warming from increasing levels of greenhouse gases, while all anthropogenic aerosols, also from biofuel burning and agriculture, contributed nearly 0.73 °C. It may be expected that significant warming is unleashed when aerosol pollution is reduced to improve air quality and reduce the public health burden (Figure 2). Aerosols have also slowed the hydrologic cycle in several areas of the world, contributing to sustained drought conditions in parts of India, Northeast China, North Africa, and Middle America. We have concluded that a rapid phase-out of fossil fuel-related emissions and major reductions of other anthropogenic greenhouse gases and air pollution are needed to save millions of lives, restore aerosol-perturbed rainfall patterns, and limit global warming to a maximum of 2 °C, which was the central commitment of the Paris Agreement.

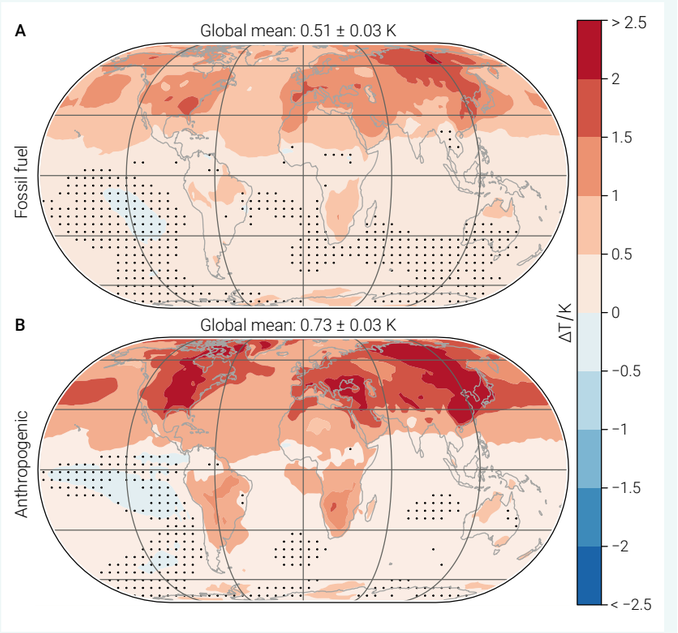

Figure 2: Modeling of two scenarios for temperature changes on the Earth's surface: (A) removing fossil-fuel-related pollution and (B) all anthropogenic pollution. The dots denote changes at 95% confidence level.

"Computer modeling supports the interpretation of field campaign observations and links atmospheric chemistry to climate and public health."

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VOLATILE ORGANIC COMPOUNDS IN THE ATMOSPHERE

JONATHAN WILLIAMS

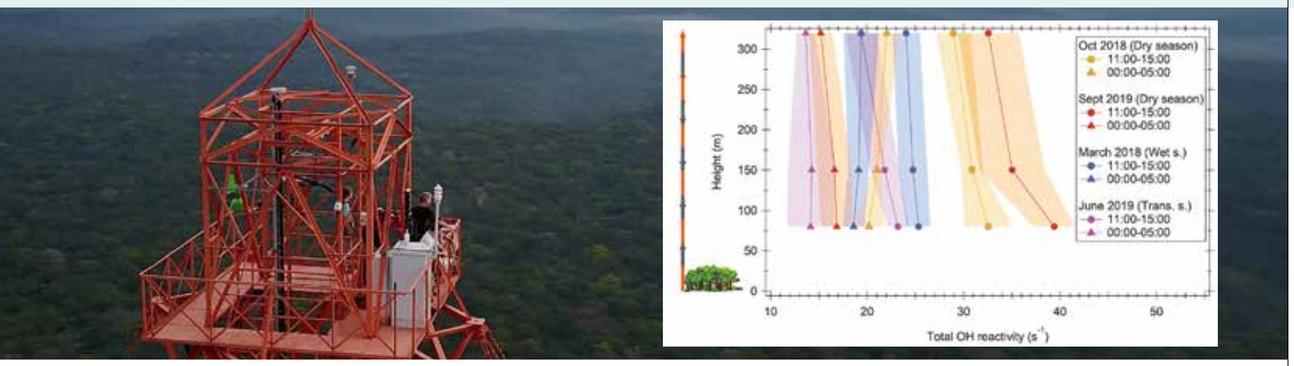

Figure 1: Dawn over the rainforest as seen from the 325-m ATTO tower, with vertical profiles of total OH reactivity.

INTRODUCTION

Our group specializes in the measurement of volatile organic compounds (VOCs). We use highly sensitive mass spectrometers to identify and quantify hundreds of VOC species in multiple environments, from the Earth's surface to the stratosphere, the second layer of the atmosphere. We develop and deploy instruments in the field at remote ground sites (Amazon Tall Tower Observatory, (ATTO), on ships (*M/V Kommander Iona*) and on aircraft such as the High Altitude and LOng Range Research Aircraft (HALO) and a Lufthansa Civil Aircraft for Regular Investigation of the atmosphere Based on an Instrumentation Container (CARIBIC). Recently, we have extended our research to investigate indoor air chemistry, in particular transport and emissions of VOCs associated with humans.

RESULTS

The Amazon rainforest is the largest source region of VOCs for the Earth's atmosphere. Our group has been active in characterizing emissions of isoprene, monoterpenes, sesquiterpenes, oxygenates, and total OH reactivity in this region. Based on measurements from the 325-m-high ATTO tower made at different heights, times of the day, and across different seasons, we have discovered an important sesquiterpene flux from tropical soil, characterized chiral emissions to reveal a potentially significant insect emission source, determined the importance of oxygenates for the OH reactivity budget, and traced the variations of these species during the 2015 El Niño drought. By deploying our instruments onboard a ship circumnavigating the Arabian Peninsula, we were able to measure VOCs in both pristine and polluted air masses. Non-methane hydrocarbons (NMHC) associated with oil and gas emissions were characterized, leading to the discovery of a new deep-water source. Furthermore, a new natural marine emission of methane sulfonamide (MSAM) emerging from upwelling regions was measured for the first time. OH reactivity in various polluted (Arabian Gulf and Suez Canal) and cleaner areas (Indian Ocean) was characterized and a significant mismatch between measured and modelled acetaldehyde was ascertained, indicating an underestimation of sources.

Aircraft have been used to gain information on VOCs in the free troposphere and stratosphere. An online proton-transfer-reaction time-of-flight mass spectrometer and a newly developed fast gas chromatography-mass spectrometry instrument were operated on-board the HALO research aircraft during three institute-led campaigns to investigate Asian monsoon outflow (OMO), African convective outflow (CAFE-AFRICA), and European emissions during the COVID-19 lockdown period (BLUESKY). Organohalogen measurements have enabled source distinction and tropopause delineation, while oxygenated VOCs have provided information on photochemical ageing as well as markers of biomass burning. Based on VOC data obtained from pressurized canisters collected from the CARIBIC flights, we have developed a method to determine global levels of OH and Cl radicals in the upper troposphere and stratosphere and found no significant changes over the past decade.

Our group has successfully participated in several EU-funded projects (IMPACT and ULTRACHIRAL) and collaborated with the Alexander von Humboldt and Albert P. Sloan foundations to investigate indoor air chemistry. The latter research has revealed how humans can transport third-hand smoke into non-smoking environments such as cinemas and how natural human emissions of VOCs, particles, and ammonia are influenced by ozone exposure, clothing, humidity, and temperature.

OUTLOOK

In the next three years, we intend to extend our characterization of VOC species in the tropical rainforest. New instrumentation will be installed at the ATTO ground site and the atmospheric chemistry of the rainforest emissions will be monitored at an altitude of up to 16 km by operating our mass spectrometer measurement systems on the HALO aircraft as part of the planned CAFE-BRAZIL field campaign. In addition, we will continue to develop novel measurement methods and use them to examine regions where volatile organic compounds play important roles in the chemistry of the atmosphere.

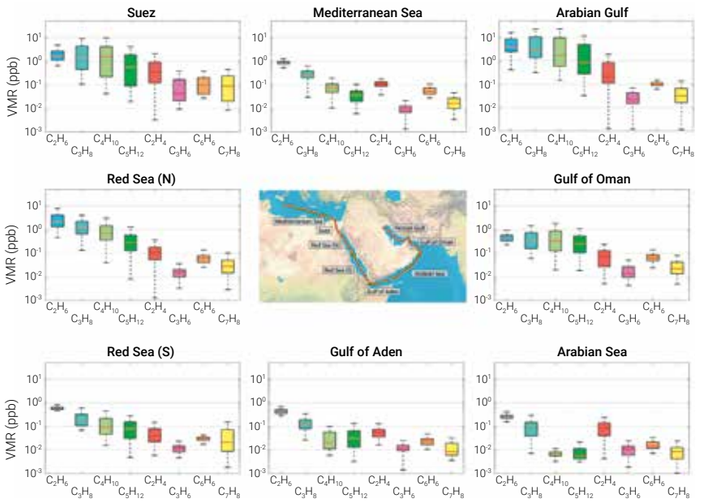

Figure 2: Sunset over the Arabian Gulf, with regional non-methane hydrocarbon measurements taken during the shipborne AQABA campaign (Volume Mixing Ratio (VMR)).

"We aim to understand how volatile organic compounds impact global atmospheric chemistry."

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COVID-19 AND AIR QUALITY

JOS LELIEVELD

Figure 1: Solitary aircraft contrail. Unusually deep blue sky over Germany, observed during the COVID-19 lockdown (left). BLUESKY group photo in front of the HALO research aircraft (right).

INTRODUCTION

The COVID-19 pandemic has brought with it unprecedented challenges, which mobilized activity throughout the Institute. In the early part of 2020, many countries worldwide had initiated lockdowns to slow the pandemic, with consequences for air pollution emissions. We analyzed measurement data from satellites and ground-based monitoring networks to assess the consequences for air quality. Then, in spring 2020 we deployed the High Altitude and LOng Range Research Aircraft (HALO), equipped with comprehensive instrumentation to measure chemically reactive gases and aerosol particles over Europe and the North Atlantic Ocean where air traffic had declined by nearly 90%. Subsequently, we studied connections between long-term exposure to air pollution and the risk of dying from COVID-19. Finally, we developed an easy-to-use model for the general public and stakeholders to estimate the risk of airborne transmission of COVID-19 by aerosol particles in indoor environments.

RESULTS

We used space-borne and ground-based data, the latter from a network of more than 10,000 measurement stations in 34 countries, to derive atmospheric composition changes during lockdowns.
After accounting for meteorological variability, we found reductions in population-weighted concentrations of NO_2 and fine particulate matter of about 60% and 30%, respectively. By incorporating Google and Apple mobility information, the decline of land transport was identified as the main cause for these reductions. Short-term air quality health benefits included the prevention of nearly 50,000 premature deaths and 90,000 pediatric asthma emergency room visits.

Notwithstanding logistical difficulties imposed by COVID-19, the HALO aircraft was instrumented for the BLUESKY measurement program to investigate the air over European metropolitan areas and in the flight corridor to North America during lockdown. By comparing measurement data with previous airborne missions, it was shown how reduced emissions from the transport sector are changing atmospheric chemistry, for example that of nitrogen oxides. Even though meteorological conditions were favorable for the formation of contrails, the near-absence of air traffic allowed Europeans to enjoy deep blue skies for the first time in decades (Figure 1).
In collaboration with medical and public health researchers, we used epidemiological data from previous US and Chinese studies of air pollution, COVID-19, and the SARS outbreak in 2003, to determine the link between long-term exposure to air pollution and increased risk of dying from COVID-19. Although there may not be a direct cause-effect relationship between air pollution and COVID-19 mortality (although it is possible), we did discover interactions between the two, i.e. air pollution aggravates co-morbidities (other health conditions) that can lead to fatal outcomes of viral infection. We estimated that nearly 20% of deaths from COVID-19 in Europe could be attributed to long-term exposure to air pollution, while in East Asia it was more than 25% (Figure 2).

In a multi-department effort of our Institute, we developed a user-friendly model to estimate the COVID-19 infection risk for different indoor environments, constrained by published data on human aerosol emissions, viral loads, infective dose, and other parameters. The results suggested that aerosols from highly infective subjects can effectively transmit COVID-19 in indoor environments. We showed that active room ventilation and the ubiquitous wearing of face masks (i.e. by all present) can reduce the individual infection risk by a factor of five to ten, similar to highly efficient particle filtering devices.

OUTLOOK

The extraordinary conditions during the COVID-19 pandemic have triggered remarkable collaborations between researchers across disciplines. Our environmental insights into the COVID-19 crisis have taught us that measures to reduce anthropogenic emissions, which cause air pollution and climate change, are more urgent than ever.

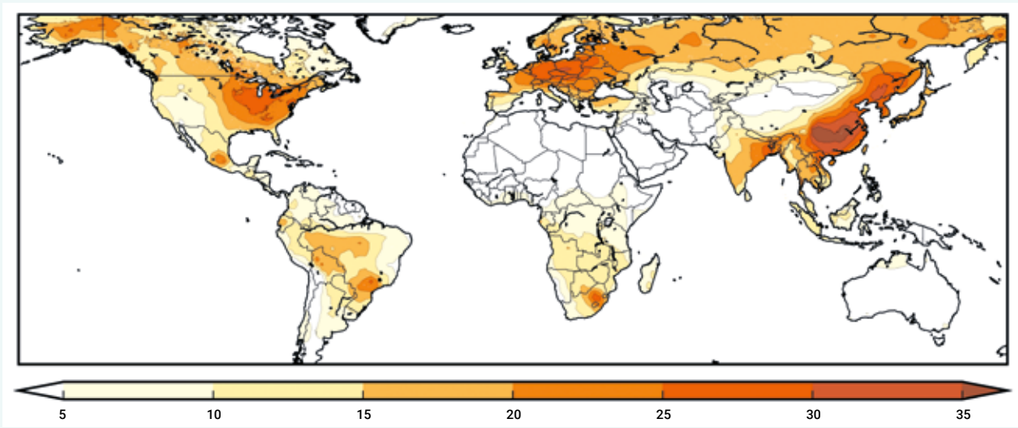

Figure 2: Estimated percentages of COVID-19 mortality attributed to co-morbidities associated with long-term exposure to air pollution.

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"Unique challenges and opportunities related to COVID-19 lockdowns and air pollution."

CLIMATE GEOCHEMISTRY

Past changes in climate, ocean-atmosphere interactions, the oceanic nutrient status, the ocean's heat transport, and atmospheric greenhouse gases.

CLIMATE GEOCHEMISTRY DEPARTMENT


Photo: Leopoldina in Halle/Saale

The department addresses climate-ocean-atmosphere processes and large scale dynamics in global biogeochemical cycles as revealed by the sedimentary and fossil record. Our department has been built to focus on three key approaches with regard to our understanding of past environmental conditions on Earth. First, we have acquired and developed sedimentary records, speleothems, and other archives, as well as the appropriate instrumentation, to undertake paleo-environmental studies of extremely high temporal resolution. Second, we run state of the art labs for novel geochemical and isotopic analyses of sedimentary deposits, fossils, and ancient organic matter; these include nanoscale trace element measurements in fossils, nitrogen and carbon isotopic measurements of fossil-bound organic matter, and high-sensitivity isotopic measurements of carbonate and water in biominerals and cave deposits. Third, with regard to these paleoproxies and others, we will mount seasonally resolved oceanographic cruises to provide a new level of understanding of paleoproxies, both those measured at MPIC and others; this effort, uses a state-of-the-art small sailing vessel, a unique tool for probing the ocean and atmosphere.

We reconstruct millennial to subdecadal scale climatic changes in the tropics and mid-latitudes. Some of this work has been centered around remarkable, often laminated, sediment archives such as those of Cariaco Basin off the coast of Venezuela, Lake Challa in the foothills of the Kilimanjaro, the Arabian Sea, Lake Van in Turkey, the Dead Sea, Eifel Maar lakes; it also includes investigation of speleothems in Asia, Africa and Central America, coral records in the tropical Pacific, amongst others. Variations recorded in these sediments correlate with high latitude northern hemisphere climate (e.g., as recorded in Greenland ice cores) and ENSO-related activity in the equatorial Pacific, and coincidences have also been observed with events in societal evolution.

A second theme, our use of organic-based tools to reconstruct biogeochemical and carbon cycle changes in the ocean. We have made major investments in the N isotopic analysis of coral-, diatom- and foraminifera-bound organic matter at unprecedented sensitivity. Our work in the polar ocean has so far focused on the Pleistocene glacial cycles as well as the major intensification of northern hemisphere glaciation at 2.7 Ma. During the past 3 years, we have also generated continuous records through the entire Cenozoic. In this context, we have worked on the evolution of climate, atmospheric CO_2 and the N cycle over the entire 65 million years of the Cenozoic, including its periods of much warmer conditions.

The Werner Siemens-Foundation donated a small (length: 22 m) but technologically advanced and seaworthy sail-powered vessel (*S/Y Eugen Seibold*) as an oceanographic sampling platform to the Max Planck Institute for Chemistry. The *S/Y Eugen Seibold* is in full operation since May 2020, after a year of intensive testing in 2019; unfortunately, the COVID-19 pandemic does not allow for the planning of cruises at the moment. Given its design, it will be able to travel safely across vast expanses of the global ocean, and it provides an excellent platform for making measurements in, and collecting samples from, the upper ~500 m of the ocean water column (as deep as 1500 m). This vessel has great potential for studying the seasonally varying processes of the upper ocean. Seasonality, both on land and in the ocean, can fairly be thought of as the dominant driver of "climate" variation after the diurnal cycle. Yet, given the disconnect between the materials used for paleoceanographic proxy calibration (e.g., foraminifera and biomarkers from surface sediments) and the environmental measurements against which they are compared (most often mean annual averages based on a compilation of measurements from prior cruises), paleoproxy calibration very rarely considers seasonality to an appropriate degree. Our sampling on *S/Y Eugen Seibold* will permit direct comparison of paleoceanographic proxies to the organisms that produce them as they respond to *in situ* environmental conditions on a seasonal basis.

Since March 2020, Gerald Haug is President of the German National Academy of Sciences Leopoldina. Founded in 1652, the Leopoldina is now the oldest continuously existing academy of medicine and the natural sciences in the world. Today, the Leopoldina has 1600 members from more than 30 countries and almost all research areas. The Leopoldina provides independent science-based advice to policy makers and society on scientific and science policy matters. These include topics such as climate change, air pollution, energy transition, disease control and health, demographic change or biodiversity conservation. To this end, the Academy develops interdisciplinary statements based on scientific findings. The Academy also detects, analyses and comments on scientifically indicated developments that may become of significance to society in the future. All findings are submitted to decision makers and interested parties in the political sphere and society to serve as a basis for discussions and further political measures. The Leopoldina also represents the German scientific community in international academic dialogue. This takes place in various forms, such as joint symposia or the issuing of joint statements. For example, the national science academies of the G7 and G20 member countries – known as the G-Science Academies – make recommendations for solving urgent global challenges to the participating heads of state and government in the run-up to each summit.

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1992 Diploma in Geology at the University of Karlsruhe

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1995–1996 Postdoctoral Research Associate at GEOMAR, Center for Marine Geosciences, Kiel

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1997–1998 Postdoctoral Guest Investigator at the Woods Hole Oceanographic Institution in Massachusetts, USA

1998–2000 Research Assistant Professor at the University of Southern California in Los Angeles, USA

2000–2002 'Oberassistent' at the ETH Zürich, Switzerland

2002 Habilitation in Earth Sciences at the ETH Zürich

2003–2007 Professor at the German Research Centre for Geosciences (GFZ) in Potsdam and the University of Potsdam, Germany

Since 2007 Ordinary Professor for Climate Geology at the ETH Zürich

Since 2015 Director at the Max Planck Institute for Chemistry and scientific member of the Max Planck Society

Since 2020 President of the German National Academy of Sciences Leopoldina.

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SAHARAN DUST SOURCES, OUTFLOW, AND AMAZON RAINFOREST FERTILIZATION

STEPHEN GALER

Figure 1: Emission of diatomite dust westwards from the Bodélé Depression, with Lake Chad below, as viewed from the ISS (right), the Amazon rainforest near Manaus is a potential receptor region where Bodélé dust might act as a chemical fertilizer (left).

The westward Saharan dust outflow is the single largest source of atmospheric mineral dust globally and has a profound impact on climate and biogeochemical cycles in the whole Earth system.

There are three ideas gaining increased traction regarding the Saharan outflow. First, the Bodélé Depression – a dried-up lake bed of vast proportions located just north of Lake Chad – is renowned as the "dustiest place on Earth" and, for this reason, it is often thought to be the principal source of emission from North Africa. Second, these North African dust outflows – often in the form of large outbreaks – are considered to reach as far as the Caribbean in boreal summer, moving further south to the Amazon Basin during the winter months. Third, contentiously, the flux of putative Bodélé-derived mineral dust may fertilize and contribute significantly to the primary biological productivity of the Amazon rainforest.

In order to determine whether these ideas are correct or not, we need to fingerprint reliably potential source areas emitting dust and form a "base map" of North African dust sources. We have been using long-lived radiogenic isotope system tracers (lead, neodymium, and strontium isotopes) which vary, depending mainly on geological age, among North African tectonostratigraphic units comprising the underlying bedrock. In addition, major and trace element abundances of a suite of some fifty elements – which are modified by weathering as well during riverine and eolian transport – provide additional information.

Our re-evaluation of potential source areas based upon the fine, deflatable fraction of North African soils is shown in Figure 2. We are able to discriminate clearly ten regions, especially between geologically older (Mauritania, Mali Centre, Niger) and younger (Libya-Egypt) terrains, with Bodélé having a unique chemical and radiogenic signature. Not all of these areas are strong sources of emission, though.

We have also been measuring time-series of eolian dust collected on filters at the Cape Verde Islands, proximal to the outflow, which can be associated with individual sources through back-trajectory analysis, lidar ranging, and time-resolved satellite imagery. These data were compared with time-series analyses of dusts from Barbados in the Caribbean and the ATTO tower site in the Amazon Basin, near Manaus.

The Cape Verde filters imply that the vast majority of the dust in the westward outflow is derived from the low-lying El Djouf desert region in Northern Mali-Southern Algeria, encompassing the source areas labelled Mali Center and Algeria-Mali in Figure 2. Surprisingly, there is no indication of Bodélé-derived dust which is thought to be a major component of the outflow. Similarly, analyses of filters exposed in Barbados show that the dust reaching the Caribbean is identical to that at Cape Verde, though with fluxes peaking in the summer rather than the winter months due to the high-level Saharan Air Layer (SAL) promoting long-range transatlantic transport.

"Quantifying how mineral dust affects climate, health, and fertilizes land and sea requires we understand its sources and chemical composition."

The ATTO tower site is distal to any African dust, and fluxes there are orders of magnitude lower than at the Cape Verdes. Our time series were collected on the towers in the "dusty" winter months in March–April 2016 and February–April 2017 above the forest canopy. Particle flux and organic data were used to distinguish Saharan from local (very weak) sources. Again, with surprise, we found that winter Bodélé dust does not appear to contribute at the ATTO site (summer dust is suppressed by the African monsoon); rather, this dust also originates from the Mali-Algeria region. It appears that the vast Bodélé emissions are not transported great distances but are mostly lost in the Sahara-Sahel region or by wet deposition in the Gulf of Guinea.

In terms of the nutrient and micronutrient mass balance, around two-thirds is internally recycled in the rainforest during vegetation death and regrowth. Of the remaining third of nutrients, lost from the system in rivers, most of this is provided by soil weathering and only a small fraction is plausibly derived from incoming Saharan dust based upon estimated fluxes. Nevertheless, this crude mass balance highlights the folly of Amazon deforestation which will have monumental consequences for the biogeochemical cycling of nutrients and the diurnal hydrological cycle in the region.

We are undertaking high-frequency sampling from aboard the *S/Y Eugen Seibold* in the Eastern Atlantic to identify smaller dust sources contributing to the Saharan dust outflow, the time-resolved progression of large outbreak events, as well as examine dust seasonality. This information will prove invaluable in deciphering the role mineral dust dissolution plays in the ocean biogeochemical cycling of micronutrients, the biological pump, the frailty of the current climate system, and paleoclimate in general.

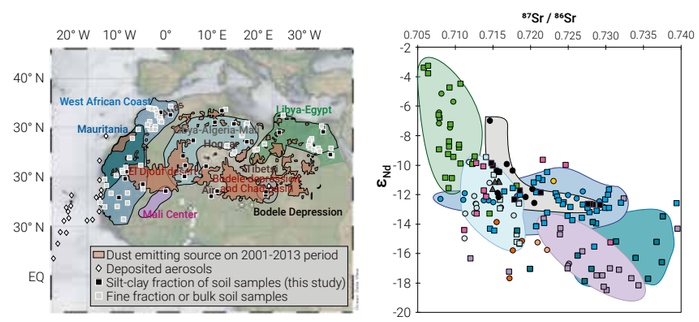

Figure 2: Ten North African potential dust emission regions discriminated by a combination of radiogenic isotope system and trace metal abundance tracers, based upon data from deflatable silt-clay fractions from soils, as well as filters collected from the Cape Verde Islands and back-trajectory analysis (left), Sr and Nd isotope data used in the evaluation, color coded to the "base map" (right).

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HIGH-RESOLUTION MICROANALYSIS OF BIOGENIC CARBONATES FOR PALEOCLIMATE RECONSTRUCTION

KLAUS PETER JOCHUM

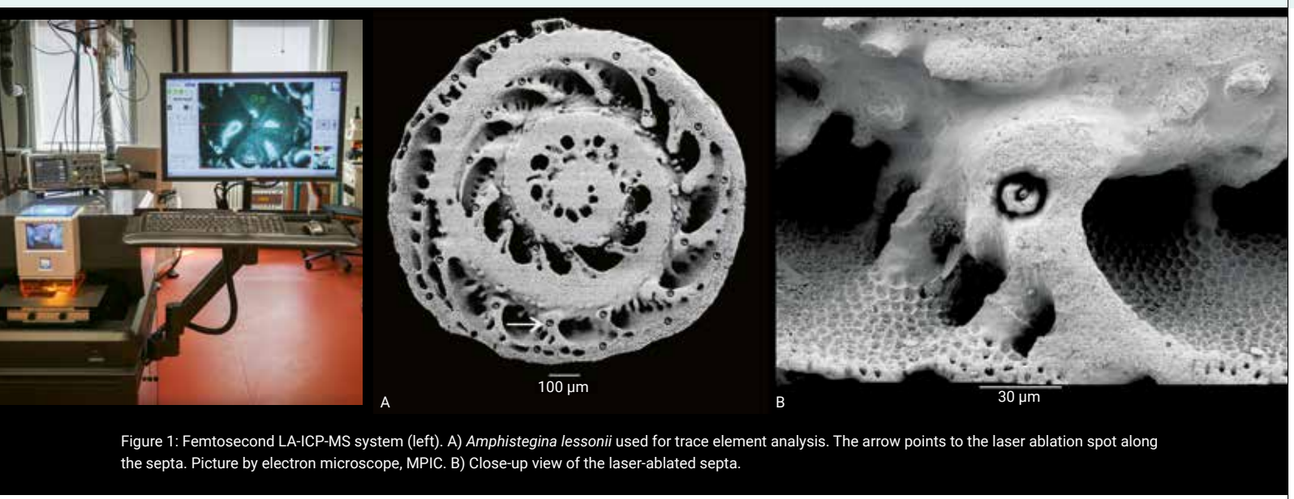

Figure 1: Femtosecond LA-ICP-MS system (left). A) *Amphistegina lessonii* used for trace element analysis. The arrow points to the laser ablation spot along the septa. Picture by electron microscope, MPIC. B) Close-up view of the laser-ablated septa.

Microanalytical investigations of foraminifers, corals, pteropods, otoliths, and other biogenic carbonates are a central focus of the Paleoclimate Research group in the Climate Geochemistry Department. Samples of these carbonates are useful archives of information on past environmental conditions, such as climate, ocean circulation, landscape, vegetation, and the influence of human activity (Figure 1).

Analyses are performed in close collaboration with the Micropaleontology group, groups from other Max Planck Institutes, and various universities and research institutions, both within Germany and internationally.

In climate geochemistry, isotope ratios of oxygen (O) and carbon (C) have long been used for climate change investigations, but trace element ratios are also suitable. We have analyzed 20 trace elements (e.g., B, Sr, Ba, Mg, Na) in many marine biogenic carbonates from different microorganisms by 200 nm femtosecond-laser ablation-ICP-mass spectrometry (200 nm fs-LA-ICP-MS) in collaboration with the Micropaleontology group (R. Schiebel). In contrast to the generally used ArF excimer and Nd:YAG ns-lasers the use of fs-laser systems avoids sample heating. This non-thermal ablation process allows for stoichiometric aerosol generation; when using a wavelength of 200 nm, elemental and isotopic fractionation are minimized or nearly absent. Of particular importance is the new cutting-edge single-shot measurement technique, where Na/Ca, Mg/Ca, and Mn/Ca, Ti/Ca ratios, respectively, can be determined nearly simultaneously in 0.5 ng sample amounts ablated by one laser shot. Using an extremely small fluence of 0.1–0.3 Jcm^{-2}, gentle ablation measurements can be performed until a depth of 10–20 µm with a resolution of 50–100 nm/laser shot. Recently produced fine-grained calcium carbonate nanomaterials (e.g., MACS-3NP) have helped to significantly improve the precision and accuracy of the microanalytical results. To better understand the different proxies (e.g., Mg/Ca, Sr/Ca, Ba/Ca, Na/Ca ratios), large numbers of foraminifers and pteropods will be analyzed for many elements by 200 nm fs-LA-ICP-MS, which will be collected by the *S/Y Eugen Seibold*, the dedicated research vessel of the Climate Geochemistry Department.

The Mg/Ca ratio in calcareous shells is a proxy for seawater temperature and is, therefore, of particular interest in paleoclimate reconstruction. This ratio can be determined precisely and accurately in nano-sized layers of micrometer-sized samples. Investigations of the Mg/Ca ratio in chambers of the foraminifera *Globorotalia menardii* revealed possible temporal changes in the Arabian Sea. NanoSIMS measurements with the NanoSIMS 50 ion probe of the P. Hoppe group are being performed to confirm the fs-LA-ICP-MS data.

Figure 2 shows the Mg/Ca profiles of various biogenic samples. Ablation took place from the outside towards the inside of the shell. Each data point represents a single-shot measurement. The measurement precision (1 relative standard deviation) of Mg/Ca is about 5 %. The Mg/Ca measurements on reference materials are in close agreement with uncertainty limits, indicating good accuracy of the single-shot technique.

Other studies that we have conducted in recent years include investigations of rock varnish and petroglyphs, paleodietary information from fossil teeth, paleoclimate studies of stalagmites, characterization of new reference materials, and support of the MPIC GeoReM database.

"Precise and accurate in-situ measurements of trace element ratios in marine biogenic carbonates are relevant to climate change investigations."

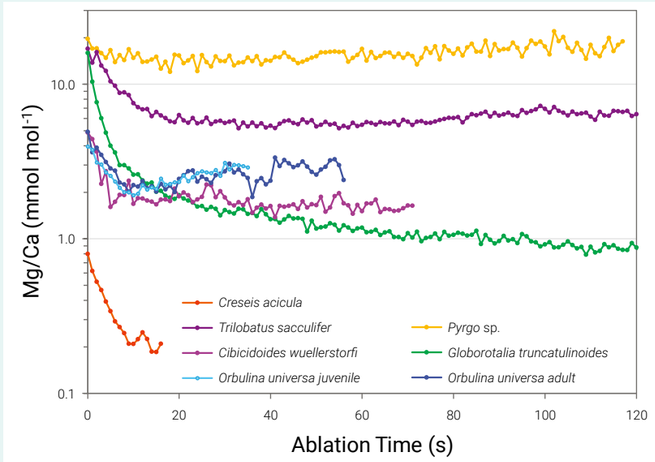

Figure 2: The Mg/Ca ratios of calcareous marine microplanktonic and microbenthic fossils. Aragonitic shells of pelagic snails (pteropods, *Creseis*) are characterized by thin shells (minimum ablation time corresponding to 1.5 µm thickness) and low Mg/Ca ratios, which are, however, significantly higher than the technique's detection limit of 0.05 mmol mol^{-1}. The low Mg/Ca ratios measured for the benthic foraminifera *C. wuellerstorfi* and the deep-dwelling planktic foraminifer *G. truncatulinoides* indicate low ambient water temperature. The planktonic foraminifera *Orbulina universa* dwells in the lower surface mixed layer, consistent with the intermediate Mg/Ca ratio in both juvenile and adult individuals. Please note the variability in Mg/Ca ratios in adult *O. universa*, which represents diurnal cycles. The high Mg/Ca ratio of the planktic foraminifer *T. sacculifer* reflects its shallow dwelling depth of around 30 m in the subtropical North Atlantic. The high Mg calcite value determined for the benthic foraminifer *Pyrgo* results in the highest Mg/Ca of the sample set.

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UNRAVELLING THE EVOLUTION OF THE MARINE CARBON AND NITROGEN CYCLES ACROSS THE CENOZOIC ERA

ALFREDO MARTÍNEZ-GARCÍA

Figure 1: The Joides Resolution drilling ship used to retrieve deep-see sediment cores (left), coral sampling during the recent expedition (2019) to the Iles Éparses (Scattered Islands) located around Madagascar (center), isotope ratio mass-spectrometer used to measure fossil-bound N isotopes at the MPIC (right).

INTRODUCTION

Human activities are changing the physical and chemical conditions of the ocean, with uncertain consequences for the ocean's uptake of anthropogenic carbon dioxide and heat from global warming as well as for the future of marine ecosystems. However, our understanding of interannual, decadal, and longer-term variations of the marine carbon (C) and nitrogen (N) cycles is still limited by the relatively short time span covered by instrumental datasets. The scarcity of information about the past can, in some cases, complicate the interpretation of current observations by hindering the attribution of observed biogeochemical trends to natural processes or anthropogenic perturbations of the system. In this context, the study of past climates can offer important insights into the background state from which anthropogenic change has occurred. In addition, looking further back in time, it can reveal the responses of the different components of the Earth system to large perturbations of the C and N cycles that occurred across the Cenozoic era (i.e. the past 65 million years).

Over the past three years, the Organic Isotope Geochemistry group has studied changes in the marine C and N cycles across different timescales (from decades to millions of years) by applying a variety of novel geochemical techniques in different environmental archives. Below, we summarize some of our most relevant findings.

RESULTS

In a recent study, we reported the first measurements of the N isotopic composition of the trace amounts of organic matter protected from alteration within the mineral structure of planktonic foraminifera extending across the Cenozoic era (Kast et al., 2019). Our data suggest that the global marine denitrification rate during the Paleocene was more than twice the modern rate (460 versus 190 Tg N/year). Between 57 and 50 Ma ago, oxygenation increased and water column denitrification dropped, while at the Eocene/Oligocene transition, $\delta^{15}N$ increased again (Figure 2). These results indicate that the N cycle underwent major long-term changes in response to tectonic and climatic changes over the Cenozoic.

In another study, we revisited the change of middle Miocene Southern Ocean temperature using two novel temperature proxies (Leutert et al., 2020). Our records indicate that Southern Ocean cooling occurred in phase with the expansion of the Antarctic ice sheet, challenging previous estimates that suggested that the thermal isolation of Antarctica encouraged ice sheet expansion. Instead, our findings suggest that a decline in atmospheric CO_2 levels likely caused both ocean cooling and ice sheet growth.

"Novel geochemical measurements reveal and explain the evolution of the carbon and nitrogen cycles at timescales ranging from decades to millions of years."

In addition, we found a reduction in deep water supply and a concomitant freshening of the surface ocean that coincided with the emergence of the high-amplitude 100,000-year glacial cycle at the end of the Middle Pleistocene Climate Transition, i.e. 0.6 Ma (Hasenfratz et al., 2019). We propose that this slowing of deep-to-surface circulation contributed to prolonging ice ages by allowing the Antarctic halocline to strengthen.

Our work also revealed a previously undocumented rise in Southern Ocean surface nitrate concentration through the Holocene (the past 10,000 years) (Studer et al., 2018). This change would have weakened the ocean's biological pump that stores CO_2 in the ocean interior, possibly explaining the rise in atmospheric CO_2 during the preindustrial Holocene.

Finally, we have examined the impact of the development of large megacities on the demise of coral communities in the Pearl river estuary over the past decades (Duprey et al., 2019). This study points to eutrophication as potentially being more important than ocean warming for coral decline along urbanized coastlines and in particular in the vicinity of megacities.

OUTLOOK

Building on these results, we are currently investigating changes in the N and C cycles across other key warm intervals of the past, including the Paleocene-Eocene Thermal Maximum (PETM), the Mid-Eocene Climate Optimum (MECO), the Mid-Miocene, and the Mid-Pliocene (Figure 2). In addition, we are generating a series of seasonal- to annual-resolution records of the N isotopic composition of globally distributed scleractinian corals, with the aim of investigating the interannual variability of the N cycle well beyond what can be observed and measured using instruments.

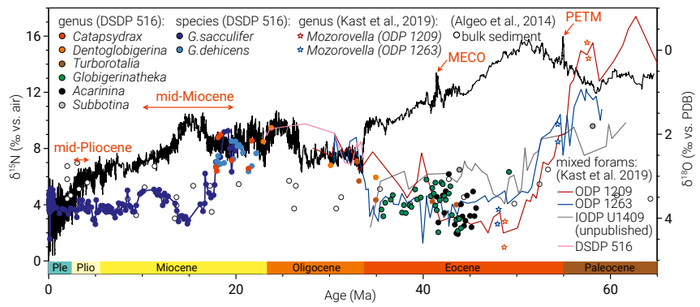

Figure 2: Preliminary measurements of foraminifera-bound $\delta^{15}N$ in samples from the Deep Sea Drilling Project (DSDP) site 516 at species (blue dots) and genus level (other colors) across the Cenozoic (Auderset et al., in preparation). These data are plotted together with the recently published mixed foraminifera-bound $\delta^{15}N$ measurements for sites 1209, 1263, and U1409 (Kast et al., 2019), older data by others on bulk sediment $\delta^{15}N$ (Algeo et al., 2014), and benthic foraminifera $\delta^{18}O$ (Zachos et al., 2008). Relevant warm periods that are currently under investigation are indicated in red.

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AN OPEN OCEAN RESEARCH PROGRAM FOR MODERN AND PAST CLIMATE CHANGE

RALF SCHIEBEL

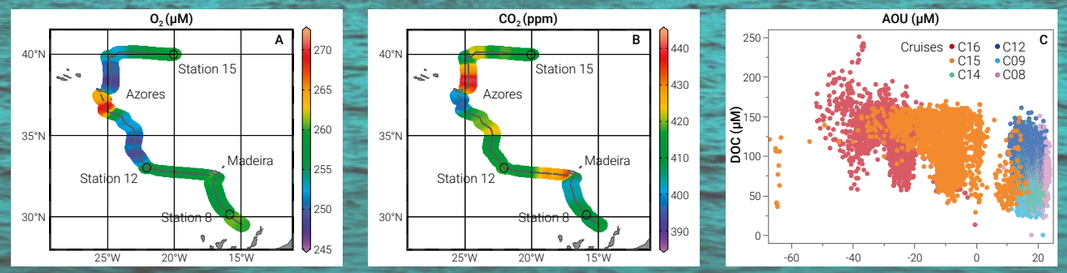

Figure 1: Ecological and geochemical variability in surface waters along the cruise track of *S/Y Eugen Seibold* across the oligotrophic Madeira Basin in summer 2019. (A) O_2 and (B) CO_2 concentrations are influenced by (C) dissolved organic carbon (DOC) and apparent oxygen utilization (AOU). Positive AOU indicates lower [O_2] than the saturation concentration, while negative AOU indicates O_2 supersaturation due to net photosynthesis. Lower surface pCO_2 than the annual mean atmospheric pCO_2 for 2019 (411.4 ppm) indicate a low capacity for biological CO_2 drawdown in a warming ocean and climate. Small-scale patterns vary among the marine provinces sampled during different cruises.

The new, fully equipped blue water research sailing yacht *S/Y Eugen Seibold* successfully sampled the eastern North Atlantic on 16 expeditions in spring and summer 2019. *S/Y Eugen Seibold* utilizes state-of-the-art technologies for the acquisition of uncontaminated samples and data from the open ocean and lower atmosphere at high temporal and spatial resolution. A multi-disciplinary approach is facilitated by close collaboration with departments and research groups at the MPIC and other Max Planck Institutes and universities.

A north-to-south transect was probed in 2020 in the eastern North Atlantic starting from the polar circle, comprising a wide range of marine provinces and environmental conditions. Continuous underway measurements and discrete sampling are used to characterize the physical, geochemical, and ecological state (Figure 1) of the surface ocean and lower atmosphere to capture systematic seasonal and interannual phenomena. Plankton such as foraminifers are analyzed as archives of ecological significance and for calibration for paleoceanographic and paleoclimate proxies (Schiebel et al., 2018).

The analytical tools installed onboard *S/Y Eugen Seibold* facilitate *in situ* analyses of seawater and atmosphere. A FerryBox measures temperature, salinity, particle-size (LISST), photosynthetic pigments (incl. chlorophyll a and phycocyanin), (CDOM), NO_3 and NO_2, pH, O_2, and pCO_2 (Figure 1). Micro- and nano-plankton (Figure 2) are quantified with a CytoSense flow cytometer. Phytoplankton community photo-physiology is measured with a Fast Repetition Rate fluorometer (FRRf). $\delta^{13}C$ and $\delta^{18}O$ of dissolved CO_2 as well as dissolved Ar, O_2, and N_2 are continuously probed with DeltaRay and miniRuedi spectrometers, respectively, connected to a custom-made flow-through sampling system. Photosynthetic active radiation (PAR) is recorded on the mast top and down the water column. An eight-channel CTD is attached to a rosette water sampler. Plankton are sampled with Bongo- and Multi-Nets (Hydrobios-midi Titanium). pCO_2 of surface seawater and overlying air are continuously analyzed for a better understanding of short-term (e.g., day-night) exchange dynamics in different trophic situations across the subpolar to tropical ocean. Macro- and micro-nutrients as well as trace metals are analyzed from seawater samples (SEAL QuAAtro) and *in situ* filtration samples (McLane pump; S. Galer group) at the MPIC.

The population dynamics of microplankton samples are being analyzed in comparison to samples from the same locations over the past 30 years, to better understand interdecadal processes in the ocean environment (Schiebel et al., 2018). Changes in ocean temperature, productivity, oxygen concentration, and nitrogen cycling in the upper ocean are quantified from $\delta^{15}N$ measurements of dissolved seawater NO_3 and microplankton coupled with studies of the $\delta^{15}N$ of the biomass and $CaCO_3$ of foraminifers (Martínez-García group; Smart et al., 2020). High-precision $\delta^{13}C$ and $\delta^{18}O$ analysis employs a newly developed method for very small $CaCO_3$ samples (< 5µg (H. Vonhof group; Vonhof et al., 2020). Pteropod and foraminifer shells are analyzed at high-resolution (sub-µm) by femtosecond-LA-ICP-MS (K. P. Jochum group; Jochum et al., 2019) and NanoSIMS (P. Hoppe group) (Buitenhuis et al., 2019). The combined information on environmental variability, the microbial community, and its physiological characteristics provide insight into the processes controlling ocean-atmosphere gas exchange, the state of the modern marine ecosystem, past ocean dynamics, and climate change.

Analyses of atmospheric particles including soot and aerosols (Y. Cheng and C. Pöhlker, MPIC) sampled from 10 m above the water line provide information on large-scale effects of wildfires and dust storms, including their fertilization of the pelagic ocean by micronutrients such as Fe (S. Galer group). Analyses of the molecular genetics of bioaerosols at the air-sea interface are generating unprecedented data on ocean-atmosphere exchange processes.

Our research is complemented by targeted projects in plankton ecology, such as in collaboration with G. Eichele, MPI for Biophysical Chemistry, Göttingen, to probe the circadian clock in plankton communities. Microbial community data from flow cytometry are integrated with (meta-) genomic studies for the identification and quantification of microbes and microbial processes in cooperation with R. Amann and B. Fuchs from the MPI for Marine Microbiology in Bremen. Air-sea interactions and the turnover of marine dissolved organic carbon (DOC) are analyzed in cooperation with O. Wurl and T. Dittmar from the University of Oldenburg.

"The present is the key to the past." (James Hutton, 1726–1797, Uniformitarian)

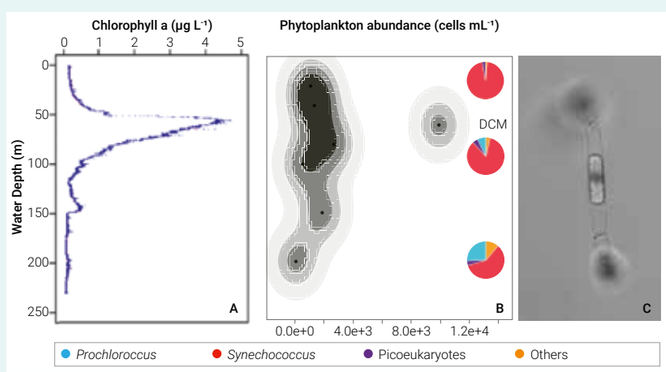

Figure 2: (A) Chlorophyll a fluorescence across the epipelagic layer in the Madeira Basin (Station. 12, Fig. 1). The deep chlorophyll maximum (DCM) at depths of between 50 m and 80 m shows (B) a stratified distribution of different phyto- and bacterio-plankton groups identified from cytograms. Pie charts show relative abundances of the four major phytoplankton groups above, within, and below the DCM. Diversity increases with decreasing cell abundance in subsurface waters. Small phytoplankton dominate the eastern North Atlantic autotrophic biomass and are predicted to increase with stratification caused by climate warming. (C) Image of a diatom acquired with CytoSense.

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ACKNOWLEDGEMENTS

We are grateful to Leon Prädel for the analyses of sea water contaminants and to Gabriele Herrmann from the XPS group of the Molecular Spectroscopy Department, Max Planck Institute for Polymer Research, Mainz, for the development of a clean seawater sampling system for S/Y Eugen Seibold.

NOVEL ISOTOPIC MEASUREMENTS IN CARBONATES FOR CLIMATE RECONSTRUCTION

HUBERT VONHOF

Figure 1: Exploration of cave systems of coastal Kenya (Collaboration with MPI-SHH, Jena).

INTRODUCTION

In the past four years we have put considerable effort in developing novel techniques and protocols for the stable isotope analysis of single-specimen planktic foraminifers smaller than 5 µg and for the stable isotope analysis of microscopic quantities of fluid inclusion water in speleothems and other fluid inclusion-bearing minerals. With this instrumentation, we have developed projects around the research themes described below.

SPELEOTHEM PALEOCLIMATE STUDIES

We are currently running several projects aimed at improving the quality of paleoclimate reconstructions based on speleothem (stalagmite) records. Complementing the recent improvements in the fluid inclusion isotope analysis technique, we have developed a collaboration with fellow MPIC researchers from the Martínez-García group, where an existing organic geochemical proxy for temperature (TEX86) was optimized for small samples of speleothem calcite. The two approaches, when combined, allow for unprecedented quantitative reconstruction of paleotemperature and isotope composition of paleorainfall from speleothem records. In the case of one of our key projects, targeting the Chinese speleothem records, this has led to much better constrained paleoclimate interpretations over the penultimate deglaciation (Figure 2).

We are engaged in a broad range of speleothem studies across the globe. The spatial dynamics of climate change in the Levant are being investigated using fluid inclusion isotope measurements on speleothems from several caves in Israel. We are studying the connection to (sub)tropical climate dynamics further south in a separate project focusing on late quaternary speleothems from Saudi Arabia (Collaboration with Nicole Boivin and Michael Petraglia; MPI-SHH in Jena). In parallel, we have started projects using the same techniques on speleothems from Brazil (collaboration with Francisco Cruz; Univ. São Paolo) and coastal Kenya (collaboration with MPI-SHH in Jena) targeted at improving our paleoclimate reconstructions of the South American and African Monsoons. In further application of the fluid inclusion isotope technique, we have commenced analysis of carbonates other than speleothems. In our work to date, we have focused on sub-surface fluids (calcite veins, travertines).

STABLE ISOTOPE ANALYSIS ON SMALL $CACO_3$ SAMPLES

The recent development of the stable isotope analysis of very small $CaCO_3$ samples (< 5 µg) in our lab supports various projects, ranging from the analysis of single-specimen diminutive planktic foraminifera to samples of structural carbonate from tooth enamel that are smaller than 100 µg in size.

Analysis of individual planktic foraminifera is yielding unique insights into past seasonal changes in the surface ocean and is being applied in several of the marine micropaleontology projects within our department (MPIC collaboration with AG Schiebel).

The isotope analysis of structural carbonate in tooth enamel has always required relatively large sample amounts (~ 1 mg), because the concentration of structural carbonate in tooth enamel is typically in the order of 5 wt %. We have successfully reduced the minimum sample volume to ~ 50 µg, enabling growth-incremental subsampling of tooth enamel from samples that were previously deemed too small.

HYDROCLIMATE OF THE EAST AFRICAN RIFT SYSTEM

Building on successful collaborations within the international Hominin Sites and Paleolakes Drilling Project, we are investigating the changing Quaternary hydroclimate of the East African Rift System (EARS). In these projects, we determine strontium isotope ratios of the skeletal carbonate of fossil lake fauna to reconstruct changing run-off patterns to EARS lakes. Our work has so far focused on the Turkana Basin, but we are now generating lacustrine Strontium isotope records from other EARS basins. These records will allow us to document hydrological connections between EARS lakes and their role in human evolution and dispersal (MPIC collaboration with AG Galer).

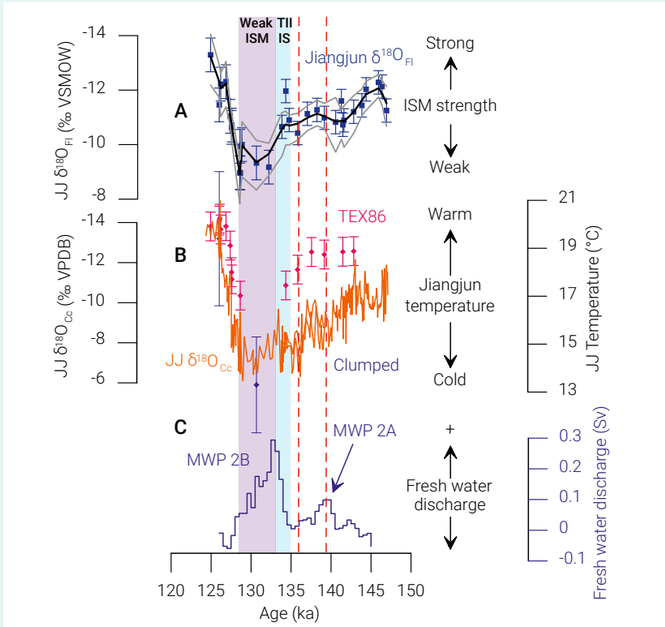

Figure 2: (A) Fluid inclusion stable isotope data of Jiangjun stalagmite (SW China), interpreted to represent rainfall isotope composition across Glacial Termination II (T-II). (B) Jiangjun temperature proxy data from TEX86 (red) and clumped isotope analyses (blue). (C) The timing and magnitude of North Atlantic Melt Water Pulse (MWP) 2A and 2B (in Sverdrup), interpreted to represent a slowdown (MWP 2A) and near-shutdown (MWP 2B) of the Atlantic Meridional Overturning Circulation (AMOC). The combined proxy records show the stepped climate response of the Asian Monsoon to the weakening (MWP 2A) and shutdown (MWP 2B) of the AMOC during T-II. (Data from Wassenburg et al., in prep).

"Using stable isotope geochemistry and other tools, our group investigates carbonate fossils and rocks with the objective of reconstructing paleo-environmental conditions."

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A NEW HOME FOR GEOROC

BÄRBEL SARBAS

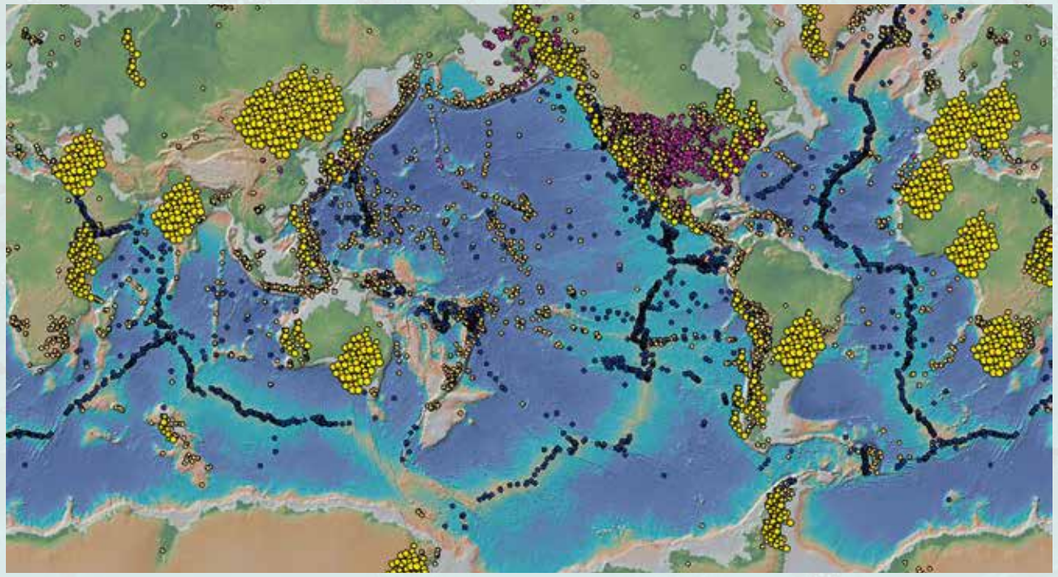

Figure 1: World map showing the distribution of samples available in the GEOROC database (yellow dots).

The Database group was established in 1998 as part of the former Geochemistry Department of the Max Planck Institute for Chemistry. Within a few years, the open-access database GEOROC (Geochemistry of Rocks of the Oceans and Continents) developed into an essential tool for geoscientists all over the world, especially but not exclusively for the so-called "hard-rock" community. The MPI database was, from the beginning, coordinated with a US-based equivalent effort that covers geochemical data from the ocean floors. This complementary database, called PetDB (Petrological Database of the Ocean Floor), was established by the Lamont-Doherty Earth Observatory of Columbia University in New York. Both databases can be accessed directly but are also jointly accessible through the Earthchem portal.

GEOROC contains published geochemical analyses of igneous rock samples from around the world and which range in age from Archean to more Recent (Figure 1). Since 2017, the database has also included entries for plutonic rocks in addition to the samples of volcanic rocks and mantle xenoliths which had been considered previously. The analyses include major and trace elements, isotope ratios, as well as analytical ages. Currently, the database contains almost 2,000,000 analyses for 600,000 samples published in 19,500 papers. The number of users per month varies between 3,000 and 4,000. The percentage of the main user countries for the time span July 2018 to July 2020 is shown in Figure 2. Many publications use GEOROC queries to establish a basis for comparison between newly analyzed samples and previously accumulated data. Sometimes, this amounts merely to a time-saving exercise for the authors, but often such comparisons are essential aspects of good scholarship and their manual preparation would require time and library resources that would exceed those available to authors. In addition to these routine applications, GEOROC is increasingly being used as a primary data source for an entirely new scientific approach, namely to address questions concerning the global chemical evolution of the Earth's crust. These publications, often appearing in top-tier journals such as *Nature* or *Science,* involve statistical analysis of thousands of geological samples. These studies also address questions of whether the tectonic processes responsible for creating and destroying continental crust have fundamentally changed over the Earth's history. In addition, this work impacts our understanding of the evolution of the Earth's atmosphere, in particular the question of when and how the atmosphere became oxygenated.

"Databases improve access to data and enable scientific breakthroughs."

The permanent personnel of the Database group were redirected to the Max Planck Institute for Chemistry from an institute which had closed in Frankfurt. From the beginning, it was clear that after retirement the personnel will not be replaced. Thus, over the last years the number of employees has decreased from four to one. A major focus during the last three years was the search for a host for GEOROC after the planned retirement of Bärbel Sarbas in 2022. A first DFG proposal from the University of Göttingen to take over and continue the database was rejected in 2017. Therefore, negotiations with other possible hosts were started, including, besides contacts with Paris and Beijing, the Goethe University Frankfurt. At the beginning of 2020, a concept was developed to migrate the database to Frankfurt where it should be merged with MetDB, a meteorite database. However, in parallel, the University of Göttingen had started preparing a revised DFG proposal, which was approved in July 2020. This approval enables the continuation of GEOROC for at least three years (with a budget of € 1,800,000), with the possibility of a continuation for a further three years after that. Thus, it was decided that the database will be transferred to Göttingen and its continued maintenance will be carried out in cooperation with Frankfurt.

After the migration to Göttingen, the web interface of GEOROC will be adjusted to the current needs of users. In cooperation with a working group on artificial intelligence of the university library in Göttingen, the literature search as well as data entry tools will be improved by automation.

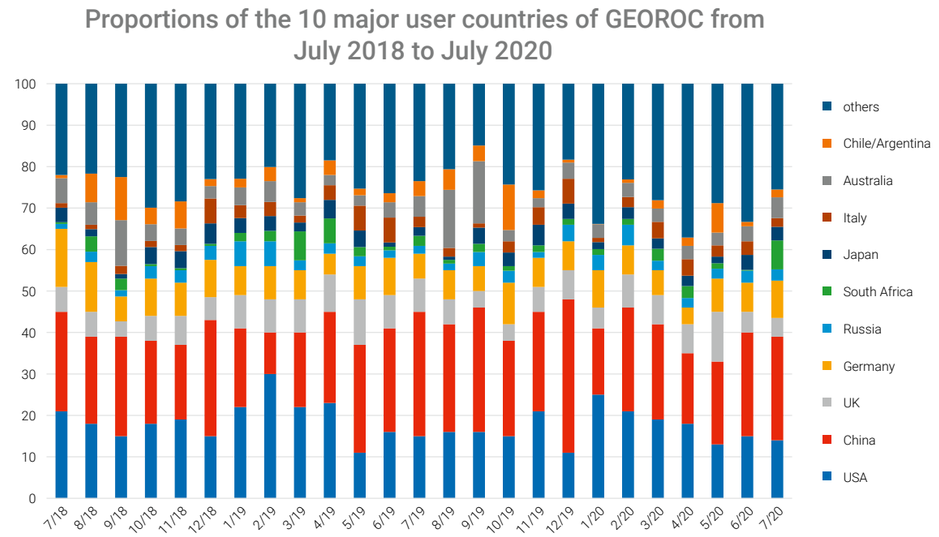

Figure 2: Percentages of the main user countries of GEOROC for the time span July 2018 to July 2020.

MULTIPHASE CHEMISTRY

Interaction and transformation of gaseous, liquid, and solid matter.
Climate and health effects of aerosols, biomolecules, and oxidants.

MULTIPHASE CHEMISTRY DEPARTMENT

Multiphase chemistry deals with reactions, transport, and transitions between different phases of matter such as gases, liquids, solids, and semi-solids. These processes are essential for the Earth system, climate, life, and public health. Prominent examples are the formation of clouds, rain, and snow or the respiration of humans, animals, and plants.

From a chemical perspective, life and the metabolism of living organisms can be regarded as multiphase processes that transform and exchange gases such as oxygen, nitrogen, and carbon dioxide; liquids such as water, blood, and lymph; and solid or semi-solid substances such as bone, skin, and cellular membranes. The global biogeochemical cycling of chemical elements and compounds, which constitutes the metabolism of planet Earth, also involves multiphase chemical reactions, mass transport, and phase transitions within and between the atmosphere, biosphere, hydrosphere, and lithosphere/pedosphere (Figure 1).

The overarching aim of the Multiphase Chemistry Department is to elucidate the role of multiphase processes that are essential in the interplay between air pollution, climate, and public health in the Anthropocene, that is, in the present era of globally pervasive human influence on Earth. Some of the key research topics addressed in the department include (a) the sources and properties of natural and anthropogenic aerosols and their effects on air quality, clouds, and precipitation; and (b) the chemical mechanisms, environmental causes, and mitigation of oxidative stress and related inflammatory disorders.

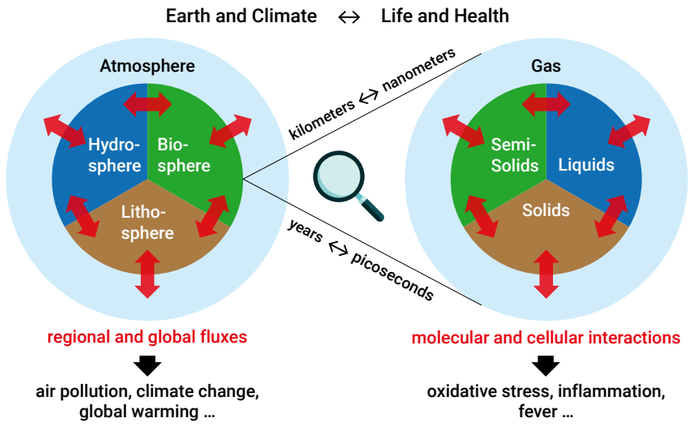

Figure 1: Chemical reactions, mass transport and phase transitions of gases, liquids and solids influencing the Earth system, climate, life, and public health (adapted from Pöschl & Shiraiwa 2015).

To explore and resolve these issues, we combine physical, chemical, and biomedical techniques in laboratory experiments, field measurements, and model studies at the interface of Earth and life sciences. We develop and apply advanced experimental and theoretical methods, including aerosol measurement techniques; spectroscopy and microscopy; bioassays and DNA analyses; kinetic process models; and regional to global atmospheric models.

The main areas of research in the Multiphase Chemistry Department are broadly reflected by the research group names as follows: Aerosol Analysis and Microscopy (*C. Pöhlker* et al.), Aerosol, Cloud, and Surface Interactions (*H. Su* et al.), Biomolecular Analyses and Interactions (*J. Fröhlich* et al.), Inflammatory Processes (*K. Lucas* et al.), Chemical Kinetics and Reaction Mechanisms (*T. Berkemeier* et al.), Organic Pollutants and Exposure (*G. Lammel* et al.), and further project teams on Cloud Condensation Nuclei (*M. Pöhlker* et al.) and Radical Chemistry (*H. Tong* et al.).

We collaborate closely with the independent Minerva Research Group on Aerosols, Air Quality, and Climate established and led by *Y. Cheng* with special funding from the Max Planck Society. Investigations of microbial communities and processes are continued in cooperation with *B. Weber* and colleagues who moved from the MPIC to the University of Graz in 2019. Moreover, we are engaged in close collaborations on the above and related topics with other alumni and research partners around the world. Among the research platforms we use are the Amazon Tall Tower Observatory (ATTO), the German High Altitude and Long-Range Research Aircraft (HALO), and the *S/Y Eugen Seibold* sailing yacht and research vessel.

Common themes and focal points include bioaerosols, proteins, and allergens; cloud condensation and ice nuclei; reactive oxygen and nitrogen species; and contrasts between pristine rainforest and polluted megacity environments. Highlights and perspectives of recent and ongoing research activities are detailed in the group and project reports that follow. They comprise insights into aerosol pH and nanoparticle phase transitions; phase change effects on the oxidation of organic aerosols and pollutants; redox reaction rates and oxidative stress in epithelial lining fluid; ice-nucleating mechanisms of water-soluble protein macromolecules; the amplification of inflammatory immune responses by chemically modified proteins, and the quantitative assessment and reduction of COVID-19 infection risks by airborne transmission.

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9 October 1969 Born in Klagenfurt, Austria.

1988 – 1995 Diploma and doctoral studies in chemistry at the Technical University of Graz.

1996 – 1997 Schrödinger fellow and postdoctoral researcher at the Massachusetts Institute of Technology.

1997 – 1998 Research scientist at the Max Planck Institute for Chemistry.

1999 – 2005 Research group leader and habilitation in chemistry at the Technical University of Munich.

2005 – 2012 Research group leader at the Max Planck Institute for Chemistry and lecturer at the Johannes Gutenberg University of Mainz.

Since 2012/2013 Director at the Max Planck Institute for Chemistry, Scientific Member of the Max Planck Society, and professor at the Johannes Gutenberg University of Mainz.

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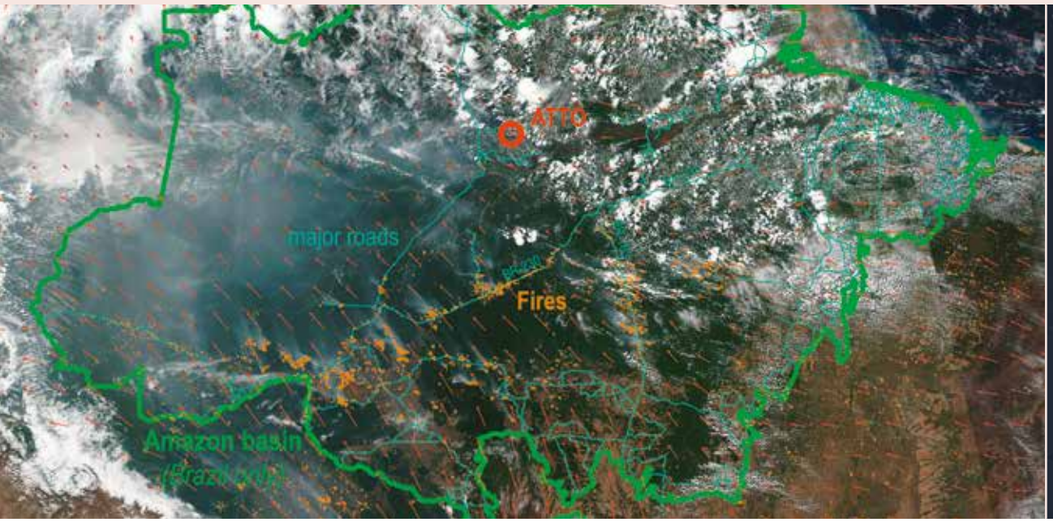
AEROSOL ANALYSIS AND MICROSCOPY

CHRISTOPHER PÖHLKER



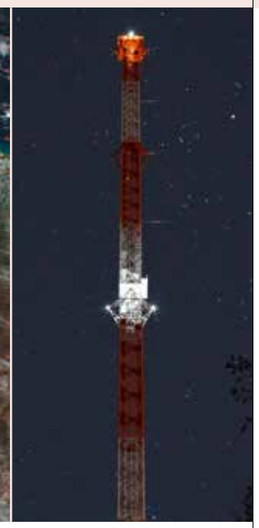


Figure 1: Left: Satellite image (corrected reflectance) with fire map and wind field of Amazon Basin on August 14, 2019 during the 'days of fire' that caused public concern worldwide. On that day, the large smoke plume also reached north towards ATTO, creating strong signals visible in the long-term datasets. Right: The 325-m-tall tower at the ATTO site, which has, since beginning operations in 2017, become a unique platform for atmospheric observations.

The Amazon rainforest is of major significance for the Earth system. It is also an ecosystem that is in rapid transition due to the combined pressure of climate change and land use transformations. The Amazon Tall Tower Observatory (ATTO) in the central Amazon Basin has become a research hub for in-depth and long-term atmospheric, climatic, and ecological studies. We analyze characteristic properties and interactions of atmospheric aerosols at ATTO and in related or contrasting environments (green vs. blue ocean; pristine vs. polluted conditions).

REGIONAL SOURCES AND LONG-RANGE TRANSPORT OF COARSE AND FINE AMAZONIAN AEROSOLS

The clean Amazonian wet season constitutes a window into the pre-industrial and unpolluted past. The prevailing aerosols under these conditions are biogenic in nature, such as microorganisms and secondary organic aerosols from regional sources in the forest. We are applying novel techniques that shed light on the properties of these particles and their roles in atmospheric and biogeochemical cycles. For instance, we have quantified the concentrations of airborne eukaryotic, bacterial, and archaeal cells and resolved their vertical profiles along the 325 m tall tower, providing new perspectives for studies of clouds and precipitation (bioprecipitation cycle). During the contrasting dry season, smoke from mostly man-made forest and savanna fires overwhelm the biogenic aerosol cycling. We found characteristically different signatures for smoke from Amazonian and African fires and determined that long-range transport of air masses from Africa influences the Amazonian atmosphere to an unexpectedly large extent. The continuous measurements at ATTO are complemented by recent and upcoming HALO aircraft missions (ACRIDICON-CHUVA, CAFE-AFRICA, CAFE-BRAZIL).

AEROSOL–CLOUD INTERACTIONS IN THE AMAZON AND OTHER REMOTE LOCATIONS

The hydrological cycle is key to the integrity and stability of the rainforest ecosystem, and a detailed understanding of aerosol-cloud-precipitation interactions in the Amazon is essential for the ATTO project. Through long-term aerosol measurements, we have obtained a climatological perspective on cloud condensation nuclei (CCN) properties and sources (pristine rainforest, biomass burning, African long-range transport). Besides ATTO, we conduct aerosol sampling and observations on the *S/Y Eugen Seibold* research sailing yacht and on the HALO research aircraft. The observed contrasts between different environments and conditions provide deep insights into the effects of anthropogenic activities on air quality and climate in the Anthropocene.

"Quo vadis, Amazonia? Atmospheric aerosols play a prime role in the hydrology and biogeochemistry of the rapidly changing rainforest ecosystem."

ADVANCED MICROSPECTROSCOPY OF ATMOSPHERIC AEROSOL PARTICLES

Chemical composition and microstructure determine the effects of aerosol particles on the Earth's radiative budget, clouds, climate, and atmospheric chemistry. To unravel single particle properties, we apply advanced microspectroscopy with high spatial and chemical resolution for the analysis of aerosol samples from ATTO, HALO, *S/Y Eugen Seibold*, and other sampling locations. It is particularly challenging to mimic and analyze the dynamic processing of aerosols in the atmosphere under laboratory conditions. To achieve this, we have developed a microreactor system for X-ray microscopy, which allows observations of standard and ambient aerosol samples under a wide range of precisely controlled conditions (e.g. temperatures down to ~250 K, relative humidity beyond 98 %, as well as variable gas phase composition). Using the microreactor, we have characterized liquid-liquid phase separation in standard and ambient aerosol samples, opening up new perspectives for further aerosol process studies.

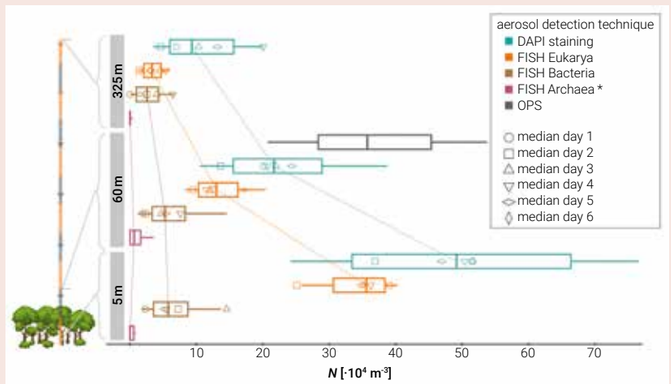


Figure 2: Vertical profiles of number concentration of airborne microorganism classes measured at the tall tower (median with 25 and 75 quartiles as boxes and 10 and 90 percentiles as whiskers). Specifically, eukarya, bacteria, and archaea were quantified with novel molecular microbiological protocols. These observations have filled important gaps in our understanding of bioaerosol abundance, taxonomy, and atmospheric mixing. Adapted from Praß et al., 2020.

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AEROSOL, CLOUD AND SURFACE INTERACTIONS

HANG SU

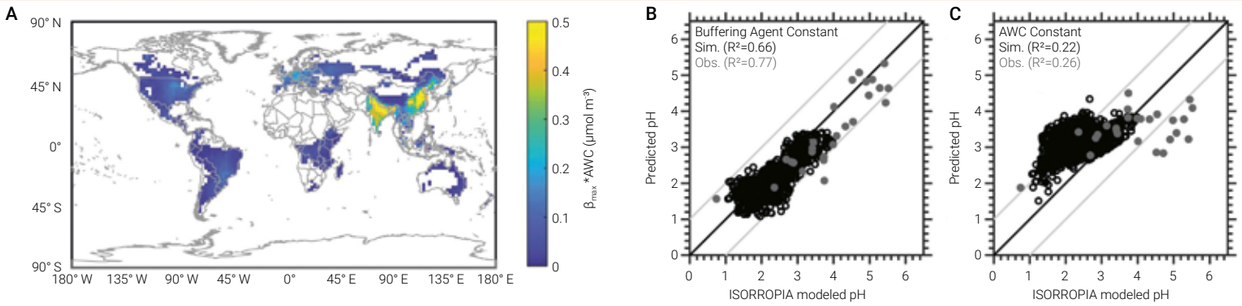

Figure 1: Drivers of aerosol pH diversity in ammonia-buffered regions. A) Global distribution of continental surface regions buffered by NH_4^+/NH_3. The color coding shows the maximum buffer capacity by NH_4^+/NH_3 (unit: mol m^{-3} air). B) Correlation of aerosol pH modelled by the ISORROPIA model with the predicted pH derived using constant buffering agent and multiphase buffer theory. C) Correlation of aerosol pH modeled by ISORROPIA with the predicted pH by ISORROPIA using constant aerosol water content (AWC) but variable compositions. Black circles and gray dots represent analysis based on model simulations and observations, respectively. Note that the observations are based on individual case studies, and thus show a wider range of aerosol pH than the annual average simulation results.

AEROSOL ACIDITY AND PHASE STATE

Aerosol acidity and phase transitions are attracting increasing interest in atmospheric research, because they influence the thermodynamics of gas-particle partitioning and the chemical kinetics of the formation and transformation of particulate matter. Understanding the temporal and spatial variations of aerosol pH and phase state in the atmosphere is crucial for accurate predictions of the properties of atmospheric aerosols and their effects on health, ecosystems, and climate. We find that aerosol pH levels in populated continental regions are widely buffered by the conjugate acid-base pair NH_4^+/NH_3. In contrast to non-buffered regions, aerosol water content and mass concentration play a more important role in determining aerosol pH in ammonia-buffered regions than variations in dry particle chemical composition. In other words, aerosol acidity can thus be approximated based on aerosol mass concentration and water content in these buffered regions. This opens up new possibilities to reconstruct long-term trends and large-scale spatial distributions of aerosol pH, which is essential to understand the global impact of atmospheric multiphase chemistry. Moreover, we have demonstrated that phase changes and the influence of temperature and humidity on multiphase chemical reactions are key to understanding and modeling the regional and global transport of hazardous air pollutants.

GLOBAL MAP OF HONO EMISSIONS FROM SOIL

Up to ~50% of the primary OH radical production in the lower troposphere is attributed to the photolysis of nitrous acid (HONO), and field observations suggest a large unidentified source of HONO. In earlier experimental and modeling studies, we found that atmosphere-surface exchange can account for this missing source of HONO. To evaluate the impact of this new source, we developed the Biogenic HONO Yield and Atmospheric Nitrogen (BOYAN) model to estimate the global soil emissions of HONO. BOYAN is a process-oriented model to simulate soil HONO emissions on regional and global scales with a spatial resolution down to 1 km. Our results show strong seasonal and spatial variations due to distinct driving parameters such as soil texture and pH, precipitation, and temperature, etc. Overall, the soil emissions of HONO are comparable to those of NO and N_2O, substantially contributing to the global nitrogen cycle.

SINGLE PARTICLE FLUORESCENCE SPECTROSCOPY OF ATMOSPHERIC AEROSOLS

Atmospheric bioaerosols, including airborne bacteria, fungal spores, and pollen, can affect human health and may influence the formation and evolution of clouds as ice nuclei or giant cloud condensation nuclei. Characteristic particle size, fluorescence intensity, and fluorescence spectra are important parameters for the detection and categorization of bioaerosols. A prototype size-resolved single particle fluorescence spectrometer (S2FS) was developed to simultaneously measure aerodynamic diameters and fluorescence spectra. The S2FS consists of an aerodynamic particle sizer and a fluorescence spectrometer with a 355-nm laser excitation source and an intensified charge-coupled device as the detector. Emission spectra are dispersed in 512 channels from 370 to 610 nm, where a major portion of biological fluorescence emission occurs. Highly fluorescent particles can be distinguished by the S2FS on a single-particle level. For weakly fluorescent particles, fluorescence spectra can only be obtained by averaging multiple particles (between 100 and 3,000) of the same kind. Preliminary ambient measurements in Mainz (Germany) show that an emission peak at ~440 nm was frequently observed for fine fluorescent particles (0.5-1 µm). Fine fluorescent particles accounted for 2.8% of total atmospheric aerosols on average based on the number fraction detected in the fine mode. Coarse fluorescent particles (>1 µm) accounted for 8.9% on average, with highest concentrations observed during morning hours and thunderstorms.

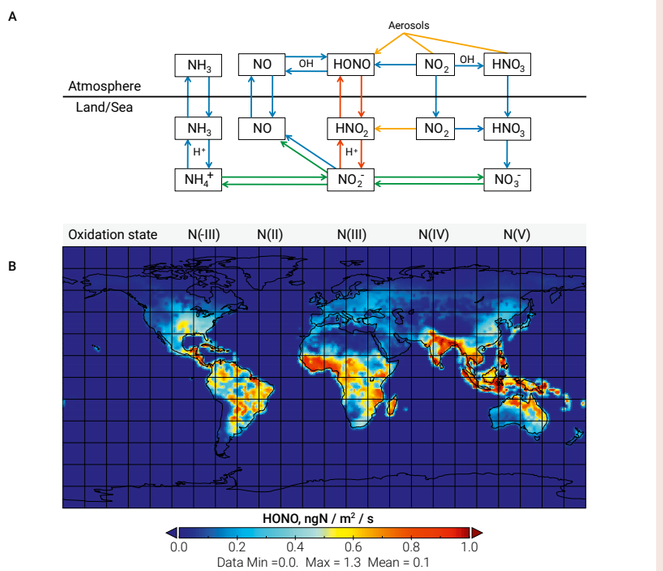

Figure 2: A) Coupling of HONO and other reactive nitrogen species in the atmosphere with biogenic nitrite and related species at the land or sea surface. Red arrows represent the multiphase processes linking gaseous HONO and nitrite (acid-base reaction and phase partitioning); green arrows represent biological processes; orange arrows represent heterogeneous chemical reactions converting NO_2 and HNO_3 into HONO; blue arrows represent other related physico-chemical processes in the nitrogen cycle (adapted from Su et al. 2011). B) Global distribution of soil HONO emission calculated by the BOYAN model.

"We investigate the mechanism and environmental impact of interactions between aerosols, clouds, and the biosphere."

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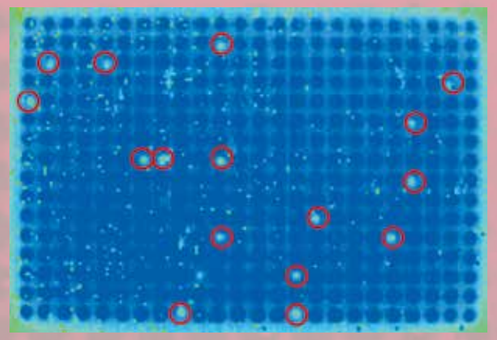
BIOMOLECULAR ANALYSES AND INTERACTIONS

JANINE FRÖHLICH



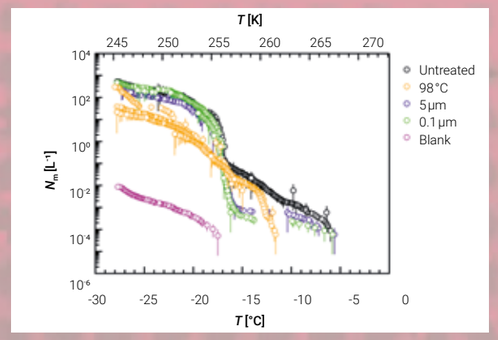


Figure 1: Infrared image of a 384-well plate during cooling in the TINA instrument. Red circles indicate freezing droplets (left). Freezing experiments of aqueous extracts of atmospheric aerosols from Mainz, Germany, after heat treatment and filtration. Cumulative number of IN (nm) per liter air (right) (Kunert et. al., 2018).

Biological aerosol particles and biomolecules are ubiquitous in the atmosphere where they influence the biosphere, climate, and public health. Airborne bacteria, fungal spores, pollen, and other bioparticles can be involved in the formation of precipitation and undergo physical and chemical transformation, stress, and biological aging before they are deposited back to the Earth surface. The abundance, impact, and multiphase chemical interactions of biological aerosols are not yet well characterized and quantified.

One focus of our research is to understand the ability of biological particles to serve as ice nuclei (IN). We have developed a new high-throughput droplet freezing instrument for efficient analysis and characterization of biological IN in laboratory and field samples under immersion freezing conditions. The Twin-plate Ice Nucleation Assay (TINA) is a fully automated setup that allows simultaneous study of ice nucleation and freezing events in hundreds of microliter-range droplets using infrared detectors.

A multitude of samples pre-treated in different ways were analyzed using TINA, allowing us to study biological IN from bacteria and fungi as well as air particulate matter. For example, the exposure of bacterial and fungal IN to atmospherically relevant concentrations of ozone and nitrogen dioxide elicited a reduction in the bacterial IN activity, but the fungal IN activity was not affected. Further experiments with fungal ice nuclei from *Fusarium* revealed that cell-free IN are smaller than 100 kDa and that IN aggregates can be formed in aqueous solutions. IN activity was not affected by long-term storage and freeze-thaw cycles but was strongly reduced by heat treatment confirming that the *Fusarium* IN are proteinaceous.

In collaboration with the Max Planck Institute for Polymer Research, we have investigated the effects of antifreeze proteins (AFPs), pH changes, and electrostatic interactions on the activity of bacterial IN from *Pseudomonas syringae*. We found that only certain AFPs inhibited the activity of bacterial IN, indicating that the ability to inhibit IN activity is not an intrinsic property of AFPs. Thus, the interactions of IN with different AFPs are mediated by protein-specific rather than universal molecular mechanisms. When pH was lowered to acidic values, we found a reduction of the activity of bacterial IN aggregates, whereas increased pH values, i.e. more alkaline conditions, did not affect IN activity. Using surface-specific sum-frequency generation spectroscopy we found that the net charge strongly correlates with the IN activity of the IN aggregates, which is minimal at the isoelectric point. Thus, electrostatic interactions play an essential role in the formation of the highly efficient functionally aligned IN aggregates. These results provide new insights that will help us to unravel the molecular mechanisms of biological ice nucleation.

Another key focus of our group is determining the influence of chemical modification on the allergenic and inflammatory potential of proteins. Upon exposure to reactive oxygen and nitrogen species, proteins can undergo chemical modifications which influence their physical, chemical, and biological properties. To elucidate the reaction kinetics and products, we perform laboratory experiments under controlled conditions. In particular, we investigate the chemical reactions of disease-related proteins with ozone, nitrogen dioxide, and peroxynitrite. In collaboration with the Lucas group, we have found that nitration and oligomerization of the α-synuclein, Heat shock protein 60, and High-mobility-group box 1 protein by peroxynitrite enhances innate immune responses mediated by pattern recognition receptors, pro-inflammatory transcription factors, and cytokines. Currently, we are studying the chemical kinetics of the nitration and oligomerization reactions of the major grass pollen allergen Phl p5, and in cooperation with the University Medical Center Mainz we are investigating the binding of modified Phl p5 to IgE antibodies from patients´ blood.

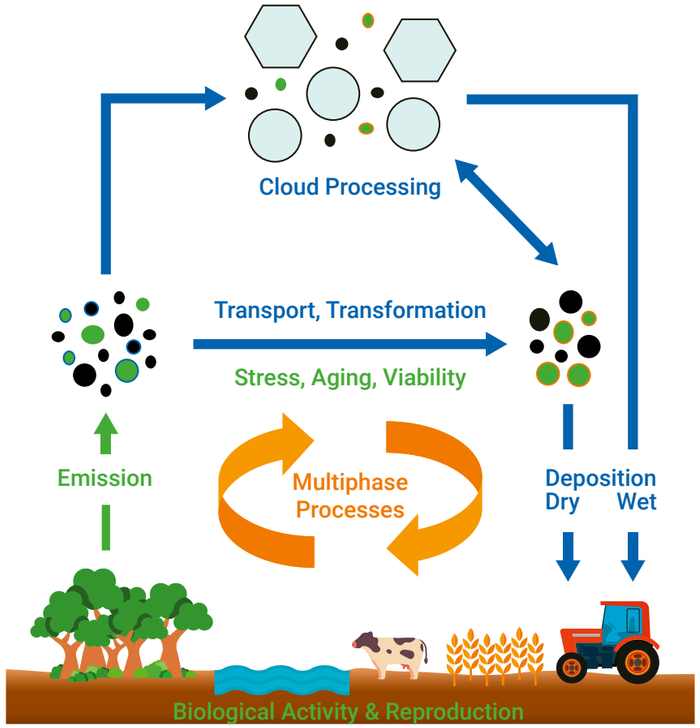


Figure 2: Bioaerosol cycling and effects in the Earth system. Adapted from Fröhlich-Nowoisky et al., 2016.

"We investigate the interactions of proteins and biological aerosol particles with air pollutants and climate and the impact on public health."

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CHEMICAL KINETICS AND REACTION MECHANISMS

THOMAS BERKEMEIER

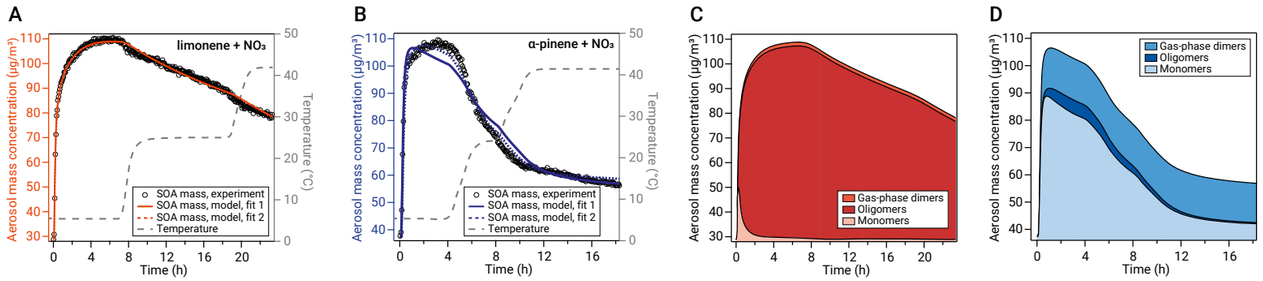


Figure 1: The evolution of secondary organic aerosol mass in a smog chamber, described with a kinetic model (panels A and B). Differences in formation and evaporation between two types of precursors can be attributed to different oligomerization kinetics (panels C and D; adapted from Berkemeier et al., 2020).

Many processes in the atmosphere and in the human body occur at and across interfaces in multiphase chemical systems (Scheme 1). Developing a detailed description of the multiphase reaction kinetics of these systems on the molecular scale is vital for understanding the rates at which particles evolve, compounds degrade, and oxidants are formed or consumed. We aim to resolve the processes and uncertainties that are characteristic for the complex reaction mechanisms of atmospheric and physiological chemistry. For this purpose, we develop and use elaborate computer models and algorithms for designing and analyzing laboratory experiments as well as understanding and predicting atmospheric and physiological phenomena.

KINETIC MULTILAYER MODELS AND MONTE CARLO GENETIC ALGORITHM

Multiphase chemical reactions are closely intertwined with transport processes and phase transitions, which requires the use of kinetic multi-layer and multi-compartment models. Due to the complex nature of the investigated systems, these models require large numbers of input parameters, including reaction rate coefficients, diffusion coefficients and the position of thermodynamic equilibria, many of which are still poorly constrained. To mitigate the need for a priori knowledge of kinetic parameters, we developed a Monte Carlo genetic algorithm (MCGA) for efficient, automated, and unbiased global optimization of model input parameters by simultaneous fitting to multiple experimental data sets. The MCGA algorithm enables an inverse modeling approach in which elusive kinetic parameters become more constrained the more training data are available. We will further develop the MCGA using statistical tools and novel machine learning algorithms.

SECONDARY ORGANIC AEROSOL FROM NITRATE RADICAL OXIDATION OF MONOTERPENES

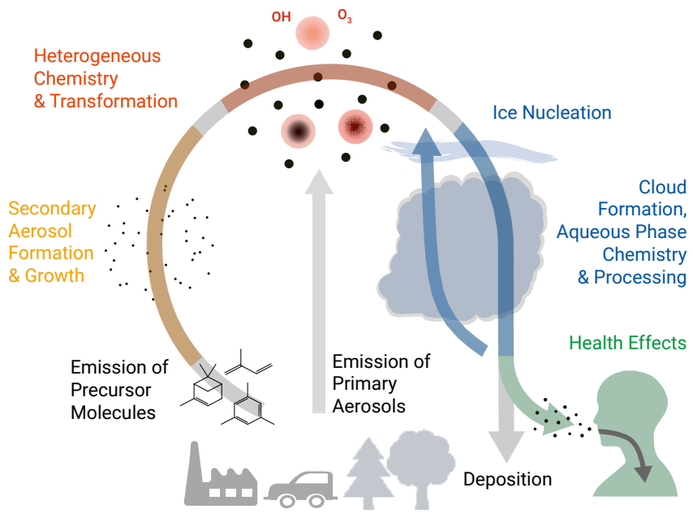
In chamber experiments and model simulations, we investigated the formation and evaporation of secondary organic aerosols (SOA), which are major components of fine particulate matter in the atmosphere. Reactions between the prominent SOA precursors monoterpenes and nitrate radicals (NO_3), which are important nighttime oxidants, revealed fundamentally different kinetics and properties for α-pinene and limonene SOA (Figure 1). The volatility distributions of the oxidation products alone cannot explain the time evolution of these processes. Hence, slow oligomerization kinetics (Figures 1 C and 1 D) and/or a viscous phase state slowing down molecular transport must be responsible for the observed mass profiles during aerosol growth as well as during evaporation at increasing temperatures. These experiments and simulations provide insights into how SOA can be formed at night and persist when temperatures rise during the day.

DIFFUSION, REACTION, AND CONCENTRATION GRADIENTS IN SEMI-SOLID PARTICLES

Atmospheric aerosols can exhibit a viscous phase state, which affects the time scales at which chemical compounds are taken up, released, or transformed in these particles. In collaboration with partners at the Paul Scherrer Institute, we were able to predict and for the first time experimentally visualize diffusion gradients in the multiphase chemical reaction of aerosol particles with ozone. A kinetic multi-layer model was utilized to simulate reactant depth profiles and infer reaction rates as well as humidity-dependent diffusion coefficients.

AEROSOL HEALTH EFFECTS AND OXIDATIVE STRESS

The health effects of aerosols are among the main focal points of our research. Air pollution can cause adverse health effects that may lead to disease or premature death. While the epidemiological evidence is clear, the underlying chemical processes are not well characterized. We will investigate how the composition of aerosols can be linked to the negative health outcomes of inhaling air pollution. It is known that redox cycling in the human lung can lead to excessive production of reactive oxygen species (ROS) that may cause oxidative stress. The goal of this investigation is to establish a connection between aerosol composition data and epidemiological health data. We will model the chemistry of redox-active components of air pollution in the fluid layer lining the human lung and investigate not only the dose-response relationship of different aerosol constituents but also the non-linear effects between them. This can be achieved by combining kinetic data from the laboratory with our kinetic models and will provide new knowledge about the mechanisms of redox chemistry in the human body.



Scheme 1: Life cycle of atmospheric aerosols with colors highlighting active research areas in the Berkemeier Group.

"We perform experiments and develop models to understand the formation, transformation, and effects of aerosol particles in the atmosphere and the human body."

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INFLAMMATORY PROCESSES

KURT LUCAS

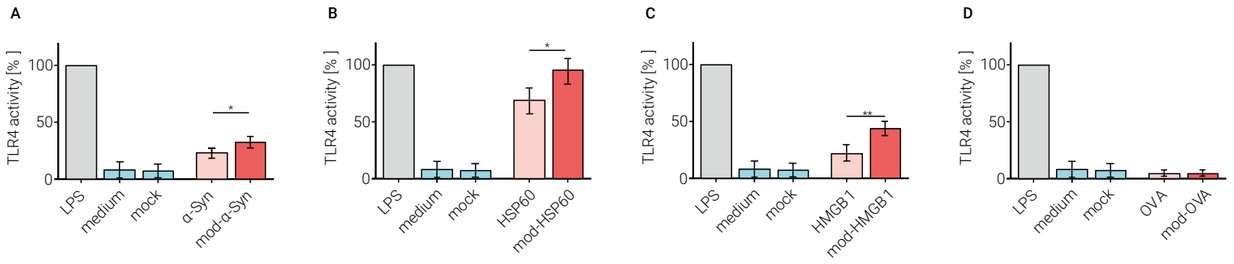


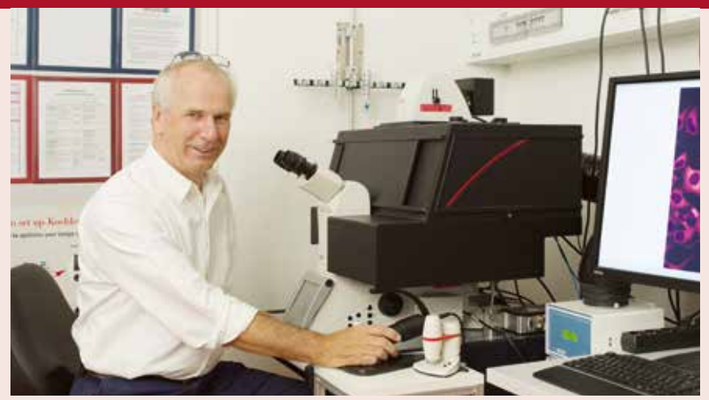
Figure 1: TLR4 activation by native and peroxynitrite-modified proteins in cell culture experiments. TLR4 activity measured in HeLa reporter cells (cancer-derived cell line) in response to treatment with α-Syn (A), HSP60 (B), HMGB1 (C), and ovalbumin (D) as a control, all normalized to lipopolysaccharide (LPS). TLR4 activity was determined using luciferase as a proxy (*p <0.05, **p <0.01).

Inflammatory processes play an essential role in the human immune system, but the underlying chemical mechanisms are not yet well understood. Our studies are focused on the immunomodulatory effects of protein modifications and related chemical interactions. For example, reactive oxygen and nitrogen species (ROS/RNS) of environmental and physiological origin can induce protein nitration and oligomerization. Such modifications can lead to enhanced activation of pattern recognition receptors (PRR) and inflammatory responses. We also investigate how substances such as plant extracts and molecular hydrogen can effectively mitigate inflammation. The aim is to unravel the molecular mechanisms of acute and chronic inflammatory diseases, determine their potential relation to environmental pollution, and open up new perspectives for their treatment and mitigation. Our research is performed in close cooperation with the Fröhlich group, University Medical Center and the Institute for Pharmacy of the Johannes Gutenberg University Mainz as well as other collaborators from the biomedical sciences.

The Toll-like receptor 4 (TLR4) is a PRR that is of central importance for the innate immune system and is found on the surface of various human cell types that can sense damage-associated molecular patterns (DAMPs). In a recent study, we investigated how the TLR4 response and pro-inflammatory potential of α-synuclein (α-Syn), Heat shock protein 60 (HSP60), and High-mobility-group box 1 protein (HMGB1), proteinaceous DAMPs with important roles in neurodegenerative and cardiovascular diseases, changes upon chemical modification by peroxynitrite, a prominent example of physiological ROS/RNS. We found that the peroxynitrite-modified proteins elicited a strongly enhanced activation of TLR4 and the pro-inflammatory transcription factor NF-κB in stable reporter cell lines as well as increased mRNA expression and secretion of the pro-inflammatory cytokines TNF-α, IL-1β, and IL-8 in human monocytes (THP-1) (Figure 1). This enhanced activation of innate immunity via TLR4 is mediated by covalent chemical modifications of the studied DAMPs. Our results show that proteinaceous DAMPs modified by peroxynitrite more potently amplify inflammation via TLR4 activation than the native DAMPs and provide first evidence that such modifications can directly enhance innate immune responses via a specific immune receptor. These findings suggest that environmental pollutants and related ROS/RNS may play a role in promoting acute and chronic inflammatory disorders by structurally modifying the body's own DAMPs. This may have important consequences for chronic neurodegenerative, cardiovascular, or gastrointestinal diseases that are prevalent in modern societies and calls for action to improve air quality and mitigate climate change in the Anthropocene (Figure 2).

In related studies, we found that peroxynitrite, tetranitromethane, and mixtures of ozone and nitrogen dioxide can also enhance the immunostimulatory potential of amylase trypsin inhibitors (ATIs), a group of proteins from gluten-containing cereals that promote inflammatory diseases, allergies, and hypersensitivities. Currently, we are investigating whether immunostimulatory potential is more efficiently enhanced by nitrated proteins, i.e., protein macromolecules that contain a nitro-group, or by protein dimers/oligomers that are formed as byproducts of nitration and oxidation.

In addition, we are studying the anti-inflammatory effects of herbal extracts and molecular hydrogen. Currently, we are investigating whether angiogenesis and overshooting immune responses to SARS-CoV-2 infections can be counteracted by cinnamon and hop extracts. Moreover, we are investigating how molecular hydrogen can be efficiently delivered and used to treat oxidative stress and chronic fatigue in the context of COVID-19 and other diseases.



"Understanding the chemical mechanisms of inflammatory processes is opening up new perspectives for the treatment of diseases."

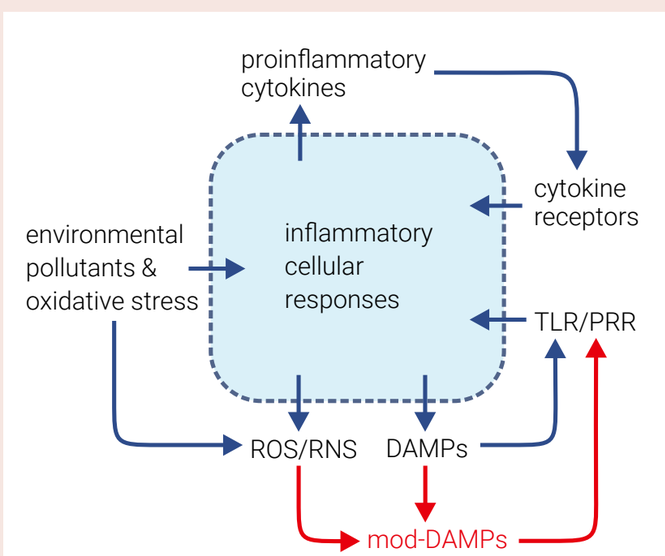


Figure 2: Amplification of inflammatory processes and innate immune responses through chemically modified DAMPs. Environmental pollutants and oxidative stress can elicit an increase in reactive oxygen and nitrogen species (ROS/RNS), the formation of chemically modified damage-associated molecular patterns (mod-DAMPs), augmented pro-inflammatory signaling via Toll-like receptors and other pattern recognition receptors (TLR/PRR), an increase of proinflammatory cytokines, and further inflammatory cellular responses.

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ORGANIC POLLUTANTS AND EXPOSURE

GERHARD LAMMEL

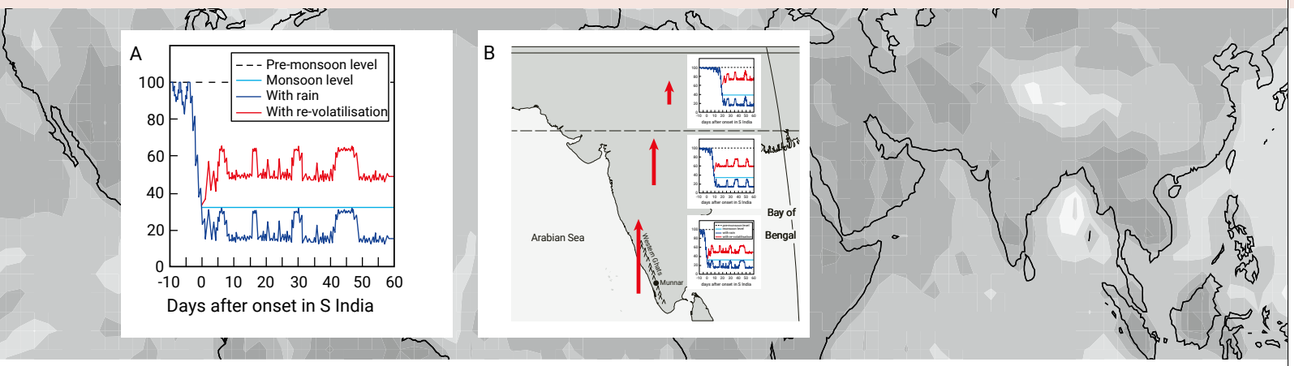

Figure 1: Illustration of temporal (A) and spatial (B) variation in semi-volatile and long-lived substances in air over southern, central, and northern India in response to the monsoon onset and its northeastward advance.

Humankind has introduced over 30,000 anthropogenic substances into the environment, including unintended by-products, many of which pose a hazard to human health and ecosystems. The cycling of long-lived organic pollutants in the Earth system is particularly complex. In atmospheric aerosols, most of these pollutants are semi-volatile and partition between the gaseous and particulate phases. Upon deposition onto soil, vegetation, and sea surfaces, they may re-volatilize to the atmosphere (so-called multihopping). Long after peak emission, such secondary sources may overrun primary sources, which are usually concentrated in highly populated and industrialized areas. The total environmental residence time of these so-called persistent organic pollutants (POPs) typically exceeds the atmospheric residence time by several orders of magnitude. The latter depends strongly on partitioning in the aerosol. Also, chronic exposure to many long-lived organic pollutants is detrimental to human health. Apart from inhalation, uptake in food is a dominant exposure path, which is relevant for the lipophilic pollutants that bio-accumulate in organisms in food webs.

POPs have in the past been heavily used as agricultural pesticides in South Asia, and the region is thus considered a hot spot. Until now, studies on environmental exposure of the Indian subcontinent have been mostly limited to urban areas, with rural inland regions scarcely addressed.

We studied the response of air-soil exchange under the influence of the South Asian summer monsoon. At the onset of this monsoon, very clean air from the southern hemisphere reaches the subcontinent. Analyses of soil and air suggest that the arrival of the summer monsoon triggers net volatilization or enhances the on-going re-volatilization of the now banned chemicals hexachlorocyclohexane (HCH, an insecticide) and polychlorinated biphenyls (PCB, used in electric installations and in construction) from soils in southern India. The modeling results showed that the re-volatilization from soils results in increasing air pollution as the monsoon advances northeastward across the subcontinent during June and July (Figure 1). In this way, each year, a small percentage of the annual atmospheric depositions of pollutants received by soils are returned to the atmosphere.

Many pollutants that are detrimental for human health are formed unintentionally as byproducts of fossil fuel or biomass combustion and further processing by atmospheric photochemistry. This includes polycyclic aromatic hydrocarbons (PAHs), nitrated, oxygenated, and halogenated PAHs, and halogenated dioxins and furans. The biological effects of nitrated PAHs are usually stronger than those of the parent compounds (PAHs). Also, the mutagenicity and carcinogenicity of many quinones, a subgroup of oxygenated PAHs, is high, because they form strong DNA adducts. Moreover, quinones, through redox cycling with the corresponding semi- and hydroquinones, promote formation of reactive oxygen species (ROS) and some of them are strong mutagens and carcinogens. ROS cause oxidative stress, which is associated with several chronic diseases. However, little is known about even the most toxic and most abundant species from these substance classes in air, soils, and surface waters, their multiphase chemistry, and long-range transport potential.

We have studied sources and distributions of nitrated 4-ring PAHs, 2-nitrofluoranthene (2-NFLT) and 2-nitropyrene (2-NPYR), by measurements at continental sites and over open ocean, as well as by modeling on regional and global scales. These nitrated PAHs are rapidly formed by radical attack of and addition of NO_2 to the corresponding parent PAHs, fluoranthene, and pyrene, in and downwind of the areas of fossil fuel and biomass combustions (Figure 2). In this way, the PAHs reach truly remote environments, including the Arctic. A fuller understanding of their atmospheric cycling is dependent on a better elucidation of their photochemical sinks.

The human health risk from inhalation exposure to air pollution can be assessed by quantifying the bioaccessible fraction of the pollutant mass and biological testing of the individual substance in pollutant mixtures. Quantification of bioaccessibility of constituents of particulate matter was so far largely limited to heavy metals. The bioaccessibility of PAHs and their nitrated and oxygenated derivatives was studied using simulated lung lining fluids for extraction of the ambient particulate matter samples. The derived inhalation bioaccessibility of the nitrated PAHs and quinones in the inhalable size fraction (PM_{10}) is found to be low, i.e., <5% of the total ambient concentration. This fraction is much higher for more polar aromatics, such as for example the nitrosalicylic acids and nitrocatechols. The main source of these and other monoaromatics, which typically represent ≈1% of the particulate organic matter, is biomass burning.

Quantification of the pollutant dose taken up as a consequence of inhalation exposure to ambient air pollution is a focus of on-going research.

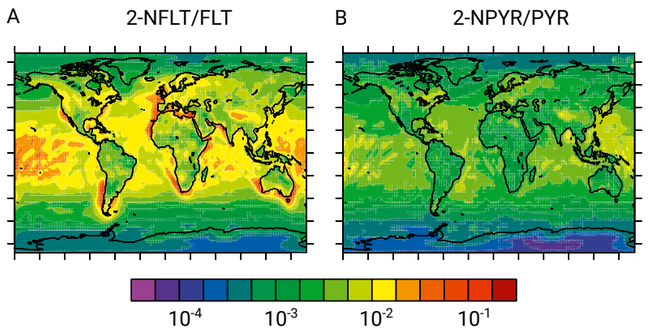

Figure 2: Ratio of nitrated PAH to parent PAH near-surface concentrations, averaged over 3 years.

"Understanding the exposure of the environment and humans to organic pollutants cycling in atmospheric aerosols and between atmosphere and surface compartments."

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MULTISCALE INTERACTIONS AND INTEGRATION

ULRICH PÖSCHL

Figure 1: A) Clouds and fog over the Amazon rainforest at the Amazon Tall Tower Observatory (ATTO); B) High Altitude and Long-Range Research Aircraft (HALO) during the EMeRGe campaign in Oberpfaffenhofen.

Chemical reactions, mass transport, and phase transitions between gaseous, liquid, and solid matter in the Earth system bridge a wide range of spatial and temporal scales. The Anthropocene, i.e., the present era of globally pervasive human influence on planet Earth, is characterized by a widespread increase of air pollutants such as combustion- or traffic-related aerosol particles, nitrogen oxides, and ozone. These pollutants can have a pronounced influence on atmospheric chemistry and physics, climate, and public health, but their actual impact remains to be fully unraveled and quantified.

The effects of aerosols on clouds and precipitation are among the largest uncertainties in the scientific understanding of climate change. This is partly due to a lack of information about how the properties and interactions of aerosols and clouds in polluted air differ from that of pristine air approximating pre-industrial background conditions.

These interactions and differences are investigated by the Cloud Condensation Nuclei (CCN) project team led by *M. Pöhlker* who holds a Minerva Fast Track position funded by the Max Planck Society. This work is carried out in close collaboration with partners at the MPIC and other institutions. Recent and ongoing studies involve long-term measurements of aerosol and CCN properties in continental and marine environments (Amazon/ATTO, Barbardos/Ragged Point; green vs. blue ocean; clean vs. polluted conditions), related aircraft and ship campaigns (ACRIDICON-CHUVA, EMeRGe, CAFE-AFRICA, CAFE-EU/BLUESKY, EUREC4A), and cloud parcel model studies using field and satellite data to constrain the properties of CCN and their effects on clouds, precipitation, and climate.

Among our key findings related to CCN and aerosols are (a) a physically meaningful parameterization of CCN spectra that is based on normal distribution functions to replace traditionally used but physically not well-defined power law functions (Figure 2); (b) a close linear relationship between the hygroscopicity parameter kappa and the organic aerosol mass fraction, which can be used for efficient parameterization of CCN properties in global climate models; (c) novel insights into the dynamic interplay of aerosol and CCN properties, water vapor supersaturations, and updraft velocities in convective clouds (secondary CCN activation); (d) characteristic differences between dry and wet season clouds over the Amazon influenced by regional sources of aerosols as well as long-range transport from Africa (biomass burning, desert dust, and sea spray); (e) substantial changes in the altitude profile of aerosols over Europe during the COVID-19 lockdown in spring 2020.

Air pollution is among the largest risk factors for premature mortality and diminished life expectancy worldwide. The chemical mechanisms responsible for the adverse health effects of fine particulate matter and other air pollutants, however, are not yet resolved. Oxidative stress is of crucial importance, but the influence, interactions, and effects of different air pollutants remain to be elucidated and quantified. The roles of free radicals and related species are investigated by the Radical Chemistry team led by *H. Tong* in close collaboration with partners at the MPIC and other institutions. Recent and ongoing studies include the investigation of air filter samples from clean and polluted environments as well as laboratory experiments with ambient particulate matter and various surrogate systems.

Among our key findings related to reactive species and the detrimental effects of air pollution are (a) characteristic concentrations and size distributions of environmentally persistent free radicals (EPFR) in air filter samples from remote tropical and boreal forests in contrast to polluted urban areas and megacities; (b) different amounts and product distributions of reactive oxygen species and organic radicals formed upon interaction of anthropogenic and biogenic secondary organic aerosols (SOA) with water and surrogate lung fluid; (c) association of radical formation by fine particulate matter with highly oxygenated organic molecules. Follow-up studies and numerical simulations are intended to relate the observed chemical species and processes to the impacts of airborne particulate matter on human health. Moreover, joint studies with partners at the MPIC and other institutions are aimed at quantitatively assessing COVID-19 infection risks by aerosol or droplet transmission and reducing them through preventive measures like face masks and ventilation.

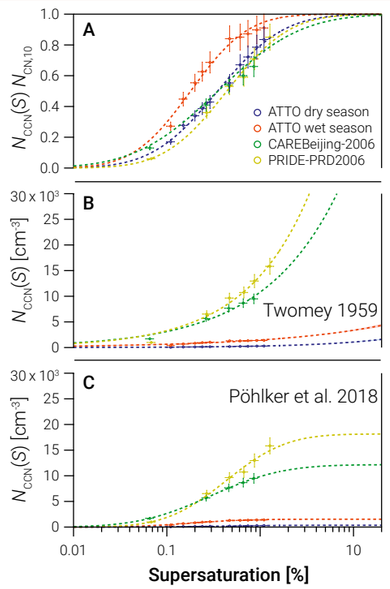

Figure 2: Regional differences and parameterizations of CCN efficiency spectra: A) ratio of CCN to aerosol particle number concentration in the Amazon rainforest compared to Asian megacity regions; B) traditionally used but physically not well-defined parameterization by power law functions (Twomey 1959); C) physically meaningful parameterization based on normal distribution functions (Pöhlker et al. 2016).

"Multiphase processes on molecular to global scales play a vital role in the co-evolution of climate, life, and health in the Earth system and in the Anthropocene."

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PARTICLE CHEMISTRY

Properties and transformation of natural and anthropogenic aerosol particles in the atmosphere, smog, cloud formation, formation of ice in the atmosphere. Meteorite and star dust.

PARTICLE CHEMISTRY DEPARTMENT

BACKGROUND

The Particle Chemistry Department (PCD) was established jointly between the Johannes Gutenberg University of Mainz (JGU) and the MPI for Chemistry (MPIC) in 2001. Prof. Stephan Borrmann, who holds a "C4" professor position at the JGU Department of Physics, Mathematics and Computer Science (here the Institute for Atmospheric Physics, IPA) and a formal part-time appointment at MPIC, is director of the department.
The department consists of five research groups: (1) Instrumental Aerosol Analytics (Frank Drewnick), (2) Aerosol and Cloud Chemistry (PD Johannes Schneider), (3) Atmospheric Hydrometeors (PD Miklós Szakáll, at IPA), (4) Aerosol and Cloud Physics (Ralf Weigel, at IPA), and (5) Nano- and Microparticle Research (NAMIP, PD Peter Hoppe).

RESEARCH FOCUS

Research in PCD is focused on the physical and chemical properties and processes of atmospheric aerosols, clouds, large hydrometeors, air pollution and its sources, as well as particulate matter of extraterrestrial origin. Experimental approaches involve ground-based, mobile, and aircraft-borne field measurements, development of state-of-the-art instrumentation, and also include intricate laboratory studies. In 2020, the department became active in experimental research on aerosols in connection with the COVID-19 pandemic (see report by F. Drewnick).

EXPERIMENTAL FOCUS

Our department operates several large facilities, including the Mainz Vertical Wind Tunnel (report by M. Szakáll), the Mobile Laboratory for Atmospheric research (MoLa), and the NanoSIMS laboratory of the NAMIP group (report by P. Hoppe). Six sophisticated mobile aerosol mass spectrometers are available for field research. Five of these instruments have been operated on eight different research aircraft (from five countries), including IAGOS-CARIBIC, the Russian M-55 "*Geophysica*", the German research aircraft *DLR HALO* (report by J. Schneider), *DLR Falcon*, the *AWI Polar P6*, the *British BAe 146 FAAM*, the *NASA DC-8*, and *NSF/UCAR HIAPER GV.* Several of our instruments have been developed in-house, such as the Aircraft-based Laser ABlation Aerosol MAss spectrometer (ALABAMA), the ERICA (i.e., ERc Instrument for Chemical composition of Aerosols) particle mass spectrometer, and the HALOHOLO holographic imaging probe (for laboratory studies, ground-based, ship, and aircraft deployment).

All of PCD's aircraft instruments as well as MoLa were deployed in many high-profile field projects both in Germany as well as internationally (e.g., ATLAS 2019 in Fez (Morocco), AQABA 2017 (around the Arabian Peninsula and in the Arabian Gulf), StratoClim (Asian monsoon, Nepal; reports by R. Weigel and S. Borrmann) EMeRGe 2018 from Taiwan, CAFE-AFRICA 2018 (Cape Verde), CAFE-EU 2020 (Europe), ACCLIP 2020 (USA), ND-MAX 2018 (USA, Germany) and others).

Stephan Borrmann giving a speech at a "Fridays For Future" demonstration in Mainz.

TEACHING AND EDUCATION

Since the department was established as a common structure for both, JGU and MPIC, in addition to research, formal education in the scope of Ph.D. programs and curricula for bachelor and master students are at the core of PCD's mission. During the reporting period, six Ph.D. theses, four M.Sc. theses, and four B.Sc. theses were completed in the department. Currently, five students are carrying out their Ph.D. projects in PCD. Altogether, since 2001 within the department a total of 56 Ph.D., 40 "Diplom", 6 M.Sc. and 6 B.Sc. theses have been (or are currently being) supervised. (Of these 108 graduate students ≈ 45 % are female.) After the successful habilitations (i.e., qualification as a postdoctoral lecturer or "Privatdozent, PD") of J. Schneider and M. Szakáll at JGU, a new habilitation procedure for Alexander Theis has now being initiated. Several members of the department – including PD J. Schneider, PD M. Szakáll, R. Weigel, S. Borrmann, and several other members of PCD – are engaged in teaching for the Meteorology curriculum at JGU. Many of our group members and graduate students, as well as the director are actively involved in several outreach activities connected with the "Scientists for Future" and "Fridays for Future" movements.

STEPHAN BORRMANN

18 January 1959 Born in Mainz, Germany

1977 – 1984 Study of Physics and Biology Johannes Gutenberg University Mainz

1985 – 1986 Adjunct Research Instructor at the Naval Postgraduate School in Monterey/CA/USA

1991 Ph.D. in Physics at the JGU University in Mainz

1991 – 1993 Postdoctoral Fellow of the Advanced Study Program (University Corporation of Atmospheric Research, UCAR) at the National Center for Atmospheric Research (NCAR) in Boulder/CO/USA

1999 German Habilitation in Meteorology

1998 – 2000 Head of the Aerosol Research Group at the Institute for Chemistry and Dynamics of the Geosphere at the Research Center Jülich Ltd.

Since 2000 Professor Johannes Gutenberg University Mainz and Scientific Member of the Max Planck Society

Since 2001 Director (part-time) at the Max Planck Institute for Chemistry

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THE ASIAN TROPOPAUSE AEROSOL LAYER – A CONUNDRUM RESOLVED

STEPHAN BORRMANN

Figure 1: Left panel: ERICA sampling inlet during takeoff. Middle panel: Takeoff of the *M-55 Geophysica* from Kathmandu, 31/7/2017. Right panel: Integration of ERICA (inside a pressurized barrel) into the aircraft.

THE ASIAN TROPOPAUSE AEROSOL LAYER (ATAL) AND THE ASIAN MONSOON ANTICYCLONE (AMA):
From mid-June until the end of October the AMA develops as a fairly "isolated" rotating air mass from East Asia to the Middle East. Extending from altitudes of roughly 12 km to 18 km, it is a component of the tropical Upper Troposphere/Lower Stratosphere (UT/LS) that is notoriously difficult to reach by experimental platforms. At various locations in the region, convective upward transport carries tropospheric source gases and aerosols into the UT/LS. These materials accumulate inside the anticyclone such that they are enriched during its life cycle and become amenable for long-range transport after the AMA dissolves. In 2009, a previously unobserved aerosol layer was discovered between 14 km and 17 km. Very faint signals of this layer became apparent in measurements obtained by the CALIOP space borne lidar on the Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations (CALIPSO), albeit only when averaging over many satellite overpasses. Since its discovery, the ATAL has posed a conundrum: What are the sizes, number densities, and the chemical composition of the ATAL aerosol particles?

It was hypothesized based on theoretical considerations that these particles largely consist of sulfuric acid/water solution droplets and sulfate. Within the EU StratoClim project, dedicated physical and chemical *in situ* measurements of clouds and aerosols were conducted (based in Kathmandu, Nepal; July/August 2017) on board the Russian high-altitude *M-55 Geophysica* research aircraft. The Particle Chemistry Department/JGU groups contributed nine instruments to the payload (see Figure 1).

PHYSICAL PROPERTIES OF THE ATAL PARTICLES
Figure 2 shows the vertical profiles of the aerosol backscatter ratio (SR, red line) as obtained from the CALIOP lidar when roughly averaging over the 2017 StratoClim period. Similar vertical profiles of SR (blue line in Figure 2) can also be calculated from the *in situ* particle size distribution measurements of our UHSAS and COPAS instruments (see report by R. Weigel). The two results are in good agreement within the altitude band of the ATAL between 15.5 km and 18 km. This closure implies that our aerosol and cloud instrument package completely covered the relevant size range with sufficient sensitivity such that the question regarding the particle sizes and number concentrations of the ATAL could be answered for the AMA of 2017 (Mahnke et al., 2020).

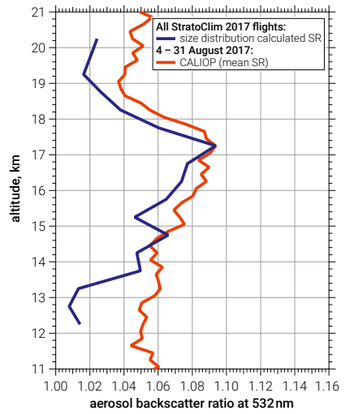
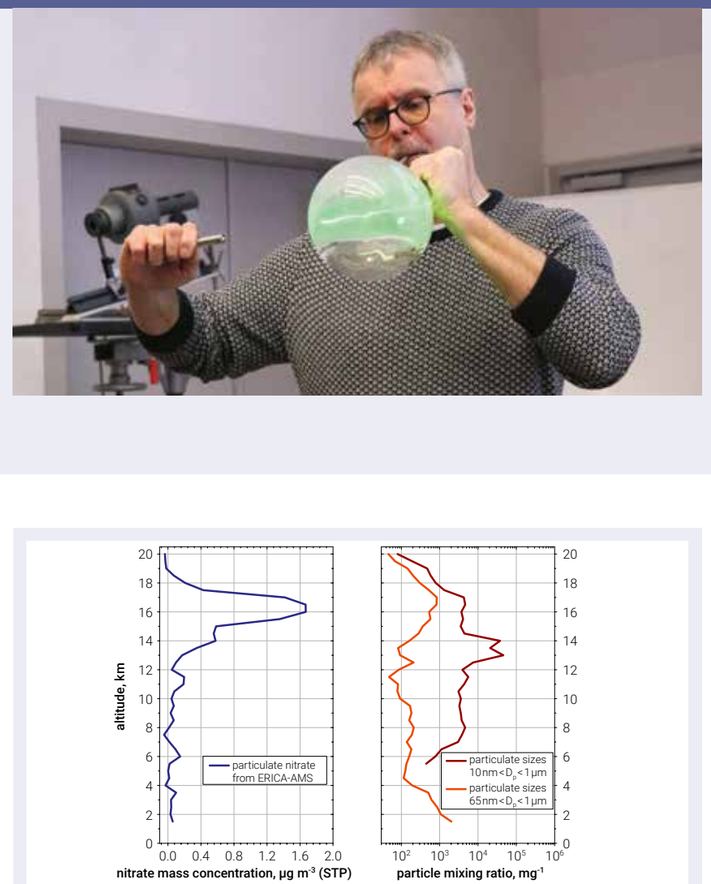


Figure 2: Vertical profiles of the ATAL signature between altitudes of 15.5 km and 18 km from remote sensing and *in situ* measurements: Red curve – aerosol backscatter ratio (SR) as measured by the spaceborne CALIOP lidar (operating at 532 nm wave length) on the CALIPSO satellite. Blue curve – backscatter SR as derived from particle size distribution measurements of the modified UHSAS (Ultra High Sensitivity Aerosol Spectrometer) and COPAS (COndensation PArticle counting System) instruments from MPIC/JGU.



"During 22 years of experimenting with the Russian high-altitude *M-55 Geophysica* research aircraft, we gained enough experience to tackle the ATAL conundrum with dedicated *in situ* measurements."

Figure 3: StratoClim flight on 4/8/2017. Left panel: Nitrate signal from the *in situ* mass spectrometric particle composition measurements of ERICA-AMS (ERc Instrument for the Chemical composition of Aerosols, an in-house instrument funded by the ERC Advanced Research grant of S. Borrmann) exhibiting a distinct nitrate peak at an altitude of 16 km. Right panel: *In situ*-measured vertical profiles of the aerosol particle mixing ratios from the UHSAS (orange curve) and COPAS (brown curve) instruments for the indicated size ranges. The ATAL is visible as a broader layer between 14 and 18 km. The "spikes" below 14 km in the COPAS data indicate new particle formation events.

CHEMICAL COMPOSITION OF THE AEROSOL:
Our novel and fully automated hybrid aerosol particle mass spectrometer ERICA (ERc Instrument for the Chemical composition of Aerosols) samples the ambient submicron aerosol and immediately converts the particulate matter into ions. In two ionization regions inside ERICA, ions are generated by means of (a) laser ablation (ERICA-LAMS) from individual particles or (b) by flash vaporization/electron impact ionization (ERICA-AMS) from small particle ensembles. The mass spectra of these ions represent the information on the particle chemical composition and are directly recorded *in situ* and online. In Figure 3, an example is shown from a research flight on August 4, 2017. A distinct peak can be seen at altitudes around 16 km, which indicates that nitrate is the major component of the ATAL aerosol. Detailed analyses (Höpfner et al., 2019; 2020) showed that anthropogenic emissions of gaseous ammonia from regional agricultural activities ultimately lead to formation of this nitrate aerosol in the AMA and the UT/LS. Thus, the combination of simultaneous remote sensing (Gimballed Limb Observer for Radiance Imaging of the Atmosphere (GLORIA) , see Höpfner et al., 2019) and *in situ* instruments on the *M-55 Geophysica* were crucial for solving the conundrum of the chemical composition of ATAL.
For further studies on the processing, aging, and atmospheric relevance of the aerosol formed within the AMA, our ERICA instrument was implemented in 2020 on the US UCAR/NSF HIAPER research aircraft for participation in the ACCLIP (Asian Summer Monsoon Chemical and Climate Impact Project) 2021 campaign based in South Korea.

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PARTICLE FILTRATION EFFICIENCY OF HOMEMADE FACE MASKS – A CONTRIBUTION FROM AEROSOL SCIENCE DURING THE COVID-19 PANDEMIC

FRANK DREWNICK

Figure 1: Setup of the testing facilities and measurement of filtration efficiencies for potential mask materials.

When the COVID-19 pandemic started spreading across the planet in 2020, it quickly became clear that countries did not have the required capacity to provide sufficient personal protective equipment, such as face masks, to effectively reduce transmission of the disease. Very quickly, simple cloth masks went into production everywhere; however, initially little was known about the filtration features of the materials used.

With this issue in mind, we began to use expertise and aerosol instrumentation which was readily available in our laboratories to test the filtration capability of various cloth materials. What started as a small-scale test on a handful of samples with a quickly assembled test setup turned rapidly into a major research effort. Initially, most new samples or suggestions to test materials came from colleagues. After the publication of a press release that conveyed the first results to the general public, we received numerous requests for testing samples and questions about potential materials.

Expressions of interest came from medical doctors and pharmacists, companies which wanted to switch their production to the fabrication of face masks, initiatives to support less developed countries, the general public, and from the state government of Rhineland-Palatinate who were in search of suitable masks for use in schools. Many samples and commercially available face masks were tested, but also systematic tests were performed in order to learn more about the properties that determine the suitability of a material for masks.

Size-dependent particle filtration efficiency of cloth samples was determined for laboratory-generated and ambient aerosol particles with diameters ranging from d_p =30 nm to 10 µm. Two measurement setups were constructed, which both applied particle counting and sizing in front of and behind the sample to determine the transmission through the material. Smaller particles (d_p≤500 nm) were generated by nebulizing an aqueous solution of NaCl and size-selecting the dried particles; the measurements were performed using condensation particles counters. In this setup, the electrical charge of the particle can be controlled, which allows investigation of the contribution of electrostatic deposition to overall filtration of small particles. Ambient particles covering the diameter range from d_p=30 nm to 10 µm were measured using optical particle counters and a scanning mobility particle spectrometer.

Particle filtration efficiency depends strongly on particle size. A filtration minimum is typically found between d_p=50 nm and 500 nm (Figure 2 A), at which all particle deposition mechanisms are inefficient. (Note: The size of an uncoated SARS-CoV-2 virion is around 60 nm to 140 nm.) Smaller particles are filtered more efficiently, due to enhanced diffusion and electrostatic deposition. The latter mechanism was mainly observed for synthetic materials, which often carry permanent electrostatic charge on their fibers. However, also a few non-synthetic materials (e.g., terry, flannel, or velvet cotton) showed significant electrostatic deposition. For larger particles, enhanced filtration efficiencies were observed for all sample materials, which increased with face velocity (Figure 2 B) due to improved impaction deposition.

A larger number of layers of cloth in a mask results in an increase of the pressure drop Δp across the material stack (Figure 2 C) but also in an increase in filtration efficiency (i.e., decreasing particle transmission T; Figure 2 D). The measurements showed that the individual layers can be treated as separate filters and that no interaction, like alignment of stitches or pores, occurs between them. Thus, the overall features of a cloth stack in a mask can readily be calculated from those of the individual layers, making laborintensive measurements unnecessary. This also means that the filter quality factor ($qf = \log(1/T)/\Delta p$) can be used for direct comparison of different potential mask materials, showing that not only professional filtration materials, but also relatively fluffy textiles like French terry, fleece, or velour can be used to make masks with reasonable filtration efficiencies, though with the need for multiple layers of material.

Importantly, measurements using samples with defined gaps showed that filtration efficiency decreases by approximately 50 % up to two-thirds with only 1–2 % relative leak area. Therefore, it is essential not only to use materials which filter particles efficiently but also to manufacture face masks which fit well and have as few gaps as possible between mask and face.

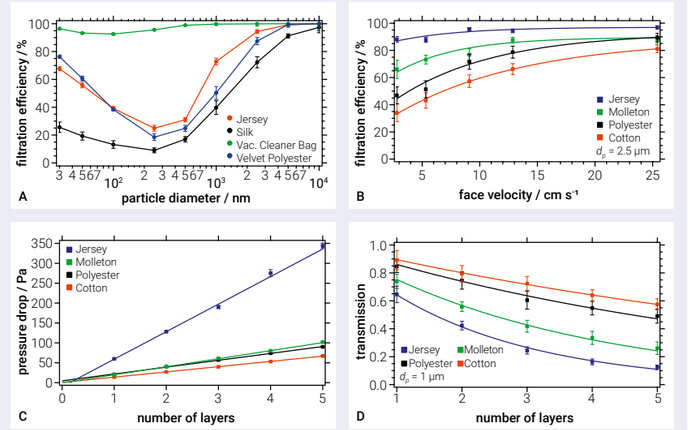

Figure 2: A) Exemplary filtration efficiency curves for d_p=30 nm–10 µm; B) filtration efficiency increases with face velocity for d_p=2.5 µm; C) pressure drop is proportional to number of layers; D) transmission decreases ($T_n = T_1^n$) with increasing number of layers n.

"We learned during the COVID-19 pandemic that aerosol science is not only relevant to society in the context of air quality and climate but also has direct implications for the day-to-day life of each individual."

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NANO- AND MICROANALYTICAL STUDIES OF MATTER FROM SPACE AND EARTH

PETER HOPPE

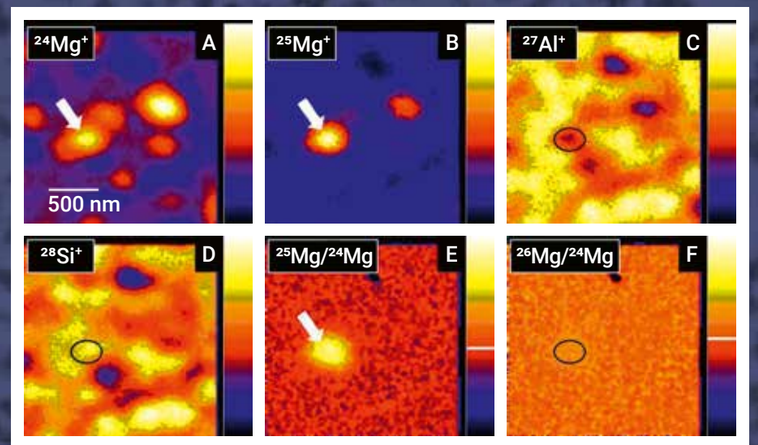

Figure 1: NanoSIMS secondary ion and isotopic ratio images of a presolar silicate (white arrows, black ellipses). The Solar System $^{25}Mg/^{24}Mg$ and $^{26}Mg/^{24}Mg$ ratios are marked by the white lines running through the color bars, in which black represents the lowest and yellow the highest ion intensities or ratios (E, F). From Leitner and Hoppe (2019).

BACKGROUND

Terrestrial and extraterrestrial matter carries specific isotopic and mineralogical signatures which can be used to trace their origins and formation histories. To address these questions, we have studied a variety of terrestrial and extraterrestrial materials with different nano- and microanalytical techniques. The key instrument for our studies is a Cameca NanoSIMS 50 ion probe, a secondary ion mass spectrometer that can be used to carry out isotope and elemental abundance studies with < 100 nm spatial resolution.

Major scientific themes addressed during the last three years include (i) the origins of the solid matter that went into the making of our Solar System (Hoppe et al., 2018a; 2018b; Leitner and Hoppe, 2019; see Results section below), (ii) transport of matter in the early Solar System (Fujiya et al., 2019), (iii) the early Earth (radioactive ^{60}Fe as a potential heat source for planetary melting and differentiation; origin of nitrogen on Earth), and (iv) foraminifera shells as proxies for paleoclimate reconstruction (in cooperation with the Climate Geochemistry Department, Jochum et al., 2019).

RESULTS

By studying isotopic compositions of stardust, so-called presolar grains, which are older than our Solar System and which are found in small quantities in primitive meteorites, it is possible to get detailed insights into stellar nucleosynthesis and dust formation and to identify the types of parent stars that contributed dust to our Solar System. Silicates are the most abundant presolar grain type. These pristine grains, which are typically 100–400 nm in size, can be found *in situ* in meteorite thin sections by NanoSIMS ion imaging. Until recently, only a few elements, e.g., oxygen, could be analyzed with the required < 100 nm spatial resolution for isotopic composition by employing a primary cesium ion beam. From a comparison of the oxygen isotope data with stellar model predictions and astronomical observations, red giant stars had been proposed as the dominant stellar sources of presolar silicates.

In 2017, we upgraded our NanoSIMS with a new oxygen primary ion source that permits to extend high-resolution isotope studies to many more elements than was previously possible. With this new capability, we were able to conduct systematic studies of Mg- and Si-isotopic compositions of more than 100 presolar silicates. These studies revealed surprising results, as a significant fraction of presolar silicates believed to come from red giant stars showed Mg-isotopic compositions incompatible with an origin in such stellar sources. Instead, the strong enhancements in ^{25}Mg (Figures 1 and 2) are best explained by nuclear reactions in the interior of supernovae. Important implications of these observations are that (i) oxygen isotopes alone are not sufficient for an unambiguous distinction between dust grains from red giant stars and supernovae, and (ii) that the fraction of supernova grains in the molecular gas and dust cloud from which our Solar System formed was significantly higher (up to 30 %) than previously thought (Leitner and Hoppe, 2019).

The majority of presolar silicates show only moderate Mg and Si isotope anomalies of typically a few percent (relative to solar compositions), compatible with origins in red giant stars. Their $^{25}Mg/^{24}Mg$ ratios correlate with $^{26}Mg/^{24}Mg$ (Figure 2), $^{29}Si/^{28}Si$, and $^{18}O/^{16}O$ ratios. These correlations are best explained by the chemical (isotopic) evolution of the Milky Way, with only minor imprints of nucleosynthetic and mixing processes in the grains' parent stars (Hoppe et al., 2018b).

OUTLOOK

We will continue and expand our nano- and microanalytical studies of different types of extraterrestrial materials (presolar grains, primitive meteorites, material from asteroid Ryugu collected by the Hayabusa 2 mission of the Japan Aerospace Exploration Agency JAXA). Of particular importance for these studies will be the new high-resolution oxygen ion source on our NanoSIMS. We will also continue our ongoing studies on the early Earth (DFG-funded projects on ^{60}Fe and on the origin of Earth's nitrogen) and microfossils.

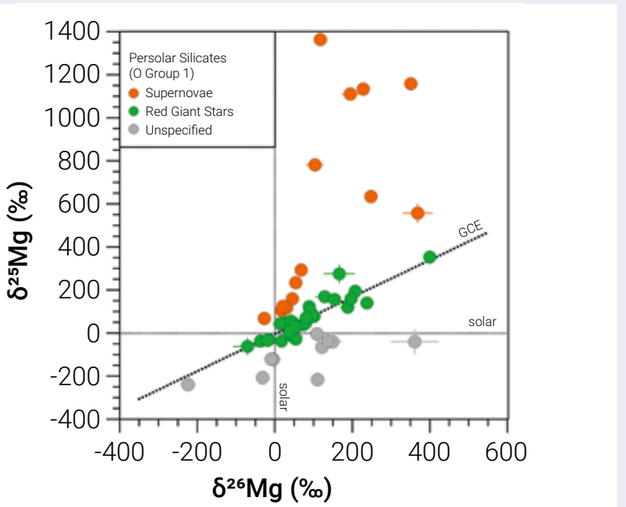

Figure 2: Mg-isotopic compositions of presolar silicates presented as per mil deviation from the solar $^{25,26}Mg/^{24}Mg$ ratios. GCE: Galactic chemical evolution. Grains above the GCE line are likely from supernovae, those along the GCE line from red giant stars.

"Isotopic and mineralogical fingerprints of terrestrial and extraterrestrial materials: A tool to trace chemical and physical processes in space and on Earth."

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ORGANIC AEROSOL PARTICLES IN THE TROPICAL UPPER TROPOSHERE

JOHANNES SCHNEIDER

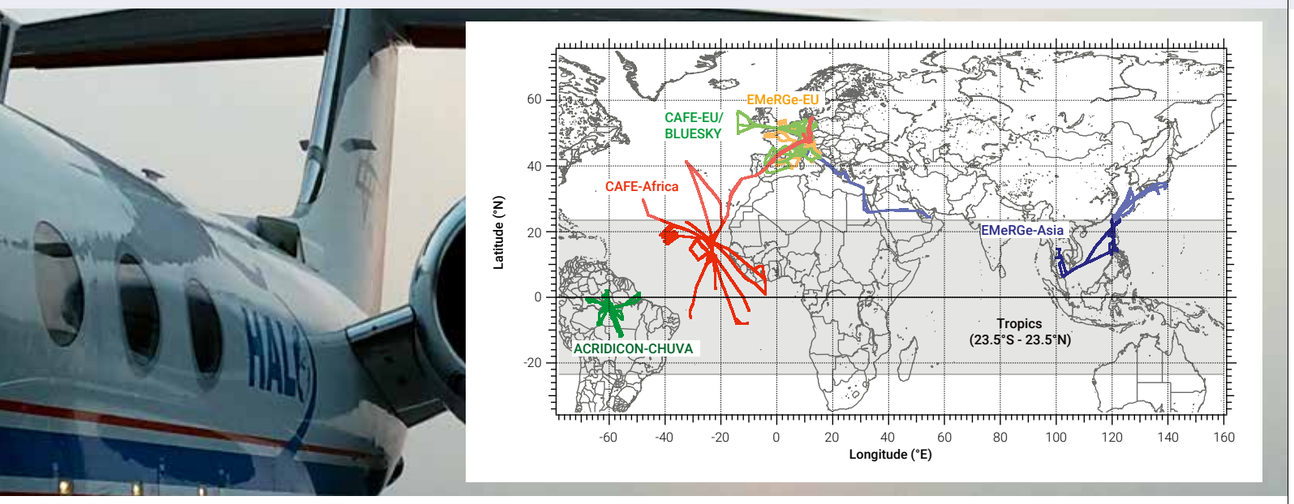
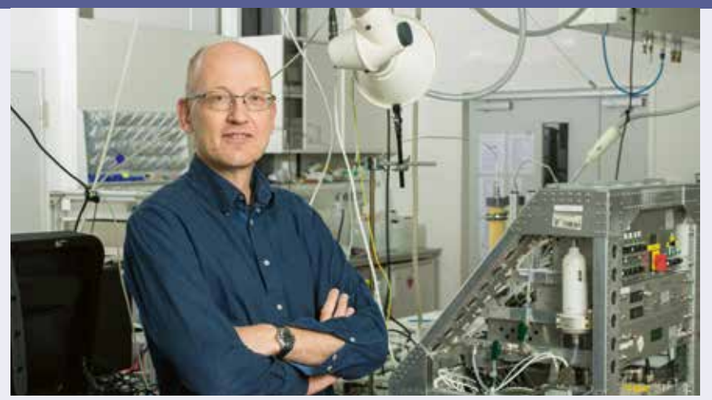


Figure 1: Map showing the flight tracks of HALO missions conducted with the Compact Time-of-Flight Aerosol Mass Spectrometer C-ToF-AMS. Darker colors indicate measurements in the tropics (23.5°S – 23.5°N).

Aerosol particles play a central role in the climate system and the hydrological cycle of the Earth system, because they regulate cloud formation by acting as cloud condensation nuclei or ice-nucleating particles. Secondary formation from organic or inorganic precursor gases is the predominant particle source at high altitudes where the influence of primary particles like sea spray, mineral dust, or biological particles is low. The upper tropical troposphere is of special interest, because the sensitivity of this region to changes in atmospheric composition with respect to radiative forcing is high. Cirrus clouds forming on aerosol particles can significantly alter the radiative balance, whereas aerosol particles can also interact directly with solar radiation. Especially in the tropics, deep convection is very effective in transporting aerosol precursor gases from the boundary layer to the upper troposphere.

The German research aircraft HALO has been available to the scientific community since 2010, and, among other applications, is being used to study the atmosphere at high altitudes. HALO's ceiling altitude of higher than 14 km and its long-operation range capability make it a unique research platform to study the tropical upper troposphere. Between 2014 and 2020, my group participated in six HALO missions (ML-CIRRUS, ACRIDICON-CHUVA, EMeRGe-EU, EMeRGe-Asia, CAFE-AFRICA, CAFE-EU/BLUESKY). In three of these missions, we conducted research flights in the tropical upper troposphere (Figure 1), operating a Compact Time-of-Flight Aerosol Mass Spectrometer (C-ToF-AMS). This instrument uses thermal vaporization of particles with subsequent ionization by electron impact, thereby allowing for a quantitative analysis of non-refractory submicron aerosol particles (with diameters between approximately 50 and 800 nm), including organics, sulfate, nitrate, and ammonium.

For the analysis presented here, we used only data between 23.5°S and 23.5°N, representing the tropics (Figure 1). Vertical profiles of the organic mass concentration and the fractional contributions to the total measured mass concentration are shown for all tropical datasets in Figure 2. The datasets show that organic particulate matter accounts for the majority of total aerosol composition in the free and upper troposphere above altitudes of about 6 km. The dataset from the Amazon region (ACRIDICON-CHUVA) additionally shows an increase in the absolute organic mass concentration above 8 km. We could show that this is partly due to secondary organic aerosol (SOA) formation from isoprene epoxydiols (IEPOX, Schulz et al., 2018).



"Secondary organic aerosol formation plays an important role in the tropical upper troposphere, creating a reservoir for lower tropospheric cloud condensation nuclei but also for stratospheric particles."

This finding demonstrated that deep convection carries aerosol precursor gases like isoprene from the boundary layer into the upper troposphere. A recent model study applying the Community Earth System Model used this dataset to validate the model results and to predict future IEPOX-SOA changes in response to changing climates (Jo et al., 2020).
In contrast to the two other tropical datasets, organic aerosol predominated over the Amazon also in the boundary layer, as has been demonstrated already in previous ground-based measurements (e.g. AMAZE-2008, GoAmazon2014/5; de Sá et al., 2018). The influence of anthropogenic emissions was much more pronounced during the EMeRGe-Asia mission, where the main target of the measurements was outflow from major Asian population centers. The high contribution of sulfate in the boundary layer during the CAFE-AFRICA mission, which was conducted out of the Cape Verde islands, is due to both low organic mass concentrations as well as sea salt sulfate and ship emissions. During CAFE-AFRICA, the upper troposphere was found to be influenced by the African monsoon, which transported biomass-burning aerosol to high altitudes. In contrast to the other two missions, HALO reached the tropopause region during CAFE-AFRICA, which is reflected by the increasing sulfate fraction above 12 km.
Overall, these data show that organic aerosol is the most important contributor to submicron aerosol mass in the upper tropical troposphere. Transport of precursor gases from the boundary layer with subsequent SOA formation is the most likely explanation for the increasing fractional contribution of particulate organics, because cloud processes remove aerosol particles transported upwards from the boundary layer during convective transport. For the Amazon region, IEPOX-SOA was identified as a major source for secondary aerosol. During the other two missions, the influence of IEPOX-SOA was much smaller, and the identification of the relevant precursor gases and particle formation pathways is still ongoing.

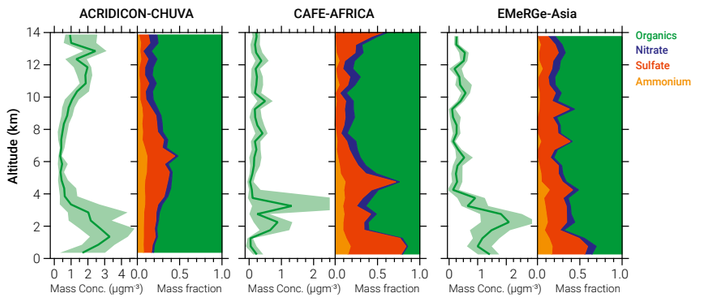


Figure 2: Vertical profiles of the organic mass concentration (left panels, medians, and quartiles) and the fractional contribution of all measured non-refractory aerosol components (right panels). Mass concentrations refer to standard pressure. Only data obtained between 23.5°S and 23.5°N were considered for this graph.

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LABORATORY INVESTIGATION OF TURBULENCE EFFECTS ON THE ACCRETIONAL GROWTH OF GRAUPEL

MIKLÓS SZAKÁLL, JOHANNES GUTENBERG UNIVERSITY GROUP

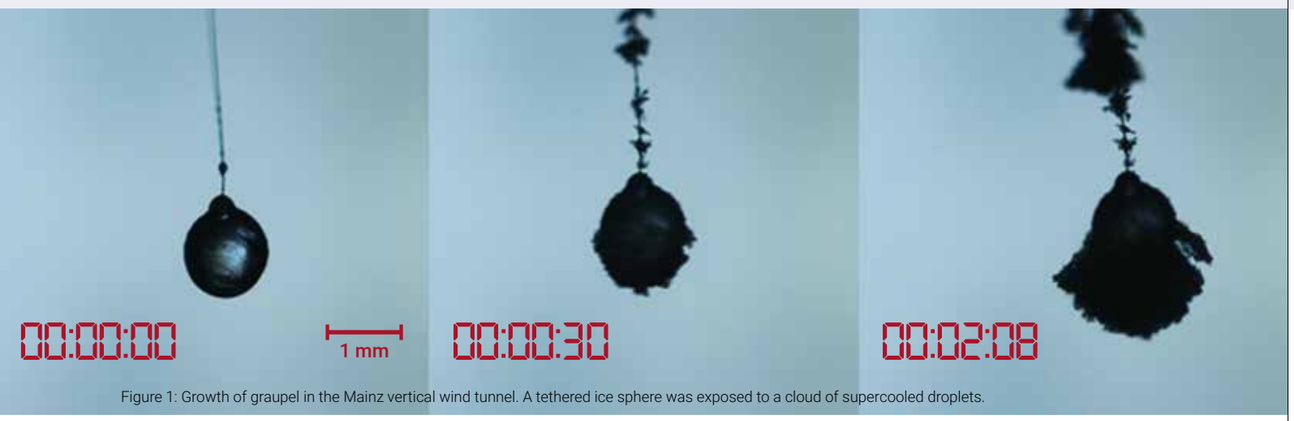


Figure 1: Growth of graupel in the Mainz vertical wind tunnel. A tethered ice sphere was exposed to a cloud of supercooled droplets.

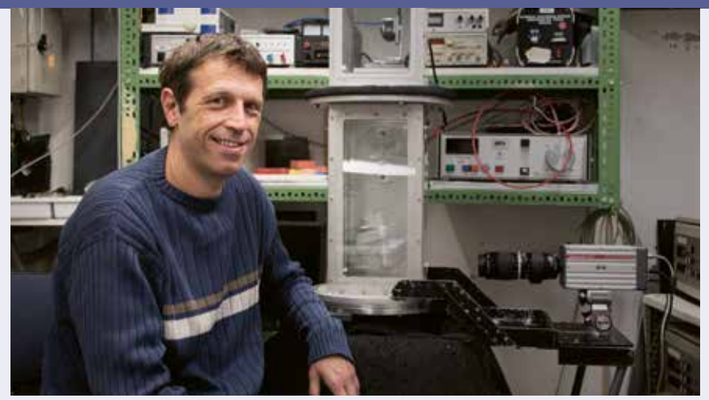
INTRODUCTION

Mixed-phase clouds play a central role in liquid and ice-phase precipitation generation. So far, the effects of turbulence on the growth of graupel, which are formed by the accretion of supercooled droplets (so-called riming), have been poorly investigated. The varying shapes, densities, surface properties, and differences in the release of latent heat during growth complicate the determination of graupel growth even in laminar flow. We have performed dedicated wind tunnel experiments to shed light on this very important piece of the puzzle of rain formation via the ice phase.

WIND TUNNEL STUDIES

Experimental studies were carried out in the Mainz vertical wind tunnel laboratory to characterize the effect of turbulence on the collisional growth of graupel. Tethered ice spheres with diameters from 220 to 340 µm were exposed to supercooled droplets with a mean diameter of 20 µm. A liquid water content of 0.9 g/m^3 and a temperature of -11 °C represented dry growth riming conditions in mixed-phase clouds. The wind tunnel air velocity was set to the terminal velocity of the initial graupel. The growth rate was characterized by the collection kernel K, which is equal to the volume swept out by the graupel per unit time and was quantified in the experiments by the mass increase of the graupel particle within a time period of 120 s (Figure 1). The experiments were performed in an alternating manner, i.e. one experiment in laminar flow and the subsequent one in turbulent flow. Turbulence was generated by placing a ring-shaped obstacle in the center of the upstream flow. The vertical root-mean-square fluctuation velocity (0.13 m/s), the dissipation rate (0.13 m^2/s^3), and the Taylor-microscale Reynolds number (48.0) of the flow represented typical low-scale turbulence in natural clouds. By comparing laminar and turbulent collection kernels, the effect of turbulence on the growth of graupel was characterized.

Figure 2 shows the measured collection kernels as a function of the mean momentum, i.e. graupel mass multiplied by its terminal velocity. The solid lines represent fits according to a power-law relationship ($K=a \times p^b$). When allowance is made for measurement errors, no significant difference between laminar and turbulent flow conditions was observed. This implies that the flow turbulence had no significant influence on the collection kernel of graupel in the investigated momentum range. We assume that turbulence effects are overcompensated for by the rapid increase in radius due to the accretion of low-density rime ice. The results suggest that disregarding turbulence effects on the initial phases of graupel growth under dry growth conditions in cloud models is justified, which greatly simplifies numerical simulations. This might change if one considers the collisional growth of low-density graupel initiated by ice crystals. Due to the lower inertia of such graupel and the related interaction with the turbulent flow, the influence on the collection kernel might be higher. These questions will be addressed in future experimental and theoretical studies.



"Wind tunnel experiments are essential to validate existing theories of turbulence effects on the collisional growth of ice particles, which is one of the major unresolved issues in cloud and precipitation microphysics."

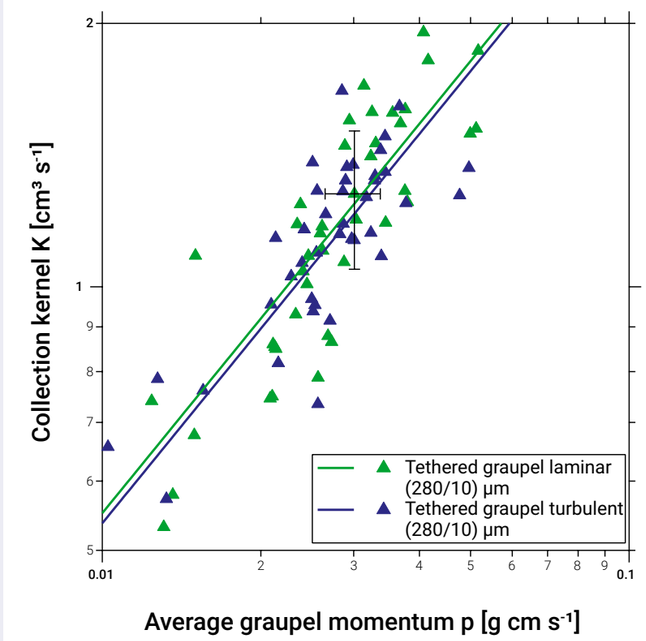


Figure 2: Comparison of graupel growth in laminar (green) and turbulent flow (blue). The lines represent the parameterizations of the data.

OUTLOOK

In the past, researchers have frequently focused on the formation of large glaciated hydrometeors, while melting has remained insufficiently investigated. We are currently investigating the melting of atmospheric ice particles, i.e. snowflakes, graupel, and hailstones, in our wind tunnel laboratory within the framework of a DFG-funded project. Besides the shapes, densities, fall speeds, meltwater contents, and the total melting time, the size distribution of the drops that shed off from the ice surface is of great importance in cloud models and radar meteorology. The Mainz vertical wind tunnel permits the characterization of the temporal change in these parameters, i.e. one obtains information from the fully glaciated to the completely molten state. We are using a digital holographic instrument which we have built in-house to continuously measure the size distribution of the shed droplets during melting of individual hailstones, which has not been quantified up to now.

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IN SITU OBSERVATION OF NEW PARTICLE FORMATION IN REGIONS OF THE TROPOPAUSE IN THE AMA AND THE ASIAN TROPOPAUSE AEROSOL LAYER

RALF WEIGEL, JOHANNES GUTENBERG UNIVERSITY GROUP

Figure 1: Pre-flight preparation of the Russian *M-55 Geophysica* (left) and during take-off for a flight during the StratoClim mission (right).

The Asian Monsoon Anticyclone (AMA) is one of Earth's most important meteorological systems and is typically associated with deep convection. The AMA mainly determines the circulation in the upper troposphere/lowermost stratosphere (UT/LS) from about June through September during the monsoon season over the Indian subcontinent, with oscillations at times extending into the Eastern Mediterranean and the Western Pacific regions. The upward transport within the AMA provides an effective way for air masses to reach the top of the AMA at ~455–465 K potential temperature (corresponding to ~60 hPa pressure level). Inside the AMA, the air is slowly lifted above the tropopause. The existence of the Asian Tropopause Aerosol Layer (ATAL) within the AMA region was proven and investigated by means of satellite observations. The constituents of convectively injected air, which further rises within the AMA, likely include precursor material from anthropogenic (Höpfner et al., 2019) and other sources, which maintain the observed ATAL. The process of New Particle Formation (NPF), as a source of aerosol material in the TTL region, may significantly contribute to the formation and persistence of the ATAL.

The four-channel COPAS (COndensation PArticle counting System) was deployed aboard the Russian research aircraft *M-55 Geophysica* (Figure 1) to investigate the properties of submicrometer-sized aerosol in the UT/LS. Three COPAS channels count particles with diameters larger than 6 nm, 10 nm, and 15 nm, respectively. The fourth COPAS channel detects aerosol particles with diameters greater than 10 nm after their exposure to heat (270 °C), providing information on the fraction (*f*) of non-volatile (nv) particles (e.g., soot, mineral dust, metallic aerosols). The upper size detection limit is about 1 µm for all channels. In this way, the COPAS measurements yield the particle number mixing ratios n_6, n_{10}, n_{15} and n_{10}nv. Eight mission flights reaching altitudes of ~20 km were conducted during the EU StratoClim 2017 mission from Kathmandu, Nepal. In total, the COPAS measurements throughout StratoClim 2017 extend to 22.5 hours at altitudes above 10 km (≳ 350 K), ~2.6 hours of which were spent under NPF conditions in the TTL region (~11–17.5 km, ~355–400 K, cf. Weigel et al 2020a). Throughout the StratoClim 2017 mission, recent NPF was identified by means of elevated mixing ratios of ultrafine particles (n_{uf}; i.e., the difference in mixing ratio between n_6 and n_{15}). From the ~2.6 hours with identified NPF, recent nucleation was encountered over a total of ~1.25 hours in the presence of ice cloud particles, e.g., in cumulonimbus (cf. Weigel et al., 2020b).

Figure 2 shows particle mixing ratios and resulting median profiles with 25th and 75th percentiles from StratoClim 2017 in direct comparison with data from earlier COPAS deployments in the tropics (TROCCINOX, Brazil (2005) and SCOUT-AMMA, West Africa (2006)) and with results from other studies (Central Pacific; Brock et al., 1995). The StratoClim 2017 data vertically structure as

- at about 350–380 K: The mixing ratios (n_6, n_{uf}, and n_{10}nv) scatter over two orders of magnitude (panels A, B, and C) and the highest n_6 values of up to 5 x 10^4 mg^{-1} are reached (panel A). The fraction *f* of non-volatile particles remains at comparatively low median values of less than 25% (panel D).

"The TTL within the Asian Monsoon Anticyclone sets new benchmarks concerning the intensity and frequency of *in situ*-observed new particle formation, and, hence, emerges as an important source of aerosols in the UT/LS."

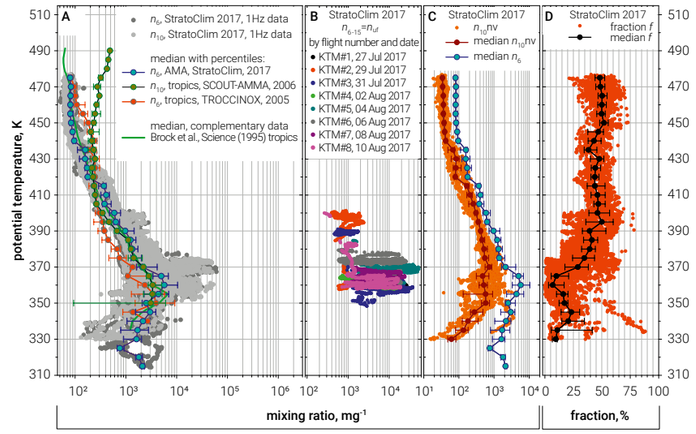

Figure 2: Vertical profiles: A) n_6 and n_{10} (gray-shaded points) from StratoClim 2017 and from earlier missions. B) The mixing ratio of ultrafine particles (n_{uf}). C) The mixing ratio of non-volatile particles. D) The fraction *f* (=n_{10}nv/n_{10}*100) of non-volatile particles. Median profiles with 25th and 75th percentiles as horizontal bars.

- at about 380–400 K: The scattering of the mixing ratio values remains high (panels A, B, and C). NPF with n_{uf} of up to 2000 mg^{-1} is observed up to altitudes corresponding to 400 K (panel B), i.e. well above the tropopause (~380 K). The total amount of non-volatile residuals remains at levels similar to those at 350–380 K (panel C), and *f* even increases towards 400 K.
- at about 400–420 K: The NPF processes have ceased (panel B). The total particle mixing ratio n_6 in the AMA remains elevated compared to earlier measurements, potentially indicating an impact of NPF several hours before the observation.

Since the *in situ* observation of NPF at and above the tropopause inside the AMA is unparalleled in terms of intensity, frequency, and spatial extent, the TTL region in the AMA likely constitutes one of the most important source regions, if not the most important, for aerosol production in the UT/LS. Although the lifetime of the smallest freshly-formed ultrafine particles is limited to a few hours due to effective coagulation (cf. Weigel et al., 2020a), the secondary aerosol material in the TTL is amenable for vertical and horizontal dispersion. It remains to be investigated whether this aerosol source affects the ATAL only, or whether the horizontal, large-scale dispersion of the aerosol material has further influence, e.g., on cirrus formation and/or the radiation balance in the UT/LS region.

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FURTHER RESEARCH GROUPS

Aerosols and regional air quality, terrestrial palaeoclimates, high pressure chemistry and physics, and satellite remote sensing.

AEROSOLS, AIR QUALITY AND CLIMATE

YAFANG CHENG – MINERVA RESEARCH GROUP

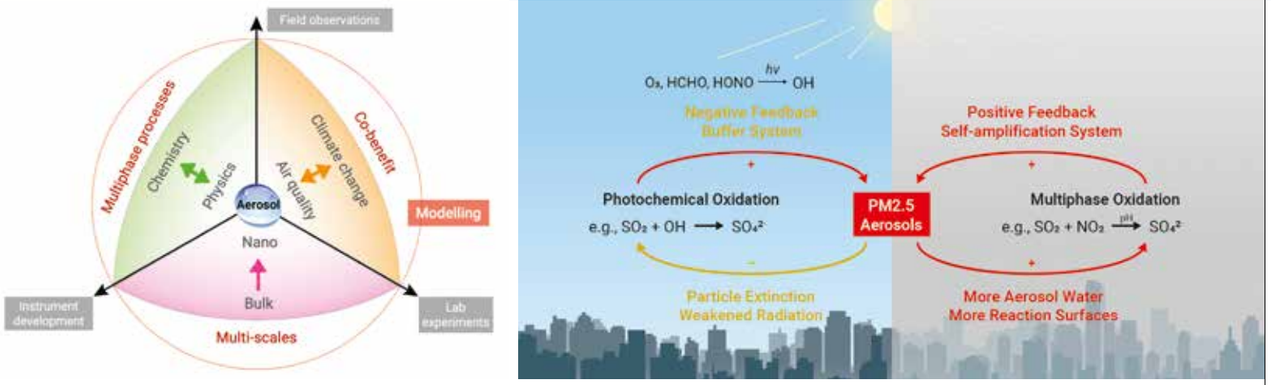

Figure 1: The broad theme and strategies of the Minerva research group and self-amplification system in the haze chemistry.

As outlined in Figure 1, we are aiming to obtain a predictive understanding of the origin, fate and impact of atmospheric aerosols to address the grand challenge of actionable projections of future climate and environment in the Anthropocene. For this purpose, we combine the development of cutting-edge instruments, lab experiments, field observations, and a synthesis approach with model simulations that involve multi-scale physical and chemical processes from molecular and nanometer scales to regional and global scales. Recent research highlights include:

DISCOVERING THE KEY ROLE OF REACTIVE NITROGEN CHEMISTRY AND MULTIPHASE BUFFERING EFFECTS IN ATMOSPHERIC AEROSOL AND HAZE FORMATION

Severe winter haze events are threatening the health of over 400 million people in the North China Plain and have been the subject of intense scientific investigations and public concern. The sources and chemical mechanisms leading to the fast formation and accumulation of fine particulate matter, however, remained unclear. Our study "Reactive nitrogen chemistry in aerosol water as a source of sulfate during haze events in China" (Science Advances 2016) revealed how the previously unexplained, infamous extreme haze events in the North China Plain around Beijing can be explained by the reaction between nitrogen dioxide and sulfur dioxide in aerosol water. The series of studies shows the essential role of multiphase reactions in aerosol water for producing sulfate, nitrate, and organic matter under haze conditions. In haze chemistry, aerosol acidity plays a key role in regulating multiple reaction rates and gas-particle partitioning. In our recent study, "Multiphase buffer theory explains contrasts in atmospheric aerosol acidity" (Science 2020), we proposed a new multiphase pH buffer theory (Figure 2) and showed that globally aerosol acidity is largely buffered by the anthropogenic ammonia. This study further demonstrates the close link between atmospheric reaction nitrogen chemistry and global nitrogen cycle.

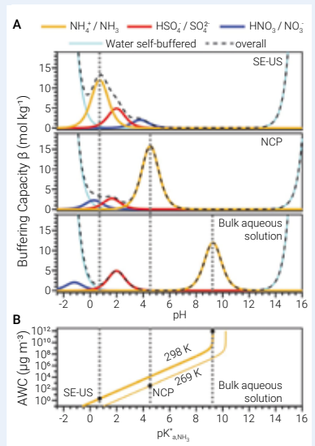

Figure 2: Multiphase buffer theory and buffering capacity for aerosol multiphase systems compared with bulk aqueous solution. (A) shows that an individual buffering agent can adopt different buffer pH values in aerosols and that aerosol pH levels in populated continental regions are widely buffered by the conjugate acid-base pair NH_4^+/NH_3 (ammonium/ammonia). (B) Dependence of the peak buffer capacity (pKa*) of NH_4^+/NH_3 on aerosol water content (AWC) and temperature.

"The broad theme of our research is to understand key processes that drive the formation and transformation of aerosols, and to elucidate and quantify the effects of atmospheric aerosols on air quality and climate."

UNVEILING THE THERMODYNAMICS AND MOLECULAR DYNAMICS OF PHASE TRANSITIONS IN HIGHLY SUPERSATURATED NANOPARTICLES

Phase transitions are of fundamental importance in aerosol research and materials science, but phenomena observed at the nanometer-scale are not yet fully understood. Our study on the "Size dependence of phase transitions in aerosol nanoparticles" (Nature Communications 2015) was the first to resolve nano-size effects on liquid-solid phase transitions of atmospheric aerosol particles with a new analytical technique (differential Köhler analysis) and including the inverse particle diameter in a multi-dimensional phase diagram. Such effects and new scientific tools are important to understand the fundamental properties and environmental impact of nanometer-sized particles in secondary aerosol formation as well as in the atmospheric transport and transformation of organic pollutants (Science Advances 2018). Towards a molecular level understanding of nano-size effects on phase transitions, we now have: (1) successfully developed a new nano-HTMDA system that can measure the hygroscopic growth of particles with diameters down to ~4nm (AMT 2020); (2) characterized the interaction of ~10nm NaCl nanoparticles with water by Atomic Force Microscopy (PCCP 2020); (3) explored the anomalies under supercooled and supersaturated conditions by molecular dynamic simulations (PCCP 2019).

GLOBAL OBSERVATIONS AND CLIMATE EFFECTS OF BLACK CARBON AEROSOLS

Black carbon (BC) is the most strongly light-absorbing component of atmospheric aerosols and one of the most important climate-warming agents. Estimations of its global radiative impact, however, are hampered by a lack of observational data, especially at high altitudes. Since 2014, I have initiated and continue to lead the international project CARIBIC-SP2, in which we perform single-particle measurements onboard a Lufthansa passenger aircraft. These measurements yielded a uniquely comprehensive dataset and unprecedented insights into the global distribution and properties of black carbon particles in the upper troposphere and lower stratosphere, which are not well constrained but crucial for the assessment and prediction of aerosol effects on climate change (Figure 3). Building on these data, our study "Strong impact of wildfires on the abundance and aging of black carbon in the lowermost stratosphere" (Proc. Natl. Acad. Sci. 2018) showed that BC particles from wildfires are frequently transported to the lower stratosphere where they can induce strong local heating and thus influence climate. As climate change is expected to increase the frequency and spread of wildfires, recording a present-day baseline will help to constrain model estimates of the radiative impact of BC on global climate change.

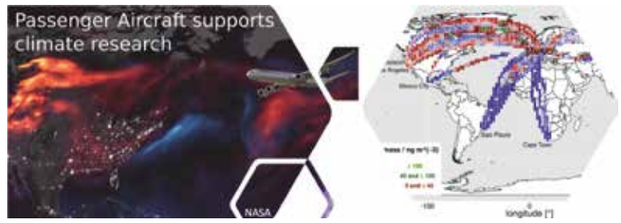

Figure 3: Global observation of black carbon and CARIBIC-SP2 project.

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NEAR-ROOM-TEMPERATURE SUPERCONDUCTIVITY AT HIGH PRESSURES

MIKHAIL EREMETS

Figure 1: In a diamond anvil cell, more than one million bars can be created between two conical cut diamonds, with hydrogen rich materials such as hydrogen sulfide or yttrium hydride becoming superconducting at relatively high temperatures.

INTRODUCTION

Is it possible to develop superconductors that operate at room temperature? Such a breakthrough would be no less revolutionary than the advances that led to electricity becoming broadly available two centuries ago. The ability to transfer electrical current without losses will obviously save large amounts of energy. The phenomenon of electricity continuing to flow in a superconducting ring even when the current source is switched off, will enable the development of new applications. For example, it is a way of storing energy that may replace accumulators. Superconducting coils create strong magnetic fields; therefore, superconducting magnets will become widespread and can be used for levitating trains, in motors, MRI scanners, accelerators, and nuclear fusion reactors. This is a dream that is now getting closer to reality.

For a long time, superconductivity was considered a low-temperature phenomenon. The first superconductor was mercury (Hg), which was discovered by Kamerlingh Onnes in 1911. Resistance sharply dropped to zero when Hg was cooled below a critical temperature (*Tc*) of 4.2 K. Gradually, other superconductors with higher *Tc* values were found.

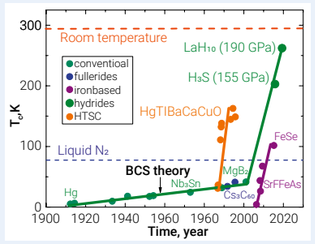

Figure 2: The evolution of high-temperature superconductivity since 1911. Green dots indicate conventional superconductors – materials that are described by the BCS theory from 1956. Orange dots indicate cuprates – a family of high-temperature superconductors. They superconduct above the temperature of liquid nitrogen (blue line). These unconventional superconductors are not described by the BCS theory. The magenta dots represent iron pnictide compounds.

Figure 2 shows the slow growth of record *Tc* values since 1911. Only in 1957 were Bardeen, Cooper, and Schrieffer (BCS) able to build a full theory of superconductivity. However, the BCS theory did not predict high *Tc* values near room temperature.

Recent research on conventional high-temperature superconductivity started with a focus on metallic hydrogen. As the main constituent of the gas giants Jupiter and Saturn, and thus the most common substance in our solar system, metallic hydrogen is an attractive candidate for such a role. In 1968, Neil Ashcroft provided qualitative arguments that metallic hydrogen can become a superconductor at high critical temperature: Since then the search for metallic hydrogen that would act a room-temperature superconductor and have other fascinating properties has been a 'Holy Grail' for many researchers. However, it remains a difficult theoretical and experimental problem as extreme high pressures of ~500 GPa are necessary. Further, measuring electrical and other properties of hydrogen in the tiny volumes of the diamond anvil cells (DACs) which are used to create high pressures is challenging. To circumvent the problem of high pressures, in 2004 Ashcroft proposed the remarkable idea of considering alloys of metallic hydrogen, for example, dense group-IVa hydrides (CH_4, SiH_4, etc.). Metallization of the hydrides should happen at much lower pressures in comparison to pure hydrogen, well within the capabilities of DACs. The reality, however, turned out to be more complex. The proposed group-IVa hydrides did not reveal substantial superconductivity.

"Our aim is to achieve room-temperature superconductivity"

RESULTS

We discovered superconductivity in hydrogen sulfide (H_2S) at high pressures ~150 GPa. The superconducting temperature of 200 K is far above that of other materials (Figure 2). The next big step towards room-temperature superconductivity was the discovery of superconductivity in hydrogen-rich lanthanum hydride (LaH_{10}) at a pressure of 170 GPa with *Tc* ~250 K, i.e., nearly at room temperature (Drozdov, Kong et al. 2019) (Somayazulu, Ahart et al. 2019) (Figure 3).

OUTLOOK

Our next candidate for room temperature 300 K superconductivity is yttrium hydride (YH_{10}), which is very similar to LaH_{10}. According to calculations, it should have a *Tc* value of ~300–330 K. We are currently trying to synthesize the YH_{10} phase. Ternary hydrides with three elements are even more promising candidates. For instance, superconductivity at 200 °C and a pressure of 250 GPa is predicted for Li_2MgH_{16}.

Practical applications require ambient pressure and temperature conditions. The success in achieving high *Tc* in H_3S – a covalent metal- clearly indicates prospect of other covalent-bond substances such as graphite, or fullerenes, diamond and many other carbon-based materials. They have the high phonon frequencies and electron–phonon coupling strengths required for high temperature superconductivity. They are intrinsically insulators, semiconductors, or semimetals but can be made metallic and superconducting by doping, i.e. through the introduction of impurities.

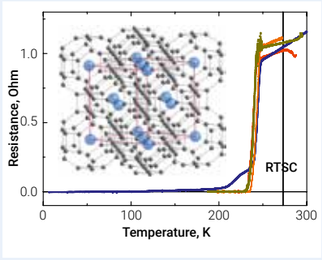

Figure 3: Superconducting transitions in lanthanum superhydride LaH_{10} measured in different samples shown with different colours. Below 250 K (-23 °C), electrical resistance drops to zero indicating a transition to a superconducting state. A vertical line drawn at 290 K marks the room temperature limit. The insert shows the structure of LaH_{10}: blue balls indicate positions of La atoms, small grey circles – hydrogen atoms. This structure can be considered to be metallic atomic hydrogen complemented with lanthanum.

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QUANTIFYING LONG-TERM CLIMATE CHANGE ON LAND

KATHRYN FITZSIMMONS – INDEPENDENT MAX PLANCK RESEARCH GROUP

Figure 1: L-R: a schematic 4D model for loess accumulation onto the Kazakh piedmont; continuous sampling by abseil in Tajikistan; first quantitative estimates of temperature change through time across Central Asia compared with the Greenland ice core framework.

Earth's climatic evolution over the last five million years – a period including the last time atmospheric carbon dioxide levels were comparable with those of today – is primarily understood from the perspective of marine mechanisms. While changes in ocean circulation go a long way towards explaining temperature modulation and the transport of moisture onto the continents, the role of terrestrial feedbacks in the opposite direction remains largely unexplored.

Our group aims to understand long-term climate dynamics in the centre of the world's largest continent, Eurasia. Central Asia is sensitive to the interplay between three major hemispheric climate systems: the temperate westerlies, tropical monsoons and the Siberian High-pressure system. Ongoing uplift of the Asian high mountain belts has driven aridification. To understand the interaction between these influences, we focus on the hitherto unrecognised potential of widespread, thick blankets of wind-blown dust – loess – as archives for past change. Long sequences of primary loess and their soils record responses to past climate, since dust accumulation intensifies during cold phases of glacier advance, and decreases with soils forming under milder conditions. In cooperation with the Climate Geochemistry Department, we apply and develop innovative new toolkits to quantitatively reconstruct past conditions from proxies embedded within the loess.

A reliable chronological framework is essential for accurate comparison with global climate records. Our age models combine multiple techniques with a focus on luminescence dating. This method measures the time elapsed since sediments were last exposed to sunlight, by means of radiation stored within the defects of quartz and feldspar crystal lattices. We used dating of multiple sites along the Central Asian piedmont to create a 4D model for loess accumulation, augmented by climate reanalysis and remote sensing of aeolian systems. We identified high-resolution deglacial loess records which enable us to model fluctuating intensities of westerly airflow through time, at the eastward margins of its influence. In addition, we are extending the applications of luminescence by investigating paramagnetic defect centres in quartz as a proxy for the origins of mineral dust.

We use stable isotope geochemistry to analyse long-term changes in precipitation and temperature. Carbonates precipitate within loess in a range of different forms. We reconstructed the last five Myr of rainfall variability based on soil carbonates from a long loess sequence in southeast Kazakhstan and quantified palaeotemperatures using clumped isotope analysis. The Charyn Canyon record highlights the long-term contribution of temperate Eurasian systems to the modulation of moisture transfer into the northern hemisphere oceans and back onto land via the westerlies, providing a missing terrestrial link within long-term global climate. Additionally, we are reconstructing temperature and precipitation from stable isotope analysis of earthworm calcite granules at high resolution to a last glacial loess sequence in the Rhine valley and investigating the applicability of calcitic root cells as palaeothermometers in Chinese loess.

Organic geochemistry provides a novel tool for quantifying past temperature and soil pH in loess, via climate-sensitive compounds deriving from bacterial lipids and plant waxes. We have developed the first biomarker calibration dataset for the semi-arid mid-latitudes. Our results so far suggest that dryland conditions influence compound distributions differently from humid environments. These insights provide the foundations for millennial-scale palaeoclimate reconstruction in loess from Kazakhstan and Tajikistan.

We are also reconstructing vegetation cover and seasonality through time by means of pollen-based modeling. This work is the first of its kind to account for differences in pollen production rates, which are considerable in the Central Asian steppe.

Our group was established in early 2017 and has so far conducted five major (and several smaller) field campaigns to Kazakhstan and Tajikistan. Continuous sampling by abseil enables the generation of records comparable with those generated from marine and ice cores. Although our fieldwork is complete, restrictions associated with COVID-19 delayed the completion of several major datasets and proxy development, and has consequently stalled publication of our main results.

Figure 2: Five Myr of climate change in Central Asia (Prud'homme et al., in review): (A) sedimentation rate, (B) soil carbonate $d^{13}C$, (C) $d^{18}O$/clumped isotope thermometry. Sea-surface temperatures from north (D) and subarctic (E) Atlantic.

"We generate long-term quantitative data for continental Eurasia, providing a terrestrial counterpart to marine and ice core records"

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PINPOINTING NO_X EMISSIONS FROM SPACE

THOMAS WAGNER

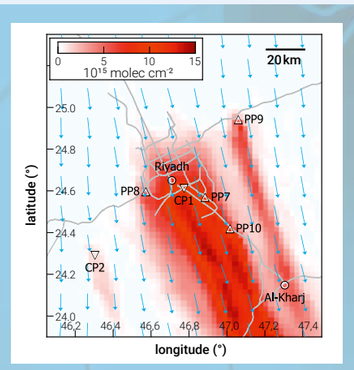

Figure 1: Tropospheric NO_2 column over the Saudi Arabian capital Riyadh as derived from TROPOMI for a single overpass on December 17, 2017. Arrows indicate ECMWF wind vectors at 450 m above the ground. Symbols mark urban centers (o), power plants (Δ) and cement plants (∇).

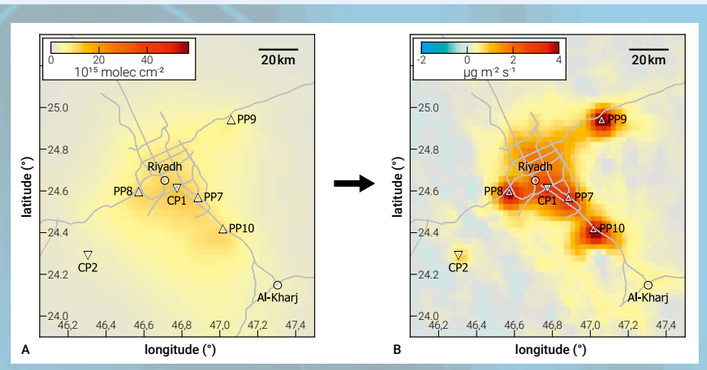

Figure 2: (A) Average NO_2 vertical column densities (VDCs) over Riyadh from TROPOMI measurements from December 2017 to October 2018. (B) NO_x emissions derived using the novel divergence method. Figure adapted from Beirle et al., 2019.

The research activities of the Satellite Remote Sensing Group focus on the exploitation of the spectral information gathered from ultraviolet/visible satellite instruments such as the Global Ozone Monitoring Experiment (GOME), and the recently launched TROPOMI sensor on the Sentinel 5 Precursor satellite (S-5P) with unprecedented spatial resolution.
Nitrogen oxides ($NO_X \equiv NO + NO_2$) are key components in urban pollution, as they negatively affect human health and control ozone production. Accurate and up-to-date NO_X emission data with high spatial resolution are thus a prerequisite for improving the power of regional atmospheric chemistry models to predict air quality.
Since the mid-1990s, NO_2 tropospheric columns derived from satellite measurements have provided an independent source of information on the spatial distribution and of tropospheric NO_2 levels and trends on a global scale, with spatial resolution of some hundreds (GOME) to tens (OMI) of km. In October 2017, the TROPOspheric Monitoring Instrument (TROPOMI) was launched on the S-5P satellite of the European Space Agency (ESA). TROPOMI measurements are characterized by high signal-to-noise ratios and unprecedented spatial resolution (up to $3.6 \times 5.6\,km^2$), thereby ushering in a new era and opening up new research vistas. For instance, individual strong power plant exhaust plumes can be directly mapped by single TROPOMI overpasses (Figure 1). However, to also identify and quantify weaker point sources, several satellite observations have to be averaged. Due to changing wind patterns on different days, the commonly applied procedure of temporally averaging the measured tropospheric NO_2 columns leads to a substantial degradation of the high spatial resolution (Figure 2a). To make full use of the high spatial resolution of TROPOMI, we developed a de-convolution approach taking into account the specific wind patterns of individual days. This novel approach acts like a magnifying glass which makes the underlying emission sources visible (Figure 2b).

A NEW APPROACH: DERIVING NO_X EMISSIONS FROM THE DIVERGENCE OF THE FLUX

Instead of averaging the tropospheric NO_2 columns themselves, first the corresponding NO_2 fluxes are calculated from the tropospheric NO_2 columns combined with European Centre for Medium-Range Weather Forecasts (ECMWF) wind fields. In a second step, the individual flux maps are averaged. Then, the divergence of the averaged flux is calculated. According to the continuity equation for the steady-state, the divergence of the flux directly yields the sources and sinks of NO_X (Beirle et al., 2019).
The sink term can be directly estimated from the TROPOMI column observations (assuming a first-order chemical loss) and added to the divergence of the flux, finally yielding the total NO_X emissions (with assumptions about the NO_2/NO_X ratio). As the NO_X flux strongly increases above a point source no matter where the wind is coming from, the divergence (i.e., spatial derivative) of horizontal fluxes proves to be highly sensitive for point sources. Thus, NO_X emissions from individual power plants can be clearly resolved even against the background of considerably high urban pollution from the Saudi Arabian capital city Riyadh, as shown in Figure 2b. By fitting a Gaussian function to the peaks in the emission maps, individual point sources were quantified with a detection limit of about 0.03–0.11 kg/s. Meanwhile, we have also applied the method globally and derived a catalog of NO_X point sources (Beirle et al., 2020). The catalog lists 451 locations which could be clearly identified as NO_X point sources by our fully automated algorithm, while ambiguous cases as well as area sources such as megacities are skipped. Out of these point sources, 242 could be automatically matched to power plants from an open access database. Besides power plants, the NO_X point sources listed in the catalog also represent metal smelters, cement plants, and industrial areas. The derived emissions in our new point source catalogue can also be used to compare the level of power plant technology and emission control efforts. The results in Figure 3 indicate large differences in NO_X emissions from power plants in different parts of the world.
Since point sources of NO_X and CO_2 are often connected, the new catalogue can also be used to improve the CO_2 emission inventories from satellite observations.

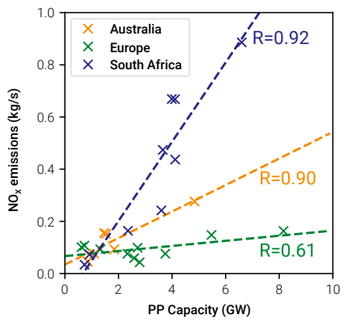

Figure 3: Correlation between power plant capacity (Global Power Plant database, World Resources Institute) and NO_X emissions (from our new point source catalog) for coal-fired power plants.

OUTLOOK

Our global catalog gives us the unique possibility of investigating the effect of point source emissions on atmospheric chemistry. Such effects will be investigated in detail in cooperation with the Modeling Group from the Atmospheric Chemistry department at the MPIC. Fundamental questions that will be addressed include the dependence of the NO_X lifetime on distance from a point source, which provides information on NO_X loss processes, i.e. OH concentrations.
The Korean GEMS satellite, launched at the beginning of 2020, is the first next-generation UV/vis satellite instrument to be operated on a geostationary platform. Together with its American and European 'sister instruments' it will, for the first time, enable investigations of diurnal cycles from space. With satellite observations available hourly, also temporal changes can be tracked and our new divergence method could be applied on a daily basis.

"Novel satellite sensors provide unprecedented spatio-temporal resolution."

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ACKNOWLEDGEMENTS

TROPOMI NO_2 data is provided by ESA and the Royal Netherlands Meteorological Institute KNMI.
The Global Power Plant database is provided by the World Resources Institute.

JOINT SERVICES

Administration, information technology, instrument development and electronics, workshops, facility management, and communications.

ASSIST AND MAINTAIN

Administration, information technologies (IT), instrument development and electronics, mechanical workshops, facility management, and communications: these Joint Services assist the scientific research departments and groups in practical aspects of the day-to-day running of the MPIC and maintain the Institute's infrastructure as well as its interactions with the outside world.

ADMINISTRATION

We provide economic, legal, and organizational support for the research at the Max Planck Institute for Chemistry. This involves the personnel administration of approximately 350 employees, implementation and monitoring of procurement policies, administrative execution of projects and third-party funding, bookkeeping and management of the Institute's budget, and travel expense accounting. The administration is organized into Human Resources, Purchasing and Finances. All provision and support facilities, including the facility management, are associated with the Institute's administration.

INFORMATION TECHNOLOGIES (IT)

The IT group ensures the smooth operation of the IT infrastructure of the Institute in Mainz and also provides support to other institutions such as the Global Fire Monitoring Center in Freiburg. The IT group comprises six employees who support all users with over 1,000 clients and network devices and a wide range of operating systems. Our team manages all physical and virtual servers necessary for work at the MPIC as well as servicing and network installations. Major projects in the last three years include migrating all administrative workplaces to virtual workplaces as a pilot project of the Max Planck Society, exchanging the central virus scanner and, jointly with the Institute's facility management, migrating the Institute's telephone system to Voice over Internet Protocol (VoIP).

In 2018, the IT group supported MPIC researchers during the CAFE-AFRICA aircraft mission locally on Sal, Cape Verde, and also equipped the *S/Y Eugen Seibold* research yacht with a satellite navigation and communication system. A specially designed router integrates the data from the navigation system, the scientific systems, and the logbook of *S/Y Eugen Seibold* in a uniform protocol. This system, unique worldwide, allows easy processing and referencing of all scientific data and is continuously developed and optimized in accordance with scientific needs.

Since 2013, we have been supporting research at the Amazon Tall Tower Observatory (ATTO) in the Brazilian rainforest. Due to ATTO's remote location, a reliable internet connection is prerequisite. The diverse research locations – be it the open ocean or the rainforest – pose special challenges for IT staff and material due to their IT-hostile environments.

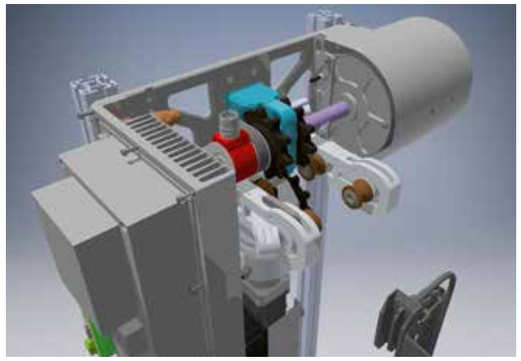
Another major challenge to be met was the sudden increase in need for mobile workplaces caused by the COVID-19 pandemic and handling the high number of support requests. Since the beginning of 2020, the IT group has mostly been working from home and is increasingly relying on an electronic ticket system to provide support to users. The group was, however, also active outside the Institute during the lockdown: For instance, in May 2020 we successfully put in place a functioning IT infrastructure for the BLUESKY aircraft measurement campaign.

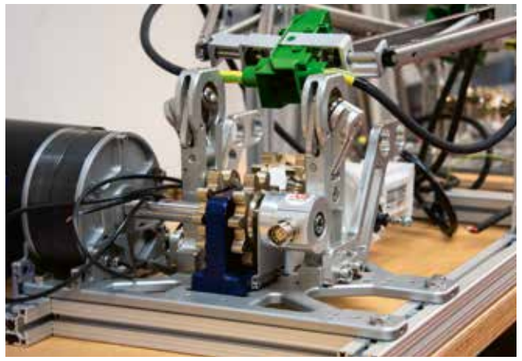
INSTRUMENT DEVELOPMENT AND ELECTRONICS

Scientific projects and missions such as HALO, ATTO, or CAFE require instrumentation for precise measurements that are typically not commercially available or which must be modified. These instruments have to comply with stringent requirements, for usage on board of satellites, aircraft, or ships. The Instrument Development and Electronics Group develops and produces electronic components, process controllers and system-to-application level software. Five staff members and two to four trainees discuss specific instrumentation needs such as air or water inlet systems for analytical instruments with scientists, engineers, and workshop staff, which are then developed and produced in-house.

Professional CAD software, the latest software development environments and unique infrastructure such as a fully automated surface mount dispense-, pick-and-place-system, an anechoic electromagnetic interference (EMI) testing chamber and special tools such as a small CNC milling machine, micro welding machine, and a bending bench enables us to design, produce, and verify custom electronic and electro-mechanical systems and components at a professional level.

A wide range of key projects realized in the last three years demonstrates the versatility of the group: For example, we developed and implemented fully automated peak integration software for a fast aircraft gas chromatograph/mass spectrometer (SOFIA), constant pressure/constant temperature gas and aerosol inlet systems for two aerosol and chemical ionization mass spectrometers (AMS, ALABAMA, PTR-TOF); control hard- and software for a Fast Aerosol Sizer; a controller for a butanol recycling system for a condensation nuclei counter; a family of more than ten differential optical absorption spectrometer (DOAS) units operating autonomously around the world and mechanics, and electronics for a gradient measurement elevator platform to be installed on the ATTO research tower.





FACILITY MANAGEMENT

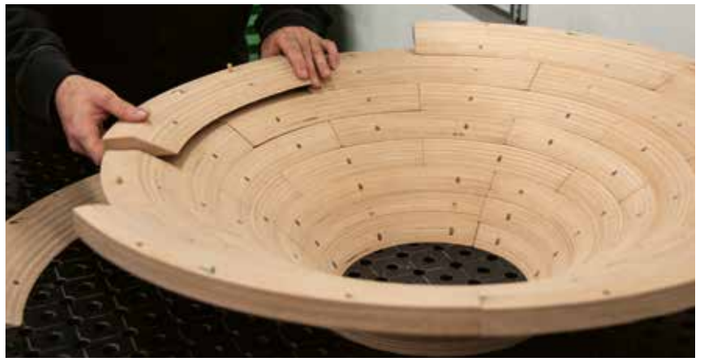
We maintain the Institute's infrastructure and take care of all building equipment including the high-tech ventilation and temperature control systems for laboratories and clean rooms. As a team, we are also committed to establishing and maintaining a proper working environment by assuming responsibility for areas ranging from general caretaker services to the inspection of all electrical equipment. In addition, our unit is also responsible for the reception desk and the receipt of goods.

MECHANICAL WORKSHOP

The mechanical workshop currently comprises 14 employees and contributes to the development of scientific instruments as well as to the maintenance of the Institute's infrastructure, closely collaborating with researchers, the instrument development and electronics group, and the facilities management. Highly qualified workshop staff perform a wide range of operations, such as welding of high-quality materials, bracing of special metals, and electroplating. New technologies such as 3D printers are being used for additive production of light and high-complexity workpieces that cannot be realized with conventional CNC machines.

Some highlights from recent years are:

- High-pressure research (Eremets group): Increasing numbers of precise diamond anvil cells are being manufactured. The CNC lathe guarantees precision in the 1/1000 mm range with the highest repeat accuracy. The cells are then finished with a precise fit ("0 game") in a manual production process.
- HALO: An highly complex camera for condensation particles (FIMS) was produced in close cooperation with the instrument development and electronics team.
- ATTO: The workshop produced the essential machinery components for the 325-m-high elevator. An employee of the workshop then installed the manufactured components at ATTO.
- COVID-19 community masks and air ventilation: Cutting devices for filter materials were manufactured and, most recently, a wooden deep-drawing mold was developed for the production of plastic ventilation funnels. The air extraction funnels are being installed in a school classroom in Mainz as part of a COVID-19 pilot project.
- The workshop is constantly building components to improve the laboratory equipment on board the *S/Y Eugen Seibold* as well as for the MoLa Mobile Laboratory (Drewnick group) that are commercially not available.



The Institute has been training apprentices in the mechanical workshop since 1949. Currently nine apprentices not only craft practice pieces, they also carry out practical machine-based tasks for the scientific departments. In addition, they are trained in CNC techniques, pneumatics/hydraulic systems, and welding technology, partly through attending inter-institutional courses. The technicians, who train for their qualification in the instrument development and electronics group, are also provided with a basic education in metal techniques.

COMMUNICATIONS

The Institute's communications and outreach group promotes and supports the overall MPIC research mission. The group of seven is not only responsible for public and media relations, but also offers several internal services to facilitate research at the Institute. Thus, the graphics office helps developing scientific illustrations and provides photos and animations, the library assists with literature search, and the international office supports new scientists and their families with matters such as applying for residence permits or settling in Germany. Furthermore, the communications group assists with seminar and event organization such as ESRP meetings and scientific lectures.

The Institute's outreach activities are directed at the media and the public in equal measure, through dissemination of press releases and information on digital media platforms, interacting with the public and showcasing our research at exhibits at local events, and opening the Institute to public visits. The Institute for instance offers internships for secondary school students and hosts several groups of visitors every year, including school children. We also participate in the nationwide Girls' Day that aims to encourage girls to enter scientific and technical professions.

In terms of public outreach, the Institute regularly presents its research activities to a broad audience, including the inhabitants of Mainz and the surrounding area. We are an active partner of the Mainzer Wissenschaftsallianz (Mainz Research Alliance) that aims at strengthening Mainz as a center of scientific activity by fostering the networking of the universities, scientific institutions, and companies and by outreach activities. Thus, many Institute members participate in events of the Wissenschaftsallianz by giving talks in the lecture series "Meenzer Science Schoppe" in local pubs or in the annual science fair (Mainzer Wissenschaftsmarkt) in the city center.

In 2018, several researchers were engaged in the central Max Planck Day in Munich where they presented an interactive videowall with our latest research campaigns and, at the same time, in a photo tour at our Institute and the neighboring Max Planck Institute for Polymer Research. The photo tour aimed at providing amateur photographers research insights and resulted in a fascinating picture exhibition that was also presented in the Rhineland-Palatinate Ministry for Education, Science, Youth and Culture. In 2019, the two Max Planck Institutes organized a family day. In 2020, however, outreach activities were heavily impacted by the COVID-19 pandemic. Formats such as the annual science fair and also internships had to be cancelled or could take place only in hybrid formats.

In terms of media outreach, from 2018 to present, we have published 56 press releases. The press releases have resulted in numerous articles and reports in national and international newspapers, magazines, and radio and television reports.

The Max Planck Institute for Chemistry is a member of two organizations which are active in climate change communication: The Deutsches Klima-Konsortium (DKK, www.deutsches-klima-konsortium.de) and the Klimanavigator (www.klimanavigator.eu). The mission of both platforms is to provide the media, educational institutions, and society with information on climate research in order to contribute to a better understanding of climate change.

STAFF AND BUDGET

In December 2019, a total of about 350 persons were employed at the Institute, among them 117 scientists, 57 PhD students and 14 technical trainees. 37% of the staff were female, 63% male.

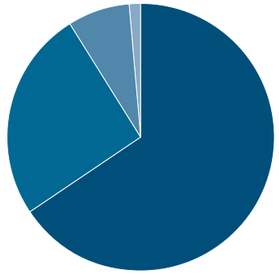
270 staff members were paid from institutional funds, 27 scientists received payment from third-party project funding, 38 from scholarships and 7 by graduate schools.

The annual budget of the Institute is approximately € 26 million. A major fraction derives from MPG institutional funds provided by federal and state governments. An overview of revenues and expenditures is given below.

The Institute has been certified according to the "berufundfamilie" audit. The audit supports companies and organizations in their efforts to implement a family-friendly personnel policy. As a strategic management tool, it serves to facilitate the compatibility of work and family. In accordance with the principles of the Max Planck Society, the Max Planck Institute for Chemistry supports its employees in their diverse life models. We offer family-friendly working conditions for both men and women.

REVENUES 2019

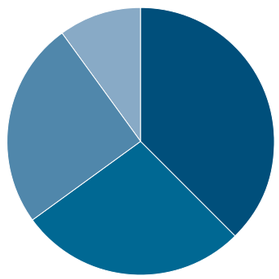
Percentage distribution excluding construction activities.



- **65.6%** MPG institutional funds
- **25.7%** MPG project funds
- **7.5%** Third-party funds
- **1.2%** Institute´s own income

EXPENDITURES 2019

Percentage distribution excluding construction activities.



- **37.7%** Personnel
- **27.5%** Materials
- **24.9%** Support of junior scientists
- **9.9%** Investments

GLOSSARY

ACCLIP
Asian Summer Monsoon Chemical and Climate Impact Project

ACRIDICON-CHUVA
Aerosol, Cloud, Precipitation, and Radiation Interactions and Dynamics of Convective Cloud Systems – Cloud processes of the main precipitation systems in Brazil: A contribution to cloud resolving modeling and to the GPM (GlobAl Precipitation Measurement)

AFPs
Antifreeze proteins

ALABAMA
Aircraft-based Laser ABlation Aerosol MAss spectrometer

AMA
Asian Monsoon Anticyclone

AMAZE
AMazonian Aerosol characterizAtion Experiment

AMOC
Atlantic Meridional Overturning Circulation

AMS
Aerosol mass spectrometer

AOU
Apparent Oxygen Utilization

APACHE
Low-pressure flow tube system

AQABA
Air Quality and climate change in the Arabian Basin

ATAL
Asian Tropopause Aerosol Layer

ATIs
Amylase trypsin inhibitors

ATLAS
Atlas Mountain Experiment in Marocco

ATTO
Amazon Tall Tower Observatory

AWC
Aerosol water content

AWI
Alfred Wegener Institute

BCO
Barbados Cloud Observatory

BCS
Bardeen, Cooper, and Schrieffer

BLUESKY
Examinations of the atmosphere during the Coronavirus lockdown

BOYAN
Biogenic HONO Yield and Atmospheric Nitrogen model

C-ToF-AMS
Compact time-of-flight aerosol mass spectrometer

CAABA/MECCA
Chemistry As A Boxmodel Application/Module Efficiently Calculating the Chemistry of the Atmosphere

CAFE-AFRICA
Chemistry of the Atmosphere Field Experiment – Africa

CAFE-BRAZIL
Chemistry of the Atmosphere Field Experiment – Brazil

CAFE-EU
Chemistry of the Atmosphere Field Experiment – Europe

CALIOP
Cloud-Aerosol Lidar with Orthogonal Polarization

CALIPSO
Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations

CARIBIC
Civil Aircraft for Regular Investigation of the atmosphere Based on an Instrumentation Container

CARIBIC-SP2
CARIBIC single particle soot photometer

CCN
Cloud condensation nuclei

CDOM
Colored dissolved organic matter

CERN
European Council for Nuclear Research

CLOUD
Cosmic Leaving Outdoor Droplets

COPAS
COndensation PArticle counting System

COVID-19
Coronavirus disease 2019

CTD
Conductivity, temperature, depth sensor

DACs
Diamonds anvil cells

DAMPs
Damage-associated molecular patterns

DFG
Deutsche Forschungsgemeinschaft (the self-governing organisation for science andresearch in Germany)

DKRZ
Deutsches Klimarechenzentrum (German Climate Computing Center)

DLR
Deutsche Zentrum für Luft- und Raumfahrt (German Aerospace Center)

DOAS
Differential Optical Absorption Spectrometer

DOC
Dissolved Organic Carbon

DSDP
Deep Sea Drilling Project

EARS
East African Rift System

ECMWF
European Centre for Medium-Range Weather Forecasts

EMAC
ECHAM/MESSy for Atmospheric Chemistry

EMeRGe
Effect of megacities on the transport and transformation of pollutants on the regional and global scale

EMeRGe-Asia
Effect of megacities on the transport and transformation of pollutants on the regional and global scale – Asia

EMeRGe-EU
Effect of megacities on the transport and transformation of pollutants on the regional and global scale - EU

ENSO
El Niño–Southern Oscillation

EPFR
Environmentally persistent free radicals

ERICA
ERc Instrument for Chemical composition of Aerosols

ESA
European Space Agency

ESRP
Earth and Solar System Research Partnership

EU
European Union

EUREC4A
Elucidating the role of clouds-circulation coupling in climate

Excimer
Short for excited dimer

ε
Efficiency

FAAM
Facility for Airborne Atmospheric Measurements

FRRf
Fast-Repetition-Rate fluorometer

GC-MS
Gas chromatography-mass spectrometry

GCE
Galactic chemical evolution

GEMS
Geostationary Environment Monitoring Spectrometer

GeoReM
Geological and Environmental Reference Materials

GEOROC
Geochemistry of Rocks of the Oceans and Continents

GLORIA
Gimballed Limb Observer for Radiance Imaging of the Atmosphere

GoAmazon2014/5
Green Ocean Amazon Experiment 2014/2015

GOME
Global Ozone Monitoring Experiment

HALO
High Altitude and Long Range Research Aircraft

HALOHOLO
Instrument for cloud particle holography developed for installation on HALO

HeLa
An immortal cell line

HMGB1
High-mobility-group box 1 protein

HSP60
Heat shock protein 60

HTMDA
Hygroscopic tandem differential mobility analyser

IAGOS-CARIBIC
In-service aircraft for a global observing system – Civil Aircraft for the Regular Investigation of the Atmosphere Based on an Instrument Container

IgE
Immunglobulin E

IL
Interleukin

IMPACT
Ion–Molecule Processes for Analytical Chemistry Technologies. EU funded project (Horizon2020)

IN
Ice nuclei

IPA
Institute of Atmospheric Physics

ISORROPIA
Thermodynamic equilibrium aerosol model, "equilibrium" in Greek

ITCZ
Intertropical Convergence Zone

IUPAC
International Union of Pure and Applied Chemistry

JGU
Johannes Gutenberg University Mainz

KNMI
Royal Netherlands Meteorological Institute

LA-ICP-MS
Laser ablation inter-coupled plasma mass spectrometry

LAMS
Laser ablation mass spectrometer

LPS
lipopolysaccharide

LS
Lower stratosphere

MCGA
Monte Carlo genetic algorithm

MECO
Mid-Eocene Climate Optimum

MetDB
Meteorite Database

ML-CIRRUS
Formation, Lifetime, Properties and Radiative Impact of Mid-Latitude Cirrus Clouds

MoLa
Mobile Laboratory

MOM
Mainz Organic Mechanism

MOZAIC/IAGOS
Measurement of OZone by Airbus In-service aircraft/ In-service Aircraft for a Global Observing System

MPG
Max Planck Society

MPI-SHH
Max Planck Institute for the Science of Human History

MPIC
Max Planck Institute for Chemistry

MRI
Magnetic resonance imaging

MWP
Melt Water Pulse

NAMIP
Nano- and Microparticle Research

NanoSIMS
Secondary ion mass spectrometer with <100 nm spatial resolution

ND-MAX
NASA/DLR-Multidisciplinary Airborne eXperiments

Nd:YAG
Neodymium-doped yttrium aluminum garnet

nm
Nanometer

NOAA
National Oceanic and Atmospheric Administration

NOPR
Net ozone production rate

NPF
New particle formation

NSF/UCAR
National Science Foundation/University Corporation for Atmospheric Research

NSF/UCAR HIAPER GV
A highly-modified Gulfstream V business jet

OMI
Ozone monitoring instrument

OMO
Oxidation Mechanism Observations

PAR
Photosynthetic active radiation

PCD
Particle Chemistry Department

pCO_2
Partial pressure of CO_2

PD
Private lecturer

PetDB
Petrological Database of the Ocean Floor

PETM
Paleocene-Eocene Thermal Maximum

Phl p5
Major grass pollen allergen

PM10
Particulate matter with diameters smaller than 10 µm

POPs
Persistent organic pollutants

ppb/h
Parts per billion per hour

ppbv
Parts per billion volume fraction

ppt
Parts per trillion

PRR
Pattern recognition receptors

PTR-ToF-MS
Proton-transfer-reaction time of flight mass spectrometry

S-5P
Sentinel 5 Precursor satellite

S/Y Eugen Seibold
Sailing yacht Eugen Seibold

S2FS
Size-resolved single particle fluorescence spectrometer

SAL
Saharan Air Layer

SARS
Severe acute respiratory syndrome

SARS-CoV-2
Severe acute respiratory syndrome coronavirus 2

SCOUT-AMMA
Stratosphere-Climate links with emphasis On the UTLS – African Monsoon Multidisciplinary Analyses

SOA
Secondary organic aerosol

SPURT
SPURenstofftransport in der Tropopausenregion (trace gas transport in the tropopause region) 2001-2003

SR
Aerosol backscatter ratio

StratoClim
Stratospheric and upper tropospheric processes for better climate predictions

Tc
Critical temperature

TEX86
An organic paleothermometer

THP-1
A human monocytic cell line

TINA
Twin-plate Ice Nucleation Assay

TLR4
Toll-like receptor 4

TNF-α
Tumor necrosis factor α

TROCCINOX
TROpical Convection, Cirrus and Nitrogen OXides experiment

TROPOMI
TROPOspheric Monitoring Instrument

TTL
Tropical tropopause layer

UHSAS
Ultra High Sensitivity Aerosol Spectrometer

ULTRACHIRAL
Ultrasensitive chiral detection by signal-reversing cavity polarimetry
EU funded project (Horizon2020)

US
United States

UTLS
Upper troposphere/lower stratosphere

UV/vis
Ultraviolet/visible

VDCs
Vertical column densities

VOCR
Volatile organic compound reactivity

wt%
Weight %

ZOTTO
Zotino Tall Tower Observatory in the Siberian taiga

α-Syn
α-synuclein

$\delta^{15}N$
Isotopic signature, measure of the ratio of stable isotopes ^{15}N and ^{14}N

$\delta^{18}O$
Isotopic signature, measure of the ratio of stable isotopes ^{18}O and ^{16}O

$\delta^{13}C$
Isotopic signature, measure of the ratio of stable isotopes ^{13}C and ^{12}C

ELEMENTS AND CHEMICAL COMPOUNDS

^{16}O
Oxygen isotope

^{18}O
Oxygen isotope

^{24}Mg
Magnesium isotope

^{25}Mg
Magnesium isotope

^{26}Mg
Magnesium isotope

^{28}Si
Silicon isotope

^{29}Si
Silicon isotope

^{60}Fe
Iron isotope, radioactive

Ar
Argon

ArF
Argon fluoride

BC
Black carbon

$CaCO_3$
Calcium carbonate

CH_4
Methane

Cl radicals
Chlorine radicals

$ClNO_2$
Nitryl chloride

CO
Carbon monoxide

CO_2
Carbon dioxide

Fe
Iron

H
Hydrogen

H_2O
Water

H_2O_2
hydrogen peroxide

H_2S
Hydrogen sulfide

H_3S
Sulfonium

HCH
Hexachlorocyclohexane

Hg
Mercury

HNO_3
Nitric acid

HO_2
Hydroperoxy radical

HONO
Nitrous acid

IEPOX
Isoprene epoxydiols

LaH_{10}
Lanthanum hydride

Li_2MgH_{16}
Example for ternary hydrides

Mg
Magnesium

MSAM
Methane sulfonamide

N
Nitrogen

N_2
Nitrogen

N_2O_5
Dinitrogen pentoxide

NaCl
Sodium chloride

NH_3
Ammonia

NH_4^+/NH_3
Ammonium/ammonia ratio

NMHC
Non-methane hydrocarbons

NO
Nitric oxide

NO_2
Nitrogen dioxide

NO_3
Nitrate radical

NO_3^-
Particulate nitrate

NO_X
Nitrogen oxides;
$= NO + NO_2$

NO_Y
Total reactive nitrogen

NO_Z
$= NO_Y - NO_X$

O_2
Oxygen

O_3
Ozone

OH
Hydroxyl

PAHs
Polycyclic aromatic hydrocarbons

PAN
Peroxyacyl nitrate

PCB
Polychlorinated biphenyls

RNO_X
Organic nitrate

RNS
Reactive nitrogen species

RO_2
Organic peroxy radicals

ROS
Reactive oxygen species

Si
Silicon

SiH_4
Silane

SO_2
Sulfur dioxide

VOCs
Volatile organic compounds

YH_{10}
Yttrium hydride

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