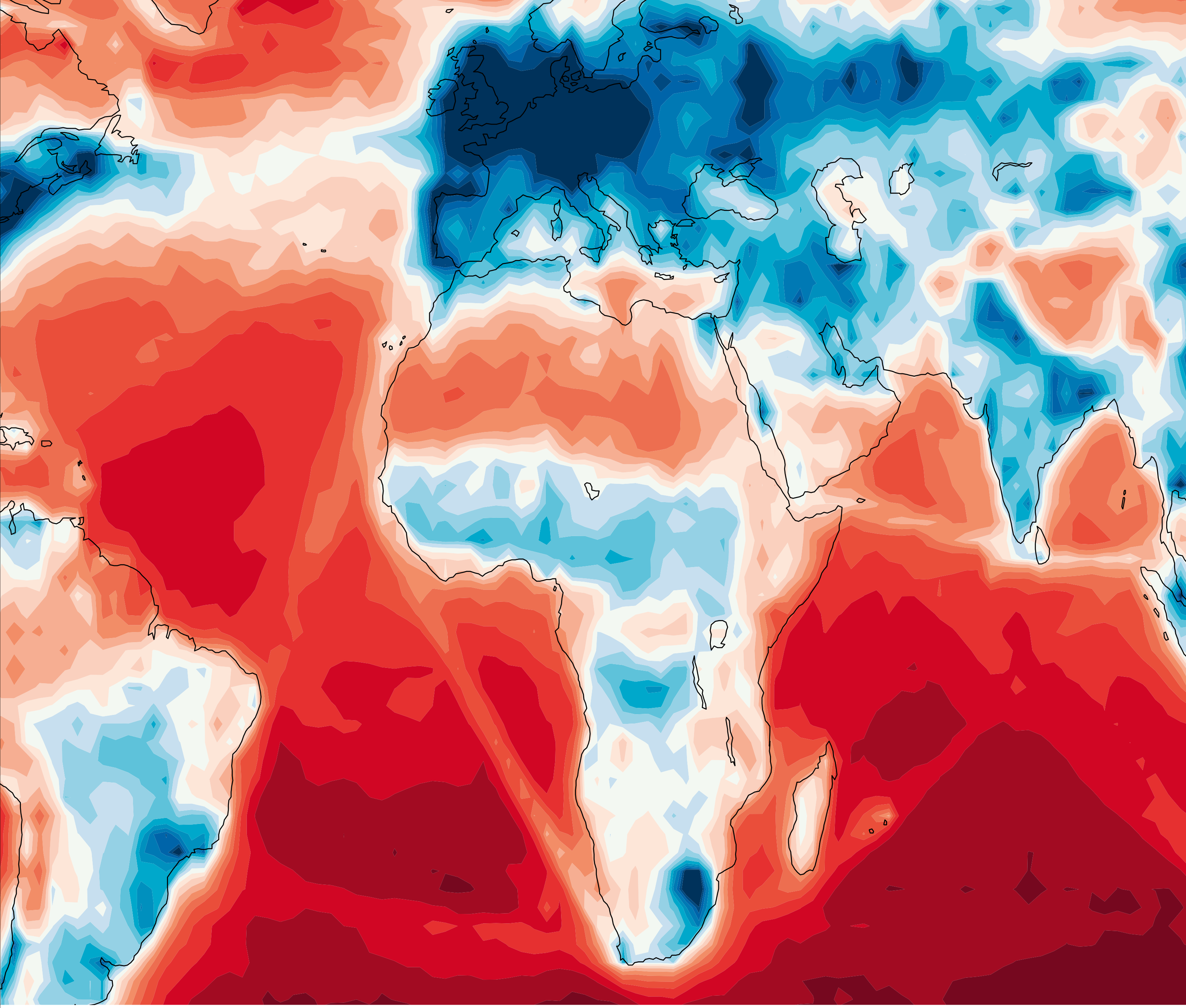


SCIENTIFIC REPORT 2021–2023

Max Planck Institute for Chemistry
(Otto Hahn Institute)

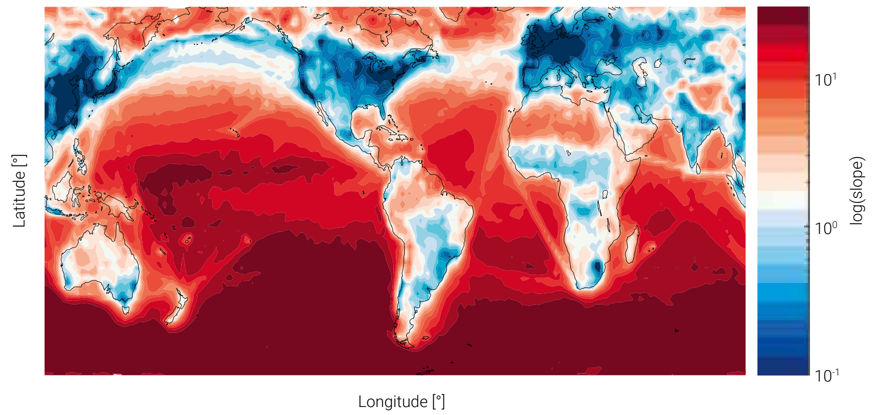
MAX PLANCK INSTITUTE
FOR CHEMISTRY

MAX PLANCK INSTITUTE
FOR CHEMISTRY

Atmospheric Chemistry · Climate Geochemistry · Multiphase Chemistry · Particle Chemistry

SCIENTIFIC REPORT 2021–2023

CONTENT



Cover picture:
Overview of O_3 sensitivity towards its precursors NO_x and VOCs at the surface based on data simulated by the EMAC model. Blue colors present VOC-sensitive and red colors show NO_x-sensitive O_3 chemistry, as indicated by the new metric $\alpha(CH_3O_2)$ in dependence of ambient mixing ratios of NO (color-code according to resulting slope). Please find details on the metric $\alpha(CH_3O_2)$ and how it characterizes O_3 sensitivity on page 36 (Adapted from Figure S13 in Nussbaumer et al., 2023, doi:10.5194/acp-23-12651-2023-supplement).

PREFACE

In the spring of 2023, Patrick Cramer, the newly elected President of the Max Planck Society, paid us a visit as part of his extensive tour of Max Planck Institutes and research facilities. During his address to the staff, he elucidated the three core principles of the Max Planck Society: a commitment to excellent research, a distinctive approach emphasizing "people over programs", and the cultivation of a feeling of belonging and togetherness within the Max Planck Society.

He encouraged us to reemphasize the importance of networking and scientific exchange, particularly in light of the restrictions imposed by the COVID-19 pandemic. He stressed that by fostering these connections, we could facilitate the emergence of novel ideas and the acquisition of knowledge that would benefit all.

During the speech and based on the questions raised, I sensed a focused atmosphere in the room, accompanied by a sense of pride. Patrick Cramer underscored the significance of our research areas, indicating a solid commitment to the continued pursuit of Earth system research in Mainz. In doing so, he also shed light on the future of the institute, especially as two of the four directors, myself included, are set to retire in 2025.

We have initiated early planning for successor appointments to ensure the institute's future and facilitate seamless transitions. I am confident that we will be able to attract two outstanding young researchers who will make substantial contributions to the institute's scientific endeavors and set new trends. Their responsibilities will involve reshaping the departments of Atmospheric Chemistry and Particle Chemistry. They will find a superbly functioning institute with a motivated and dedicated staff.

Nevertheless, the previous report highlighted the challenges of predicting the future. When I penned the foreword for the previous Scientific Report in December 2020, it could not be foreseen that the COVID-19 pandemic would persist for another two years. The conflicts in Ukraine and the Middle East and their profound political, economic, and social ramifications were even more unforeseeable. The global landscape has grown increasingly complex.

The passing of our esteemed colleague and Nobel Laureate, Paul Crutzen, in February 2021, was another significant moment. Paul would undoubtedly find satisfaction in knowing that the term he coined, "the Anthropocene", to describe the human-influenced era of the Earth, has been widely accepted within the scientific community. In the summer of 2023, the Anthropocene Working Group (AWG) of the International Commission on Stratigraphy proposed Crawford Lake in the southern Canadian province of Ontario as a geological reference. This marks a pivotal step towards officially recognizing the Anthropocene as a new geological epoch.

Many of our research groups are dedicated to investigating and quantifying the impact of human activities on the Earth system. This includes examining how burning fossil fuels and biomass affects atmospheric composition, air quality, and climate. Furthermore, our institute is increasingly delving into health-related aspects of air pollution, aligning with the new "planetary health" concept.

However, in Earth system research, it's often not the laboratory but rather the rainforest, savannah, or ocean where the fascinating data is to be found. Therefore, measurement campaigns involving research aircraft like the High Altitude and Long Range Research Aircraft (HALO), the research yacht *S/Y Eugen Seibold*, and the Amazon Tall Tower Observatory (ATTO) are at the core of our work. Many of these campaigns are conducted in collaboration with the Max Planck Institutes of the Earth and Solar System Research Partnership.

A few of these endeavors are described in this report, which provides an overview of our scientific activities and accomplishments from 2021 to 2023. The report is divided into a general institute section and specific reports from our Atmospheric Chemistry, Climate Geochemistry, Multiphase Chemistry, and Particle Chemistry Departments, each with their scientific groups plus a number of independent research groups.

Successful science relies on the support of reliable and efficient services. Consider our electronics and workshops, essential for tasks like repairing a damaged ship's shaft or designing a lift for 325-meter altitude profiles on ATTO. Our IT colleagues ensure seamless data transfer, even from the most remote ocean and forest environments. We also must mention the teams managing our finances, security, and intricate export processes. Like a smooth-running machine, each component of our institute functions harmoniously – a testament to the dedication of our staff.

It's heartening to see how science unites individuals from diverse countries and cultures around shared values and goals when collaborating on projects or issues in an increasingly intricate world. The commitment of our young scientists to climate and environmental protection, evident in all aspects of their lives, fills me with optimism about the future. This commitment can foster the feelings that Patrick Cramer mentioned. After all, science flourishes through collaboration built on principles of honesty, trust, and transparency.

This is my final Scientific Report as Managing Director, and I want to express my heartfelt gratitude to all the Max Planck Institute for Chemistry members for their exceptional work.

I hope readers will enjoy exploring the 2021 to 2023 activities at MPIC in this report.

Jos Lelieveld

Jos Lelieveld
Managing Director
December 2023



From the left: The President of the Max Planck Society, Patrick Cramer, at the institute; researchers onboard the HALO aircraft preparing for the next flight of the CAFE-BRAZIL campaign; drilling a coral core as geochemical archive to better predict the consequences of climate change for the world's oceans.



From the left: The Federal President, Frank-Walter Steinmeier (r.), at the German-Brazilian research station ATTO; ocean water sampling onboard the research yacht *S/Y Eugen Seibold*; virtual visits to the ATTO research station during the science fair in Mainz.

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 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's history up to the Anthropocene – the current geological epoch characterized by significant human impact on the Earth's geology and ecosystems.

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

Scientists at the MPIC 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 the 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 air-sea exchange and biogeochemical cycling of greenhouse gases, oceanic nutrients, and related substances.

At present, the institute employs about 300 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 is responsible for defining the scientific objectives and guiding the department's research. The directors jointly lead the institute's development and take turns in serving as the spokesperson of the board of directors and managing director of the institute. Jos Lelieveld has been serving in this position since 2020.

DEPARTMENTS

The **Atmospheric Chemistry Department** led 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 atmosphere's self-cleaning capacity, are studied through laboratory investigations and field measurement campaigns, particularly 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 also holds a part-time professorship at the Cyprus Institute in Nicosia, Cyprus.

The **Climate Geochemistry Department** led 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 the Earth's environment, the department employs diverse geochemical methods that include light stable isotopes of foraminifera shells and organic matter, biomarkers, and trace metals as well as high-resolution non-destructive analytical techniques. Gerald Haug has also been President of the German National Academy of Sciences Leopoldina, since March 2020.

The **Multiphase Chemistry Department** led 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. The department's research focuses on the composition and physical properties of micro- and nanoparticles in the 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.

INDEPENDENT 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 with the goal of achieving superconductivity. This research has been supported by an Advanced Grant from the European Research Council and central funds of the Max Planck Society.

The **Emmy Noether Research Group "Hominin Meat Consumption" (HoMeCo)** led by Tina Lüdecke addresses questions about the onset and intensification of meat consumption in early hominins using a method they developed to analyze nitrogen isotopes in tooth enamel.

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 Heidelberg University, 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:

Edouard Bard, Climate and Ocean Evolution, Collège de France, Aix-en-Provence, France

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

Christian George, IRCELYON, CNRS-University of Lyon 1, Lyon, France

Colette Heald, Department of Environmental Systems Science, Institute for Atmospheric and Climate Science, ETH Zürich, Zürich, Switzerland

Dwayne Heard, School of Chemistry, University of Leeds, Leeds, 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

Jean Lynch-Stieglitz, School of Earth and Atmospheric Sciences, Georgia Institute of Technology, Atlanta, GA, USA

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 (until 2022)
- **Organic isotope geochemistry** – A. Martínez-García
- **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

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)
- **Physics and chemistry of the UTLS aerosol** – S. Borrmann, F. Köllner

Independent Research Groups

- **Aerosols, air quality and climate** – Y. Cheng
- **High pressure chemistry and physics** – M. Eremets
- **Hominin Meat Consumption** – T. Lüdecke
- **Satellite remote sensing** – T. Wagner

Central Services

- **Communications** – S. Benner
- **Administration & technical services** – I. Lemm
- **IT** – T. Disper
- **Administration** – I. Lemm
- **Instrument development & electronics** – F. Helleis
- **Facility management & operational technology** – C. Pallien
- **Researchers support** – K. Sulsky
- **Workshops** – R. Wittkowski
- **Shipping & Export Control** – M. Carswell

December 2023

Group picture during the institute meeting in April 2023.

MAJOR COLLABORATIONS AND PROJECTS

The institute's research departments and groups engage in collaborations with numerous international partners. Selected collaborations that span multiple departments and groups are detailed below.

Additional projects can be found in the reports provided by individual departments and groups.

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 after 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 consequences 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 can be expected. To find solutions to the challenges posed by these changes, the ESRP studies the complex interactions and feedbacks between land, ocean, atmosphere, biosphere, and human actions through investigations in the field, the laboratory, and through numerical modeling. For this purpose, the ESRP develops, maintains, and utilizes joint research infrastructures, e.g., the German Climate Computing Center (DKRZ) for Earth system modeling 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.

HALO AIRCRAFT

The institute's atmospheric research and Earth observations are greatly supported by HALO, 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. The following are the main missions in which the MPIC has been involved since then.

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 elucidation of the 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 studied 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 BLUESKY research mission was to investigate the impact of reduced emissions from industry and transport during the COVID-19 lockdown on 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.

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 studied tropospheric oxidant photochemistry in combination with particle formation and growth mechanisms under pristine conditions found over the Amazon rainforest.

Researchers from the MPIC, the Goethe University Frankfurt, the Universidade de São Paulo, and the Instituto Nacional de Pesquisas Espaciais collected data by aircraft, balloons, drones, a ship, and from the ground at the German–Brazilian research station ATTO. Originally, this mission was planned for spring 2020 but had to be postponed due to the COVID-19 pandemic (replaced by the BLUESKY campaign).

2024 – CAFE-PACIFIC
Flying from Cairns in Northeast Australia, this mission has targeted the area around Indonesia and the Pacific warm pool, where deep convection is most intense on Earth. The region is sometimes referred to as the Earth's "heat engine". While continental (forest) emissions dominated tropospheric chemistry in CAFE-BRAZIL, clean marine conditions were predominant during CAFE-PACIFIC.

The CAFE missions were performed to investigate tropical tropospheric oxidant photochemistry in combination with aerosol particle formation and growth under clean, pristine conditions over land. The measurements were then contrasted with results from marine and polluted conditions. The measurements constrain computer models that represent chemical processes and environmental feedback mechanisms across the tropics.

AMAZON TALL TOWER OBSERVATORY (ATTO)

The Amazon Basin plays a key role in the carbon and water cycles, climate change, atmospheric chemistry, and biodiversity. Human activities have an impact on the basin, 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. 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.

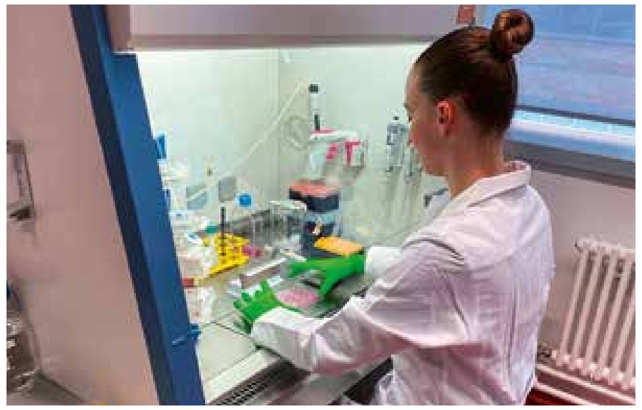
Two 80-m towers have been operated at the site since 2012, and a 325-m-tall tower was completed in 2015. The ATTO project is a collaboration between the Instituto Nacional de Pesquisas da Amazonia (INPA), the Universidade do Estado do Amazonas (UEA), the Max Planck Society, and further research partners. 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.

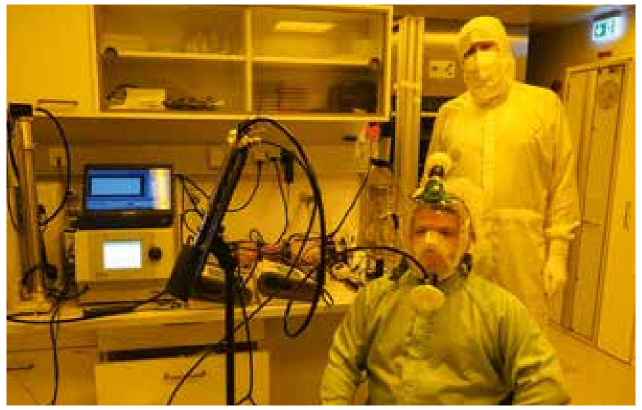
S/Y EUGEN SEIBOLD

The *S/Y Eugen Seibold* is a modern research yacht that has been operated by the MPI for Chemistry since 2018. The focus is on analyzing the marine atmosphere, plankton, and seawater to gain a deeper understanding of the complex interactions between the ocean and the atmosphere, shedding light on both historical and contemporary climates. Various marine regions and environmental conditions, from the polar circle to the equator in the eastern North Atlantic, have been explored. Subsequent ship tracks across the Atlantic and Caribbean Sea collected samples at 13 °N. Future plans include an in-depth analysis of the tropical eastern Pacific to investigate the effects related to the El Niño–Southern Oscillation (ENSO) throughout a full El Niño cycle.

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 the Middle East (EMME) region, which has been identified as a global climate change hotspot. Starting in 2019 and integrated into the Cyprus Institute in Nicosia, it focuses on the causes and effects of climate change in the area and on developing regional research networks, mitigation and adaptation solutions though the new "Climate and Atmosphere Research Center (CARE-C)". It 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 this long-term teaming project, supported by the European Union and the Cypriot government.





FIELD MEASUREMENTS AND EXPEDITIONS 2018–2023

SCIENTIFIC PUBLICATIONS

PUBLICATION STATISTICS

The results of the scientific research conducted at the institute are mainly published in peer-reviewed scientific journals. From 2012 to 2022, 2,406 peer-reviewed journal articles and reviews were published by researchers from the MPIC, corresponding to an average of 219 publications per annum. According to the Web of Science, nearly 76 % of the total set are open access papers. Compared to the previous reporting period (2009–2019), this is an increase of 11 %.

As of late 2023, MPIC-authored publications from 2012 to 2020 were cited 85,846 times. This is an average of 44 citations per paper and an increase of 4 % compared to the previous reporting period.* Between 2012 and 2020, the institute published papers that belong, on average, to the top 29.1 % most cited papers and thus well above the average citation impact compared to all publications from the same subject areas and years. An overview of relevant subject areas is given in Figure 1.

About a fifth (20.6 %) of the papers published between 2012 and 2020 belong to the 10 % of most cited papers within their subject categories, and 3.1 % belong to the 1 % of most cited papers within their subject categories, which is greater than the community average by a factor of three. The MPIC citation impact and related performance indicators are comparable to other world-leading academic institutions and significantly higher than the average values for Germany, the United States of America, and the Chemistry, Physics and Technology (CPT) section of the Max Planck Society (MPS).

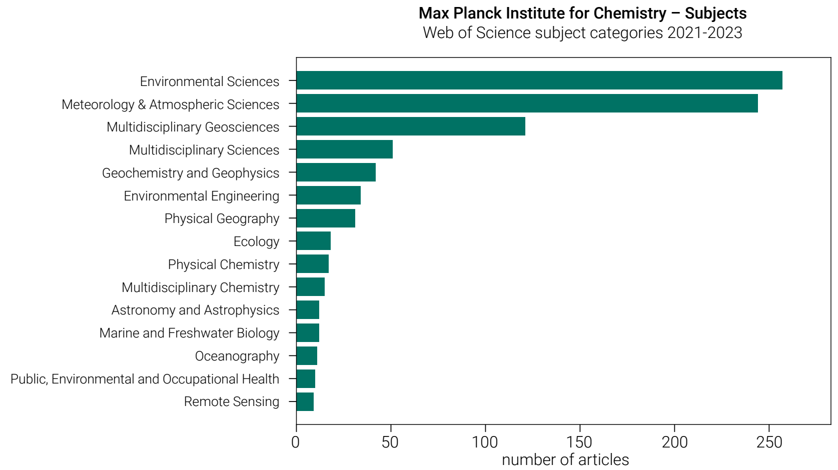


Figure 1: Main subject areas in which papers from the MPIC have been published according to the Web of Science during the years 2021 to 2023 (MPDL 2023).

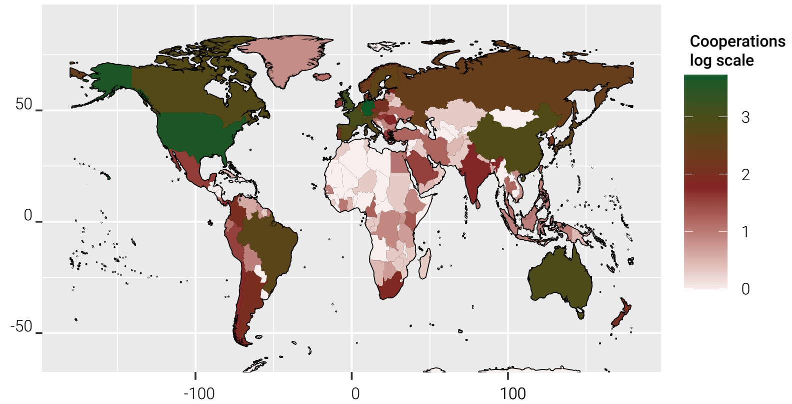


Figure 2: Scientific collaborations and joint publications of the MPIC with partners around the world. The color-coding indicates the number of publications co-authored by partners in each country between 2012 and 2022 (logarithmic scale; Scheidsteger & Haunschild 2023).

Moreover, individual institute members have been ranked repeatedly as "Highly Cited Researchers" (top 0.1 %) according to the Web of Science. A comprehensive listing of scientific publications during the past decades is available on the institute's website (www.mpic.de/3625125/Publications); further information and citation statistics are provided on the web pages of individual researchers (Researcher ID, Google Scholar, etc.), and selected studies have also been highlighted in press releases (www.mpic.de/3538502/press-releases). An overview of the geographic distribution of scientific collaborations and joint publications with partners around the world is given in Figure 2, illustrating the highly international nature of the research conducted at the MPIC.

OPEN ACCESS

The MPS and the MPIC are among the leading proponents of open access (OA) to scientific publications and support the widest possible dissemination of scholarly knowledge for the benefit of humanity.

Since the year 2003, the MPS has hosted and supported a series of international meetings, the Berlin Open Access Conferences, which are dedicated to the promotion of OA and which have been responsible for some of the key declarations and developments in the global move toward OA. From the beginning, scientists from the MPIC have been actively involved in these efforts and they continue to play a leading role.

The Declaration on Open Access to Knowledge in the Sciences and Humanities (openaccess.mpg.de/Berlin-Declaration) issued in 2003 has been signed by over 750 leading scholarly organizations around the world and continues to attract further signatories. Building on the Berlin Declaration, the global initiative OA2020 aims to transform existing scholarly journals from subscription to OA and at the same time to continue to support new and improved forms of OA publishing like interactive OA journals with open peer review as outlined below. An overview and detailed information on the approach and achievements of OA2020, which was initiated and is co-chaired by MPIC director Ulrich Pöschl, are available at https://oa2020.org.

Among the most efficient pathways to OA are transformative agreements between scientific institutions and traditional publishers, converting former subscription fees into so-called "publish-and-read" fees to have the institution's papers published under a proper OA license (ideally a Creative Commons Attribution license, CC-BY) while maintaining the institution's access to the non-OA journal content of the publisher. In this way, the MPS, together with other leading international scientific organization, and a growing number of countries have managed to ensure that large fractions of their publication output, i.e., up to 90 % and more, are open access, as illustrated in Figure 3.

In a consortium with other major scientific organizations in Germany (DEAL, https://deal-konsortium.de/en/), the MPS and its digital library (MPDL) also succeeded in establishing nation-wide transformative agreements with large international publishers that had previously resisted the transition to OA. In 2023, several years after letting subscription contracts expire, the consortium finally arrived at a scholarly oriented transformative agreement with the publisher Elsevier, enabling not only OA for papers in this publisher's journals but also substantial financial savings compared to the costly subscriptions of the past (www.mpg.de/20820489/deal-open-access-elsevier-2023). Moreover, successful earlier transformative agreements with Wiley, Springer Nature, and other publishers were extended (https://deal-konsortium.de/en/news).

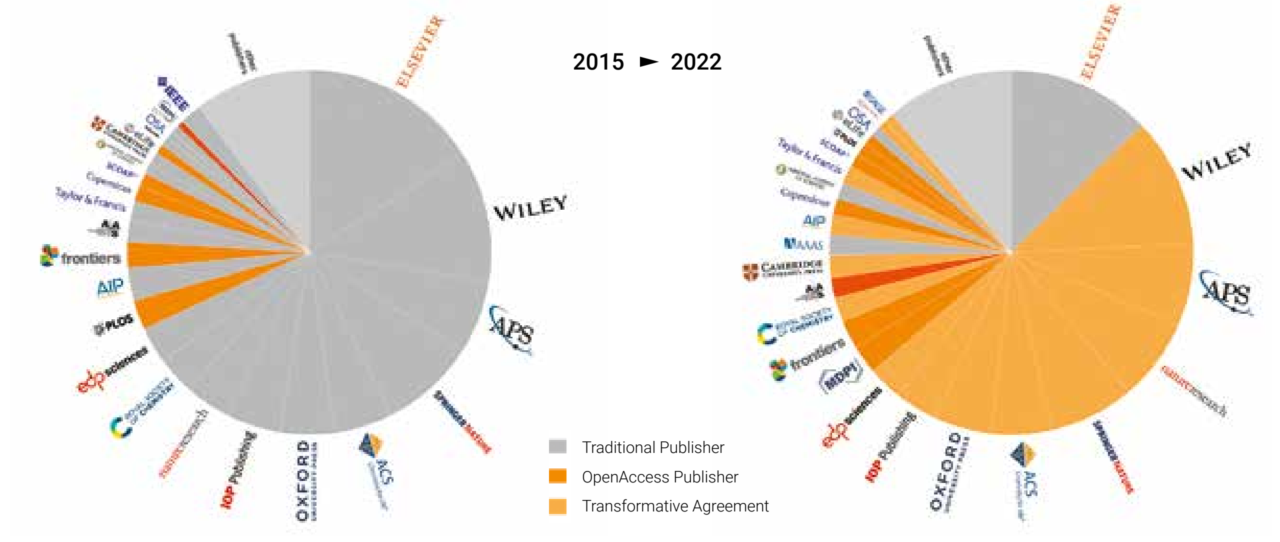


Figure 3: Progress in OA of the Max Planck Society (MPDL 2023).

SCIENTIFIC PUBLICATIONS

To gain the full benefits of open access and open science, complementary approaches are required ("as-well-as", not "either-or"): top-down approaches to achieve large-scale progress as well as bottom-up initiatives to maintain scholarly diversity. Appropriate transformative agreements with traditional publishers are needed to achieve an efficient conversion of subscription journals that are still important for some communities, while funding for proper OA publishers and new publishing platforms has to be provided to maintain competition and innovation.

Even before the term open access was coined and the Berlin Declaration was issued, MPIC scientists were pioneers in developing new and improved forms of OA publishing going back to the years 2000/2001. In collaboration with the European Geosciences Union (EGU) and the OA publisher Copernicus, the MPIC researchers developed and successfully established the concept of interactive open access publishing with multi-stage open peer review and interactive public discussion, which is also spreading to other fields in the sciences and humanities. In fact, some of the first and most successful international open access journals have been founded and developed into highly reputable publications under the aegis of MPIC researchers: 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.**

In addition to these journals, and following ACP as a role model, EGU launched 15 other interactive OA journals covering the entire field of geosciences, which brought this field to the forefront of the global evolution in OA. Accordingly, the OA fraction of papers published by the MPIC and other institutes in the geosciences was consistently higher than the OA fraction of institutions in other fields of research as illustrated in Figure 5 by comparison with average values for the CPT section of the MPS. The recent boost to transformative agreements provided by OA2020 has meant that all fields including the geosciences have reached even higher levels of OA (> 90 %, Fig. 5).

To celebrate past achievements and explore future directions in OA publishing and open peer review, the EGU publications committee, which has long been chaired by U. Pöschl, recently held a workshop at the MPIC. New initiatives discussed and advanced at this workshop include a virtual highlight magazine (EGU Letters) and an interactive community platform (EGUsphere) to further facilitate, improve, and document the scientific discourse and quality assurance in an epistemic web of preprints, journal articles, reviewer reports, commentaries, replies, and conference contributions from the geoscientific community (see/copy press release text; add link to press release). Through the above and related activities, the MPIC continues to serve as a pace-setter for open science for the benefit of scientific and societal progress.

Participants of the 16th Berlin Open Access Conference at the Harnack Haus, June 6 - 7, 2023.

Figure 4: Covers of open access journals founded and shaped by MPIC researchers with the European Geosciences Union (EGU).

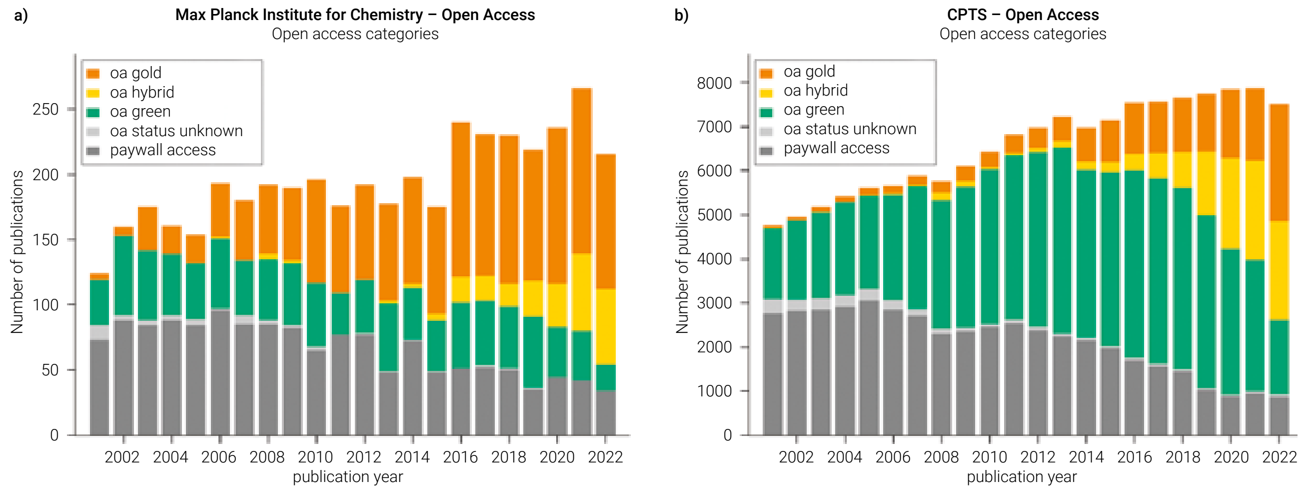


Figure 5: Publication output by OA categories comparing the MPIC (a) to the entire Chemistry, Physics, and Technology (CPT) section comprising 33 institutes of the Max Planck Society (b). At the beginning of the OA2020 initiative in 2016, the OA publishing percentage (orange/yellow) was already higher than 50 %, while it was still less than 20 % for the entire CPT section. By now and through OA2020, the total OA percentage of both the MPIC and the entire CPT section has increased to approx. 90 % (OA publishing in orange/yellow plus and OA archiving in green).

The publication list of the institute is available at www.mpic.de/3625125/Publications

* *The bibliometric data are taken from the report "A bibliometric analysis of the MPI for Chemistry, in the publication period 2012–2022" by Thomas Scheidsteger and Robin Haunschild, Max Planck Society, Information Retrieval Services.*

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

JUNIOR SCIENTIST, RESEARCHER SUPPORT, AND GUEST PROGRAM

PhD students and postdoctoral researchers contribute greatly to the success of the institute. As these career phases are a challenging time not only in professional but also in private life, the institute aims to offer junior scientists the best possible support during their stay at the MPIC and to prepare them for the next career steps.

In addition to the structured doctoral programs for PhD students – the Paul Crutzen Graduate School (PCGS) and the Max Planck Graduate Center (MPGC) – a postdoctoral program was set up to meet the particular needs of researchers in this career stage. The curricula of both graduate programs combine research with education. They are tailored to the needs of students and provide advice and supervision during the entire PhD period. Social events are supported to promote intercultural exchange among PhD students from all over the world and to foster a healthy work-life balance. Annually elected PhD representative committees are established to communicate and pursue the interests and perspectives of PhD students at the institute.

PAUL CRUTZEN GRADUATE SCHOOL (PCGS)

Paul Crutzen Graduate School

All PhD students associated with the institute are automatically members of the PCGS. At the beginning of their PhD studies, a Thesis Advisory Committee (TAC) is established in consultation with the student and their main supervisor. This committee provides guidance, support, and feedback not only on scientific matters but also with regard to soft skills and future career steps and perspectives.

For TAC meetings and written reports, regular schedules are foreseen. Students have the freedom to adapt their schedules in consultation with the supervisors and graduate school coordinator, especially with respect to research campaigns and university teaching commitments. The PhD students are encouraged to invite additional guests with special expertise on their topic, and they can also request additional support if any problems or conflicts arise. In such cases, the graduate school coordinator as well as general ombudspersons can be approached and act as mediators or arrange for external support and professional counseling for both students and supervisors. The coordinator also provides further academic and practical support for bureaucratic and other issues of student life in the institute and its environment. Moreover, the PCGS has its own budget to provide financial support for students attending conferences and courses, including a mandatory course on Good Scientific Practice and other in-house courses according to suggestions of students and supervisors (www.mpic.de/3538568/pcgs-paul-crutzen-graduate-school).
Currently, 54 students from 14 countries, 28 female and 26 male, are enrolled in the PCGS (38 from Germany, 16 from abroad).

MAX PLANCK GRADUATE CENTER (MPGC)

Max Planck Graduate Center mit der Johannes Gutenberg-Universität

The MPGC is a cross-institutional graduate program of the MPIC, the neighboring Max Planck Institute for Polymer Research (MPIP), and four departments of the Johannes Gutenberg University (JGU) in Mainz.

It is especially aimed at PhD students with highly interdisciplinary research topics and has its own doctoral regulations. Students whose project or study background does not fit to a single university department can apply for admission to the MPGC, serving as a kind of virtual interdisciplinary department. The curriculum and structures of advice and supervision are similar to the PCGS. The MPGC offers scientific focus groups bundling expert knowledge and research interests from across the MPIC, MPIP, JGU, and other scientific institutions in Mainz and beyond. Faculty members and other affiliates contribute their expertise as principal investigators or associates of the MPGC and its focus groups. In this way, the MPGC promotes interdisciplinary scientific exchange and excellence among all participating institutions. Structurally and scientifically, the PCGS benefits from the interconnection with the MPGC and vice versa. Currently, 19 students from the MPIC and PCGS are also members of the MPGC.

After an evaluation in spring 2023, the MPGC has been institutionalized as a permanent graduate program connecting the MPIC, MPIP, and JGU. It is financed in equal parts by the Max Planck Society and by the federal state of Rhineland-Palatinate.

POSTDOCTORAL SUPPORT

To give postdoctoral researchers the best possible support and help them prepare for future career steps within or outside academia, the institute offers a program with elements similar to the PhD programs and its own budget. It provides counseling on funding and career opportunities and fosters professional networking within and beyond the institute. Individual coaching and further support are also provided through central programs of the Max Planck Society (Planck Academy, see below).

GUEST PROGRAM

The Guest Program provides scholarships to scientists who visit the institute for a limited period of time to engage in ongoing research projects or to use the MPIC infrastructure and expertise for their own research projects (PhD students up to six months; postdocs up to two years; individual arrangements for senior scientists). The straight-forward application and admission process of the Guest Program is an important, flexible tool to enhance scientific exchange and to expand international collaborations. Guests can also participate in the institute's junior scientists support programs as outlined above.

RESEARCHER SUPPORT

Since early 2023, the Junior Scientist Support, Guest Program, and the International Office are embedded in the umbrella unit Researcher Support, which provides general assistance to students, scientists, and visiting scholars with regard to getting settled in Mainz/Germany, administrative matters, funding opportunities, and career development. Working in close cooperation with the institute administration and department secretariats, the Researcher Support unit helps to ensure efficient exchange and avoid duplication of efforts. This bundling of supporting activities and expertise has proven to work well also under difficult conditions such as the COVID pandemic and related issues.
Since February 2020, the Max Planck Society offers a central program, called Planck Academy, for target-group-specific professional and personal career development to all employees: senior and early career researchers as well as administrative and technical staff (https://www.mpg.de/career/planck-academy).
Moreover, the MPIC provides support for child care and families as detailed in the next section and on the institute´s web pages (www.mpic.de/4161235/equal-opportunities).

DIVERSITY, COLLABORATION, AND WORKPLACE SAFETY

As part of the Max Planck Society, the Max Planck Institute for Chemistry places a strong emphasis on outstanding scientific talent, creativity, and passion. Regardless of gender, nationality, religion, physical abilities, age, cultural background, or sexual identity, the institute promotes and supports all of its employees and guests. It is committed to creating a working environment where everyone can perform at their best. In creating equal opportunities, it focusses on the compatibility of family and research, in particular on supporting female scientists in the family and career start-up phase. An equality plan and elected equal opportunities officers at the institute help to achieve this goal. The officers are involved in all personnel, organizational, and social measures relating to equality between genders, the reconciliation of family life and work as well as protection from sexual harassment at the workplace. They take part in job interviews and in regular meetings with the board of directors. Furthermore, the officers are well integrated into the everyday life at the institute by participating in discussions and meetings.

The institute provides a welcome service and organizes special events for international researchers upon their arrival in Mainz, including regular German courses at the institute, aiming to ease the transition into living and working in Germany.

In a comprehensive institute-wide survey on work and management culture conducted in 2022, it was revealed that the vast majority of MPIC employees take pride in their association with the institute. The survey also highlighted excellent collaboration within teams and between science and service facilities, surpassing comparable institutes both nationally and internationally.

The positive spirit of internal collaboration finds expression in various initiatives. For instance, the dedicated MPIC PhD Committee consistently organizes events like the MPIC Literature Club, lecture series, and social gatherings. These activities cater not only to doctoral and postdoctoral researchers but to all institute members.

The sustainability group actively pursues more responsible resource use through themed days, a swap meet, and a gardening project and thus helps achieving the goal of transitioning to green energy. Additionally, employees autonomously organize diverse fundraising campaigns.

To uphold and enhance the mental and physical well-being of our staff, the MPIC routinely offers health courses and mental stress prevention programs. This is complemented by a comprehensive support system, which includes structured conflict and crisis management with clearly communicated advice and reporting points. Additionally, self-management and project management services are provided, with harassment awareness lectures being an integral part of this program.

Ensuring workplace safety is a paramount concern for the institute, which is pursued through biannual work safety weeks and related events. During these events, employees receive training on correct behavior in emergencies such as fires, as well as safe driving practices. Specialized courses further provide safety training tailored to research campaigns and individual laboratories.

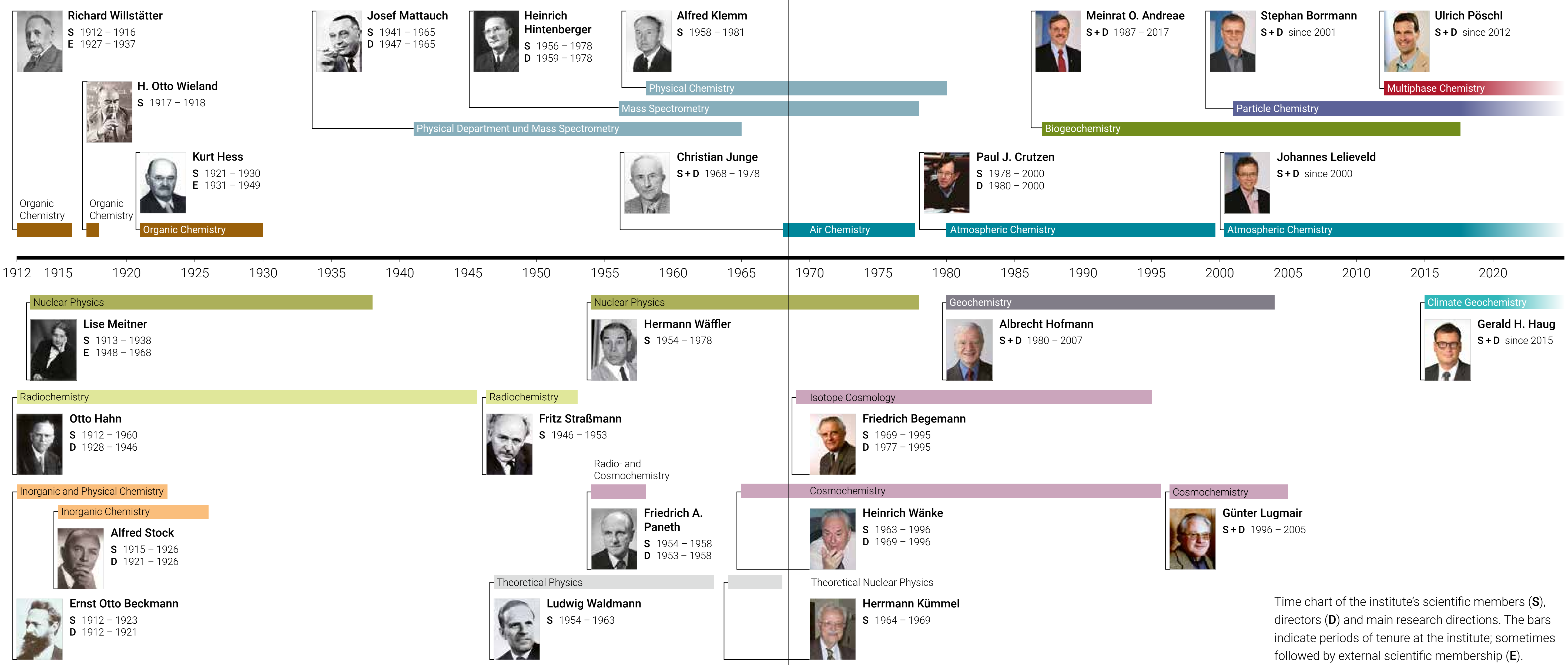








HISTORY



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**).

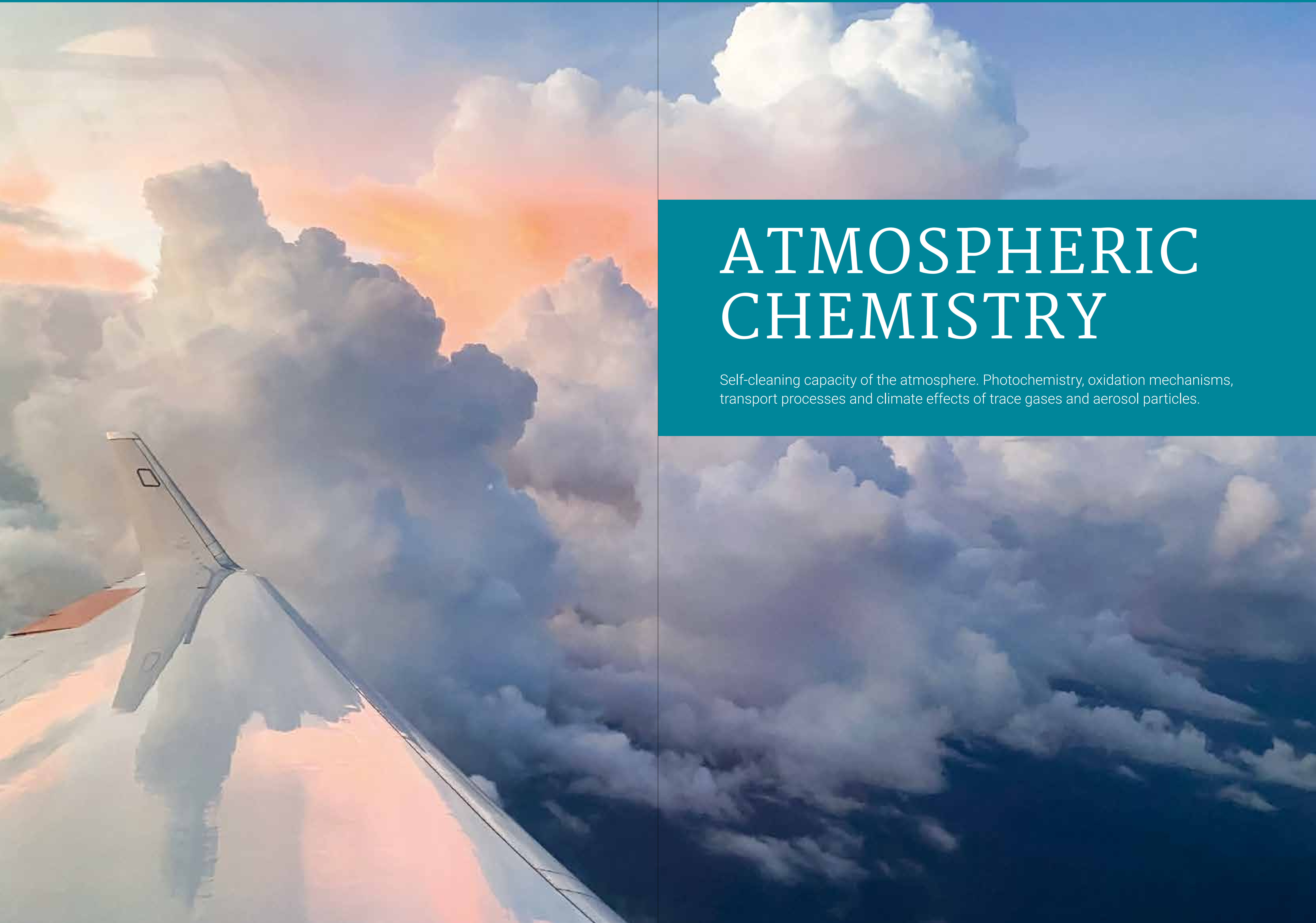
Research at the Max Planck Institute for Chemistry has been at the forefront of science throughout its existence. Since the institute's foundation in 1912, three of its directors were awarded with the Nobel Prize for Chemistry: Richard Willstätter in 1915 for the revelation of the structure of chlorophyll 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

"CHANGING ATMOSPHERIC COMPOSITION" – NEW INSTRUMENTAL AND SOFTWARE TOOLS FOR ATMOSPHERIC CHEMISTRY

Our department studies the physical–chemical processes that govern the composition and self-cleaning capacity of the Earth's atmosphere. The atmosphere removes natural and anthropogenic pollutants through photo-oxidation chemistry and radical reactions. The hydroxyl (OH) radical plays a central role in these processes as a powerful oxidant, and we are uncovering the mechanisms that control its concentration from local to global scales. This is achieved by laboratory experiments of atmospheric chemical reactions and by employing instrumented platforms such as aircraft, ships, and ground-based stations in diverse environments. These measurements provide critical insights into interdependencies between emissions, chemical transformations and atmospheric transport processes. We measure many reactive species with custom-built instrumentation, from highly reactive radicals to large organic molecules and a myriad of reaction products.

In recent years we have carried out a series of field measurement campaigns with the High Altitude Long-range (HALO) research aircraft under the overarching title "CAFE" (Chemistry of the Atmosphere: Field Experiment). CAFE-AFRICA, CAFE-BRAZIL, and CAFE-PACIFIC have focused on the tropical troposphere, where atmospheric chemistry measurements have thus far been scarce. The measurements have provided evidence for the long-distance transport of pollutants, new particle formation from low-volatile precursor gases, and the role of deep cloud convection in the vertical redistribution of gases and particles. For example, the results have illuminated how nitrogen oxides from lightning control ozone and OH chemistry. By juxtaposing different conditions that span very clean to highly polluted settings in both marine and terrestrial environments, we have significantly improved our understanding of atmospheric mechanisms and the accuracy of our Earth system chemistry model (described below). Further, we took advantage of the lockdowns during the COVID-19 pandemic, when air and road traffic pollution temporarily declined in Europe. These measurements in the BLUESKY campaign during spring 2020 could be contrasted with prior European campaigns, documenting the transport sector's immense influence on the troposphere's chemistry.

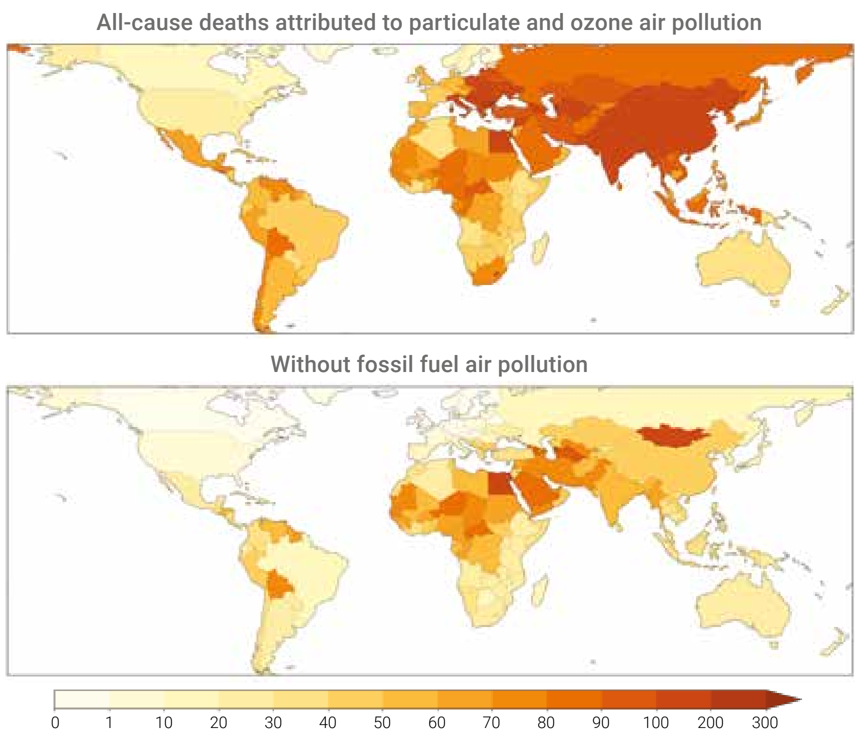


Figure 1: Country-average, excess mortality per 100,000 population per year attributable to fine particulate matter ($PM_{2.5}$) and ozone (O_3). Lower panel: after removing fossil fuel-related emissions, accounting for 80 % of the health impacts of all anthropogenic emissions.

Such studies are more important than ever, as the atmosphere's chemical composition changes significantly. For example, the atmospheric concentration of methane (CH_4), the second major greenhouse gas after CO_2 (nearly 30 % of the total climate forcing), is increasing at an accelerating pace, despite the commitment of 150 nations to decrease anthropogenic emissions by at least 30 % from 2020 to 2030. It is conceivable that tropical wetlands respond to climate change by intensifying CH_4 emissions. Methane's lifetime is limited by reaction with OH radicals, and new challenges may arise from changing sources and removal processes. Within the near future it is possible that fossil fuel-related emissions will decline in high-income countries and rise in low- and middle-income countries that are striving for income equality. Such shifts may involve a north–south redistribution of pollution emissions and more significant pressure on tropical environments.

The wealth of data obtained from field measurements and observations from space has supported the development of our Earth system chemistry model that simulates interactions between the atmosphere, terrestrial and marine environments, and anthropogenic influence. The model has become a versatile tool in analysing measurement data, including methane in recent decades and has been used to perform scenario calculations of possible future atmospheric composition and climate. We also use it to investigate the historical climate system that was affected by (super)volcanoes, glacial-interglacial cycles, and supernova explosions that influenced the evolution of life. We considered star–planet configurations in the universe, informed by the Earth and solar system, in the search for habitable planets. Further, the model allows for "what-if" scenarios that provide evidence of air quality and climate impacts from specific sources (Figure 1). These studies reveal the prominent role of fossil fuel use in climate change and the loss of human life expectancy and suggest that carbon neutrality will have significant co-benefits for public health and climate.

JOS LELIEVELD

25 July 1955 Born in The Hague, The Netherlands

1984 Study of natural sciences at Leiden University, The Netherlands

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

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

Professor in Atmospheric Physics, Johannes Gutenberg University Mainz (JGU), and Professor at the Cyprus Institute, Nicosia, Cyprus

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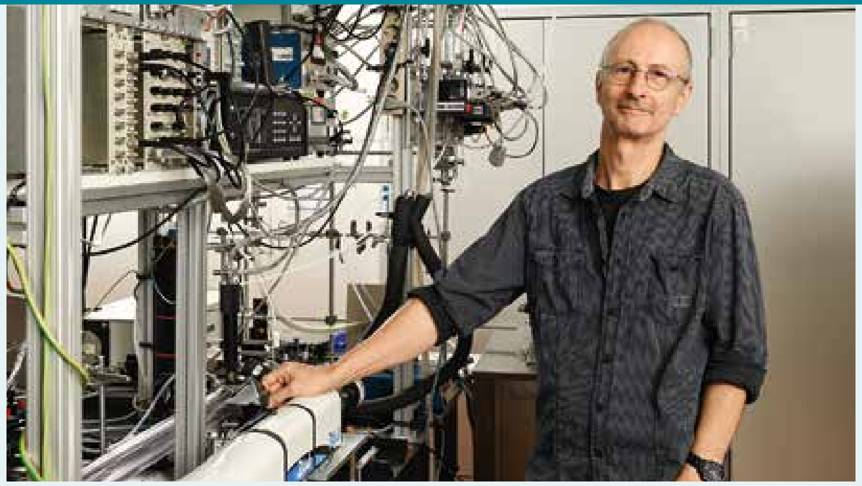
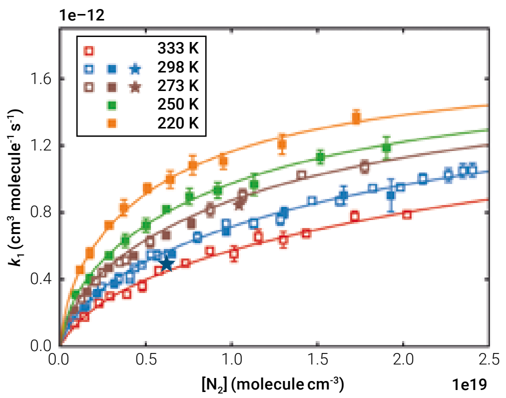
LABORATORY AND FIELD STUDIES OF REACTIVE TRACE GASES

JOHN CROWLEY – KINETICS AND PHOTOCHEMISTRY GROUP



"The 'Reactive Processes' group combines *in situ* observations with laboratory studies to provide insight into the chemical processes that define atmospheric composition from the boundary layer to the lower stratosphere."



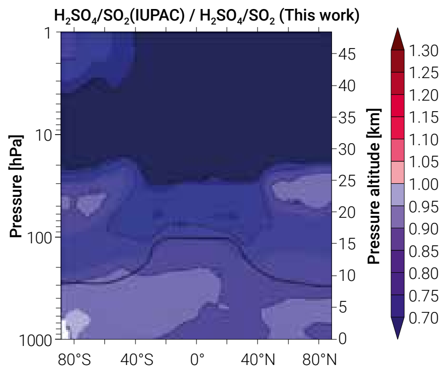


Figure 1: Rate coefficients (k_1) for OH + SO_2. Open squares, closed squares, and stars represent data obtained using H_2O_2, HNO_3, and HONO as OH precursors, respectively.

Figure 2: Effect of different parameterizations of k_1 on the global (zonal and yearly averaged) H_2SO_4 to SO_2 ratio.

LABORATORY STUDIES OF OH KINETICS

Reaction with the OH radical is the first step in the daytime oxidation of the vast majority of biogenic and anthropogenic emissions into the atmosphere. Termolecular (or "three-body") reactions may display a strong, positive dependence on pressure and a negative dependence on temperature, which is related to the formation and stabilization of an initially formed association complex. A parameterization of such reactions for atmospheric modelling requires measuring rate coefficients that cover pressures from the surface to the lower stratosphere (50 to 1000 hPa) and temperatures between 220 and 310 K. Even for some centrally important reactions, the experimental database is often not of sufficient quality, and the recommendations of evaluation panels (JPL-NASA, IUPAC) diverge. We have carried out detailed studies of the following termolecular reactions using pulsed-UV-laser generation of the OH radical and pulsed laser-induced fluorescence to directly detect OH in real-time.

$$OH + SO_2 + M\ (N_2/H_2O) \rightarrow HOSO_2 + M$$
$$OH + NO + M\ (N_2/H_2O) \rightarrow HONO + M$$

The reaction between OH and SO_2 leads ultimately to the formation of sulfuric acid, H_2SO_4. Figure 1 displays a set of rate coefficients (k_1, in total > 100 measurements) for the reaction of OH with SO_2 obtained at various temperatures (220–333 K) and pressures (19–990 hPa) and associated fits (fall-off curves) to the data. This represents the first temperature-dependent data set in an atmospherically relevant bath gas. We found that the presence of water vapour accelerated the reaction, presumably as H_2O is a better 3rd-body quencher of the $HOSO_2$* association complex (by a factor of ~ 5) than N_2. A data set of similar quality was obtained for the OH + NO reaction, the rate coefficient of which was also enhanced (by a comparable factor) in the presence of H_2O.

To investigate the impact of the new dataset on the atmospheric sulfur cycle, we introduced a parameterization into the chemistry-climate model EMAC, using either the OH + SO_2 rate coefficient derived in the present study, or using the IUPAC recommendation.The results are displayed in Figure 2, which compares the H_2SO_4-to-SO_2 ratio obtained under both scenarios. The new data indicate a significant reduction in the SO_2-to-H_2SO_4 conversion rate in the upper troposphere and lower stratosphere. In contrast, the effect of H_2O increases the rate coefficient by ≈ 5 % in the humid, tropical boundary layer.

AIRBORNE MEASUREMENTS OF PAN AND PAA (PEROXYACETIC ACID)

PAN ($CH_3C(O)OONO_2$) is the most abundant peroxynitrate in the atmosphere, and PAA ($CH_3C(O)OOH$) is often the second most abundant organic peroxide (after CH_3OOH). Both are believed to be formed solely from reactions of the acetyl-peroxy radical ($CH_3C(O)OO$) with NO_2 (for PAN) and HO_2 (for PAA). During the CAFE-AFRICA (2018) and BLUESKY (2020) campaigns, we deployed an iodide-chemical ionisation mass spectrometer on the HALO aircraft to measure PAN and PAA as well as their C3 homologues PPN ($C_2H_5C(O)OONO_2$) and PPA ($C_2H_5C(O)OOH$). Vertical profiles of PAN and PAA are given in Figures 3 (CAFE-AFRICA) and 4 (BLUESKY).

During CAFE-AFRICA, PAN displayed a well-defined maximum mixing ratio at altitudes close to 8 km, resulting from a combination of its thermal instability at lower altitudes (where its mixing ratio tends to zero) and a vertical gradient in its production term. PAN was still observable at 14 km in the tropical upper troposphere (UT). Elevated mixing ratios of both PAN and PAA during CAFE-AFRICA were correlated with elevated black carbon, CH_3CN, and CO, indicating a heavy influence of biomass burning in southern African and the Northwestern US. The lifetime of PAA is defined almost entirely by its photolysis, and its mixing ratios decrease monotonically from the ground to the UT. Molar enhancement ratios of PAA/CO of between ≈ 3 and 10 × 10^{-4} were derived for four flights, which enabled the influence of biomass burning on PAA mixing ratios to be assessed. Over Europe, mean PAN mixing ratios were similar though the PAN maximum is less well-defined owing to lower temperatures and higher production terms at low altitudes over this industrialized continent. In contrast to CAFE-AFRICA, some of the highest mixing ratios were observed in the boundary layer. PAA levels at lower altitudes over Europe were about a factor of two larger than over the North Atlantic, which likely reflects an increase in the fraction of acetyl-peroxy radicals that stem from anthropogenic processes.

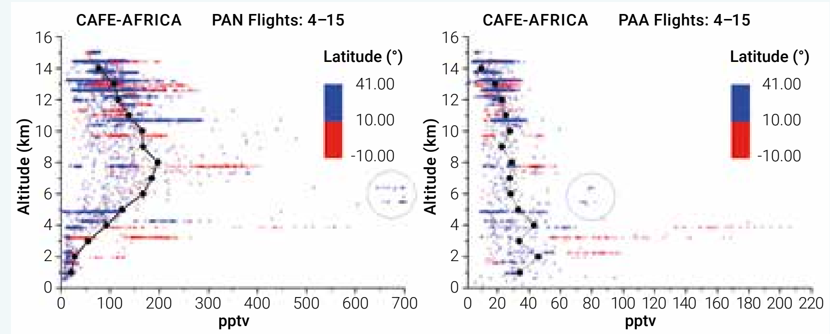


Figure 3: Vertical gradients of PAN (left) and PAA (right) during CAFE-AFRICA. Red and blue data points were obtained south and north of the ITCZ located at ~ 10 °N. Black data points are averages over 1 km vertical bins. The circled data were obtained when the HALO aircraft intercepted a biomass burning plume originating in the Northwestern US.

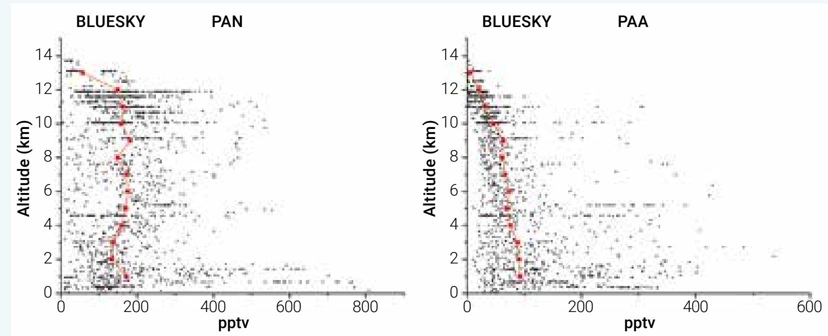


Figure 4: Vertical gradients of PAN (left) and PAA (right) during BLUESKY. Red data points are averages over 1 km vertical bins.

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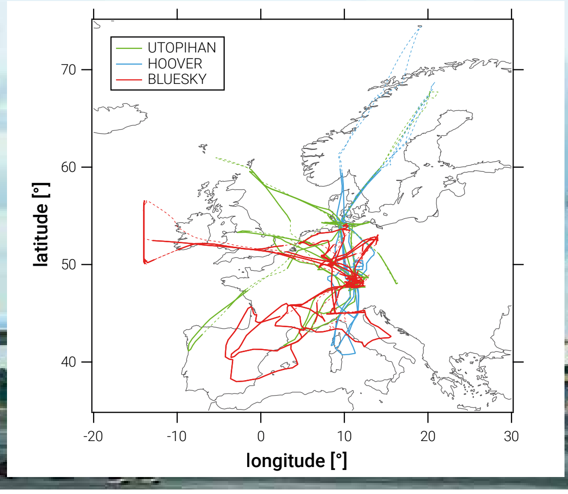
A NEW METRIC FOR OZONE SENSITIVITY TO NO_x AND VOCS AND ITS APPLICATION THROUGHOUT THE TROPOSPHERE

HORST FISCHER – OPTICAL SPECTROSCOPY GROUP

Map showing the flight tracks of HALO missions.

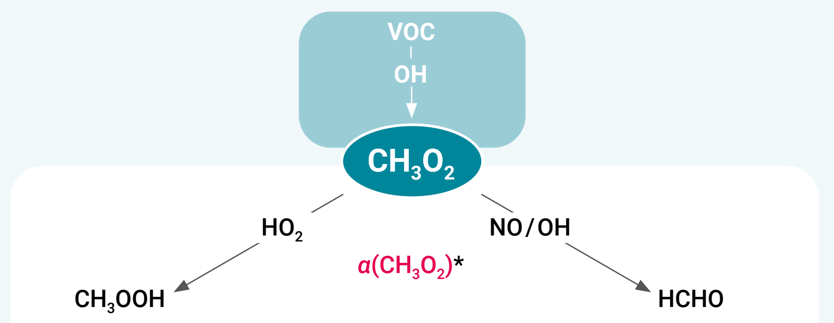


INTRODUCTION

Tropospheric ozone plays a pivotal role in atmospheric chemistry, air pollution, and climate change. The concentration of ozone (O_3) is central to the primary formation rates of the hydroxyl (OH) and NO_3 radicals. Close to the ground, O_3 can be a hazard to human health, and it is also a potent greenhouse gas, in particular in the upper troposphere. Its formation in the troposphere is a nonlinear function of nitric oxide (NO) and peroxy radicals (HO_2 and RO_2) formed from volatile organic compounds (VOCs) via oxidation by OH.

RESULTS

In order to determine whether changes in O_3 formation are more sensitive to changes in NO or changes in peroxy radicals, a number of metrics and indicators have been used. Some are based on observed trace gases, whose ratios indicate either NO_x- or VOC-sensitive ozone chemistry, e.g., H_2O_2/HNO_3 or $HCHO/NO_2$ ratios. Another example is the change of O_3 formation in response to changes in NO. The application of the majority of these indicators is limited to low altitudes and relatively high temperatures. Recently, we have developed a new metric, $\alpha(CH_3O_2)$, to determine O_3-sensitivity from *in situ* observations of HO_2 and NO that can be used throughout the whole tropospheric column. It is based on the fate of the methyl peroxy radical (CH_3O_2) that can either react with NO to form formaldehyde (HCHO) and contribute to O_3 or with HO_2 to form methyl hydrogen peroxide (CH_3OOH) without O_3 formation (Figure 1). At low values of $\alpha(CH_3O_2)$, increases of NO lead to relatively high O_3 formation rates (NO_x-sensitive) while at higher NO values, $\alpha(CH_3O_2)$ is mostly unresponsive to further increases in NO (VOC-sensitive). The concept was first tested using data from three ground-based campaigns across Europe and shown to lead to consistent results compared to other indicators. A first application to the free and upper troposphere was based on airborne data from the BLUESKY campaign over Europe in spring 2020 when restrictions in air traffic during the lockdowns led to a decrease in NO concentrations in the upper troposphere compared to measurements from earlier aircraft campaigns in 2003/04 and 2006/07. Application of the $\alpha(CH_3O_2)$ metric indicated that during the lockdown O_3 formation in the upper troposphere switched to being NO_x-sensitive, while it was VOC-sensitive in previous years (Figure 2). A subsequent model study on $\alpha(CH_3O_2)$ in the tropical upper troposphere demonstrated that lightning is the dominant NO_x source in this area of the world. In particular, lightning NO_x significantly fuels O_3 production in the tropical upper troposphere over continents, which is associated with high $\alpha(CH_3O_2)$ values (VOC-sensitive), while oceanic environments are NO_x-sensitive. This is attributed to the weak NO formation via lightning associated with deep convection in oceanic environments, as demonstrated by in situ observations of the tropical storm (later hurricane) Florence in 2018 over the Atlantic Ocean. Observations showed that although deep convective transport led to enhancements of a large number of boundary layer-derived tracers in the upper troposphere, NO enhancements were not observed due to the absence of lightning in this phase of the storm development.



$$^{*}\alpha_{CH_3O_2} = \frac{k_{CH_3O_2+NO}\times[NO] + k_{CH_3O_2+OH}\times[OH]}{k_{CH_3O_2+NO}\times[NO] + k_{CH_3O_2+OH}\times[OH] + k_{CH_3O_2+HO_2}\times[HO_2]}$$

Figure 1: Definition of $\alpha(CH_3O_2)$ based on the photochemical fate of the CH_3O_2 peroxy radical.

“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.”

OUTLOOK

During December 2022/January 2023, airborne measurements of a large suite of trace gases, aerosols, and radicals were performed from the HALO research aircraft over the Amazon during the wet season. In a further campaign, scheduled for January/February 2024 to probe the maritime continent from northwestern Australia, additional data will be obtained. This will permit further testing of the predictions of the EMAC model study on O_3 sensitivities towards NO_x and VOCs in the tropical upper troposphere over continental and maritime regions. It will also allow further studies on NO formation in deep convective systems with and without lightning and their role in the oxidation capacity of the troposphere.

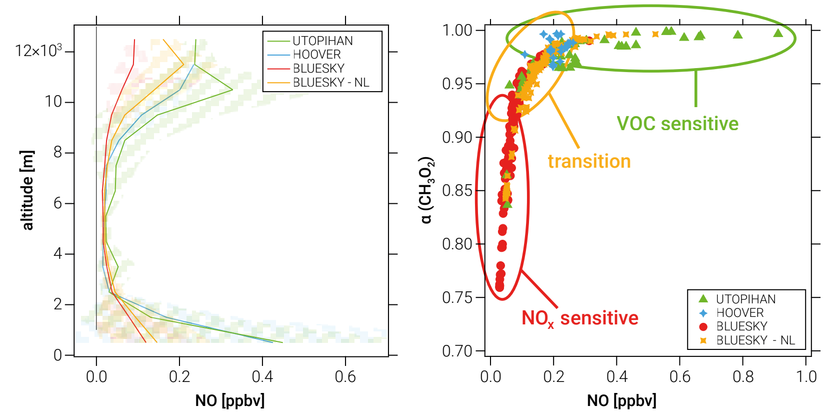


Figure 2: Vertical profile of NO (left) and $\alpha(CH_3O_2)$ (right) at altitudes above 10 km measured during the UTOPIHAN, HOOVER, and BLUESKY campaigns. The yellow data points are EMAC model results under no lockdown (NL) conditions.

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THE IMPACT OF CHANGES IN COMPOSITION ON THE SELF-CLEANING CAPACITY OF THE ATMOSPHERE

HARTWIG HARDER – RADICAL MEASUREMENTS GROUP

"*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 of the atmosphere."

Figure 1: HALO research aircraft in Brazil (left), CLOUD chamber at CERN (center), and photochemical experiment inside CLOUD (right).

INTRODUCTION

The abundance of radicals in the atmosphere is heavily influenced by recycling reactions e.g. the regeneration of OH radicals after their reaction with reduced or partly oxidised gases. We study the mechanisms governing this process using chamber, ship, and aircraft measurements in different parts of the world.

TROPICS

During the CAFE-AFRICA campaign, OH production in the upper troposphere was found to be significantly increased in air, as a direct influence of convection over the ocean and land. This was more pronounced in continental than in marine air. Over the ocean, peroxides were transported by convection to the upper troposphere, where water vapor concentrations are low, serving as a source of OH through photolysis. Continental air contains more volatile organic compounds (VOC) and higher organic peroxide concentrations, while lightning, resulting in the production of NO, is more frequent over land. As a result, in the continental upper troposphere, the HO_x (HO_x = OH + HO_2) balance shifts from HO_2 towards OH, increasing the OH-initiated oxidation of VOC, and allowing OH recycling from oxidation products. Furthermore, the oxidation of VOC by OH in continental conditions forms additional HO_x that contributes to the atmosphere's self-cleaning capacity.

SUBTROPICS

Our AQABA ship campaign observations showed that even though the lower atmosphere over the Arabian Gulf exhibited an extraordinarily high mean primary production of hydroxyl radicals up to 2.5 × 107 molecules cm^{-3} s^{-1}, the OH concentration was more than 50 % lower than over the Mediterranean Sea, even though the primary OH production was 50 % higher. We attribute the lower OH concentration in the Gulf region to a recycling probability of about 15 %, which is markedly lower compared to that over the Mediterranean (nearly 60 %). Our analysis suggests that the low recycling probability over the Gulf is due to radical–radical reactions, influenced by high local organic peroxy (RO_2) radical concentrations. The direct loss of radicals over the Arabian Gulf decreases the recycling probability and, therefore, the self-cleaning capacity compared to the Mediterranean atmosphere.

TEMPERATE LATITUDES

The analysis of our HO_x data collected over Europe during the campaign in the summer of 2020, compared with our data from the HOOVER campaign a few years earlier, revealed a considerable decrease in OH mixing ratios in the upper troposphere. We showed that this was primarily a result of markedly lower NO_x emissions from road and particularly air traffic during the pandemic shutdown, leading to suppressed OH recycling and, therefore, a reduced oxidation capacity of the upper troposphere. This might be a forerunner of the effects of reduced NO_x emissions in a future climate-neutral society.

At the CLOUD chamber experiment CERN, we study radical chemistry, new particle formation, and growth in the chemical regimes encountered during our expeditions. By comparison of our HO_2 measurements with results from the Br-CIMS from the University of Helsinki, we validated our HO_2 measurements under high isoprene and monoterpene concentrations.

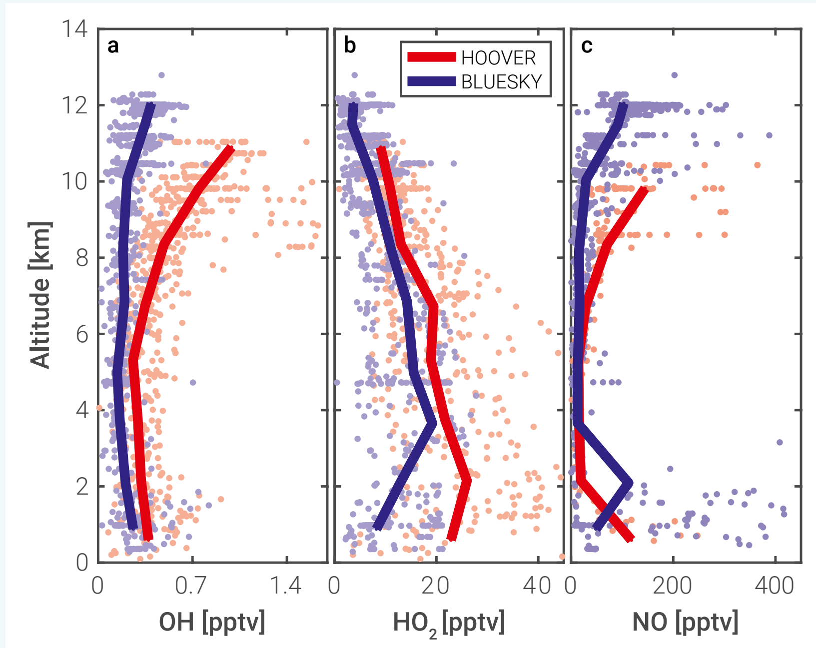

Figure 2: Vertical profiles of atmospheric trace gases (a) OH, (b) HO_2, (c) NO for the BLUESKY and HOOVER campaigns. While the HO_2 concentration is similar for BLUESKY as for HOOVER, the OH concentration, with less NO, is significantly lower. (Source: Sreedev Sreekumar, PhD thesis)

OUTLOOK

We aim to continue aircraft studies to investigate radical chemistry in the thus far understudied upper troposphere.

We are developing a new instrument to add highly sensitive SO_2 measurements based on the same principle as our HO_x measurements during upcoming field and CLOUD chamber campaigns.

At the ATTO tower in the Amazon, we will determine the canopy reduction factor for NO_x and measure the fluxes of NO_x and SO_2 in conjunction with HO_x measurements to study the atmospheric self-cleaning capacity within and above the rainforest.

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NUMERICAL MODELING OF ATMOSPHERIC CHEMISTRY

ANDREA POZZER – ATMOSPHERIC MODELLING GROUP

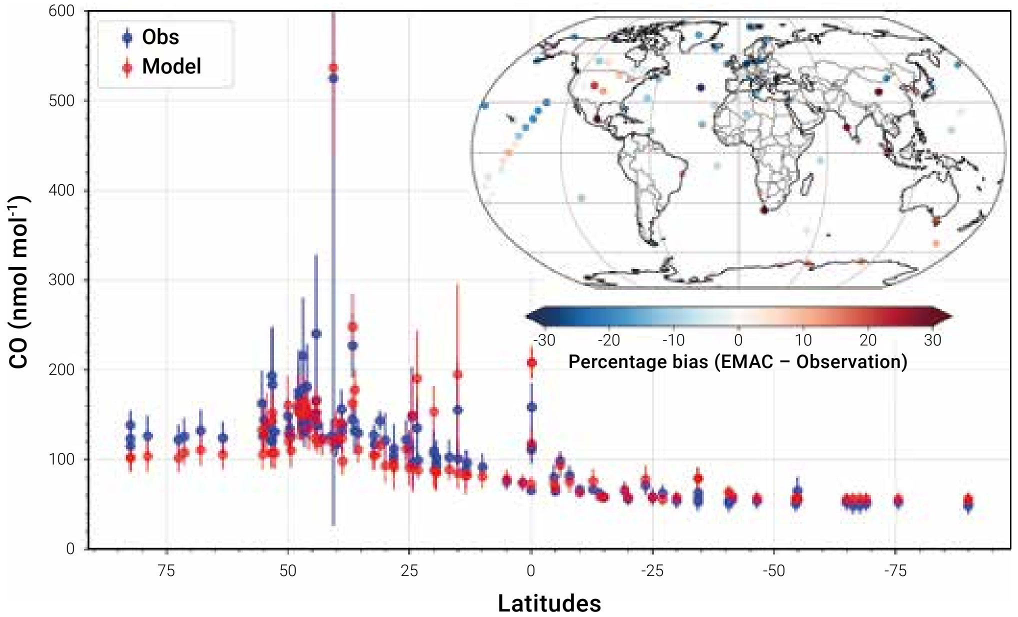


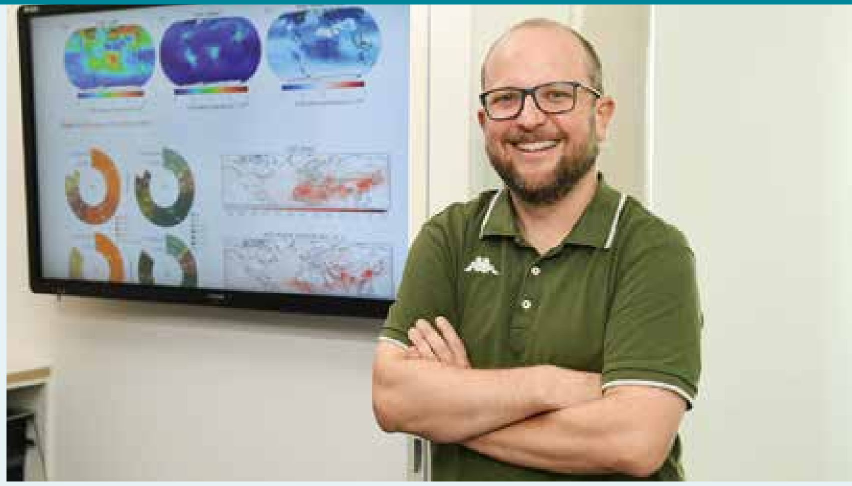
Figure 1: Annual means of measured and simulated CO mixing ratio at measurement stations. The error bars show the 1σ standard deviation of the annual mean (based on daily mean output). The map in the inset shows the annual bias between the simulation and measurements at the locations of the stations.

INTRODUCTION

The composition of our atmosphere is the result of a complex interplay between different processes, such as emissions, deposition, transport, and chemical and phase transformations. Aerosol particles and gases are strongly interconnected and influence the concentrations of atmospheric oxidants, pollutants, radiatively active species, clouds and the climate. Numerical models that incorporate these processes and the feedbacks between them can improve our theoretical understanding of the atmosphere.

RESULTS

In recent years, our team has made substantial progress in enhancing the capabilities of the EMAC (Earth system Model for Atmospheric Chemistry) global numerical model to account for reactive gases and aerosols. A detailed and comprehensive evaluation of the EMAC model, accounting for approximately 700 organic species, has been published using a detailed oxidation mechanism with more than 1,500 reactions and explicit phase transitions (Pozzer et al., 2022). This version of EMAC is one of the most comprehensive atmospheric chemistry climate model available to date. While the number of modelled non-methane volatile organic compounds (NMVOCs) is very large, their chemical decomposition mechanisms are well simulated, as illustrated by the comparison between the model results and observations of reaction intermediates such as carbon monoxide from observational networks (see Figure 1). The detailed data on the NMVOCs are unprecedented, allowing new studies on specific trace gases, secondary organic particle formation, and feedbacks between natural and anthropogenic emissions and atmospheric oxidation processes. For instance, the role of aromatics in our atmosphere has been investigated, revealing their regional significance for various other species and global air quality (Taraborrelli et al., 2021). We showed that in areas with high concentrations of NO_x, the chemistry of aromatics increases ozone and OH concentrations up to 12 % and 17 %, respectively. Further, the reaction of ozone with phenoxy radicals is a significant mechanism for loss of tropospheric O_3, the order of 200–300 Tg yr^{-1}, which is similar to the estimated ozone loss due to global bromine chemistry.



“Numerical models are integrative tools that facilitate the analysis of measurement data and the development of a comprehensive understanding of atmospheric composition.”

Apart from gas-phase chemistry, significant attention has been dedicated to aerosol modelling. The comprehensive NMVOC simulations with EMAC feed into detailed aerosol thermodynamics and microphysics schemes for more than 200 low-volatile species. Furthermore, the model now integrates and simulates the chemical and climatic impact of new particle nucleation pathways based on experiments performed in the CLOUD (Cosmics Leaving Outdoor Droplets) experimental facility at CERN. An illustration of EMAC's capabilities can be found in the study of Wang et al. (2022), which introduced a novel "synergistic nucleation" pathway, discovered in CLOUD laboratory experiments involving HNO_3–H_2SO_4–NH_3 interactions. The EMAC model was employed in this study to underscore the significance of this nucleation process in the control of particle number concentrations in the upper troposphere. The results reveal that this new nucleation pathway increases particle number concentrations by a factor of three to five in the outflow of the Asian monsoon and downwind over the Pacific Ocean; thus, this atmospheric transport mechanism is an important source of precursor gases to aerosol particles in the upper troposphere.

Another recent breakthrough with the EMAC model involves the first global simulation of ultrafine particle concentrations (UFP, with a diameter smaller than 100 nm), accounting for direct emissions from combustion processes, new particle formation, and growth (Kohl et al., 2023). Furthermore, the numerically simulated UFP distribution has been downscaled based on observations to an unprecedented 9 km horizontal resolution (Figure 2), obtaining a logarithmic scale correlation between observed and simulated UFP concentrations of $r = 0.95$. These model results are available for studies on public health, other impacts of atmospheric UFP, and for intercomparison with other regional and global models and datasets.

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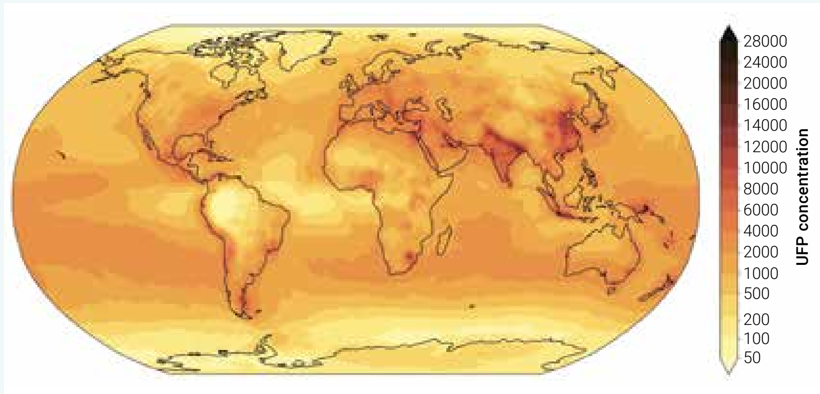


Figure 2: Annual average of global UFP for the year 2015 at high resolution (0.1° × 0.1°) in [1/cm³].

VOLATILE ORGANIC COMPOUNDS IN THE ATMOSPHERE

JONATHAN WILLIAMS – ORGANIC REACTIVE SPECIES GROUP

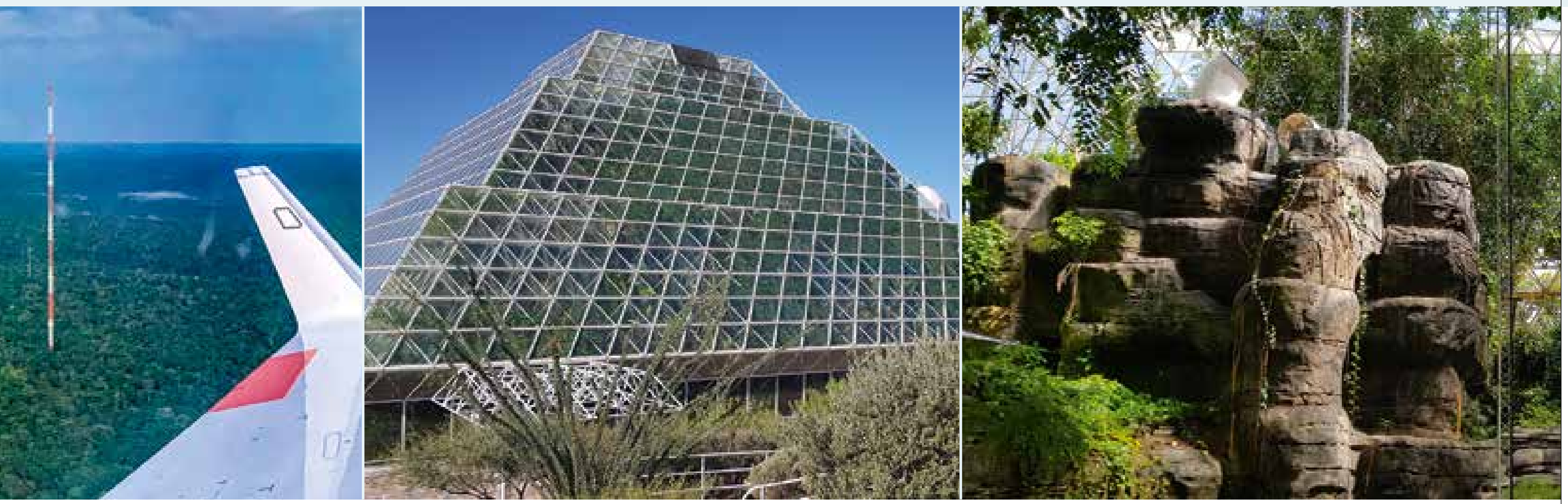


Figure 1: The HALO research aircraft flies past the ATTO tower (left). The BIOSPHERE, a controlled tropical rainforest ecosystem in Arizona, USA. Within this enclosed system, we are able to vary the meteorological conditions (center and right).

INTRODUCTION

Our group specializes in the measurement of volatile organic compounds (VOCs) in the atmosphere. We use highly sensitive mass spectrometers to identify and quantify hundreds of VOC species that are emitted from various sources and then oxidized in the air. We operate our instruments at remote ground sites (Amazon Tall Tower Observatory, ATTO), in enclosed mesocosms (BIOSPHERE), on ships (AQABA), and aircraft such as the High-Altitude Long Range (HALO) research aircraft. Recently, we have also used our instruments to investigate the indoor air chemistry of VOCs emitted by humans.

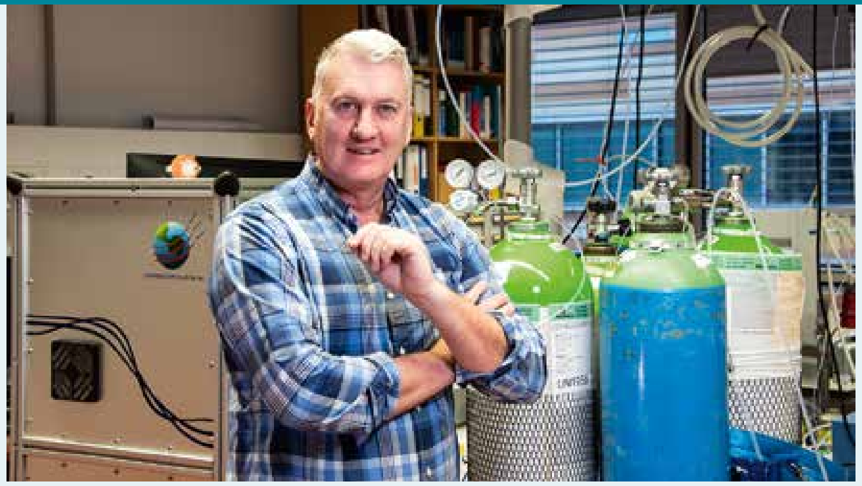
RESULTS

The Amazon rainforest is the largest source of VOCs for the Earth's atmosphere. Based on measurements from the 325-m-high ATTO tower made at different heights, times of the day, and across different seasons, we have comprehensively characterized biogenic VOCs, discovering important sesquiterpene fluxes from tropical soil, chiral terpene emissions, the importance of oxygenates for the OH reactivity budget, and how moss and lichen (cryptogamic covers) emit reactive sesquiterpenes but up-take oxygenated products. Further, we have used VOC measurements to indirectly determine atmospheric OH radical levels.

The HALO Aircraft has been used to gain information on the vertical distribution of VOCs from 300 m over the rainforest up to altitudes of 15 km. An online proton-transfer-reaction time-of-flight mass spectrometer and a custom-made fast gas chromatography-mass spectrometry instrument were operated in parallel on-board the HALO research aircraft during the BLUESKY and CAFE-BRAZIL campaigns (2020–2023). This enabled us to explore the fate of compounds emitted at ground level and convected to the upper troposphere where particle production occurs.

To complement the measurements made at the ATTO tower in the rainforest, we also conducted a large-scale experiment within the enclosed tropical rainforest mesocosm BIOSPHERE. Within this facility, the ecosystem was subjected to a prolonged three-month drought, simulating future conditions for the Amazon. We focused on how chiral monoterpene emissions changed in response to drought, finding that the two mirror-image forms of alpha pinene responded differently to progressive drying. Isotopic labelling established that vegetation emitted mainly de novo-synthesized (−)-α-pinene, whereas (+)-α-pinene was emitted from storage pools, so that we could follow enzymatic changes occurring within the leaves through air measurements.

As we spend an important part of our lives inside, indoor VOC emissions and chemistry are important for our overall exposure to airborne chemicals. Through a collaboration with the Danish Technical University (DTU), we comprehensively characterized indoor emissions from humans, including skin and breath-borne chemicals. Ozone exposure, clothing, temperature, and humidity were found to be important factors in these emissions. The measurements led to the discovery of the presence of an OH field that generates itself in the presence of ozone. This means that people are not only potent mobile emission sources but also a source of OH radicals indoors.



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

OUTLOOK

Over the next three years, 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. We intend to extend our characterization of VOC species in the Amazon rainforest at the ATTO site and to use the HALO aircraft to examine the chemistry of clean marine background atmospheric chemistry and transport in the CAFE-PACIFIC aircraft campaign.

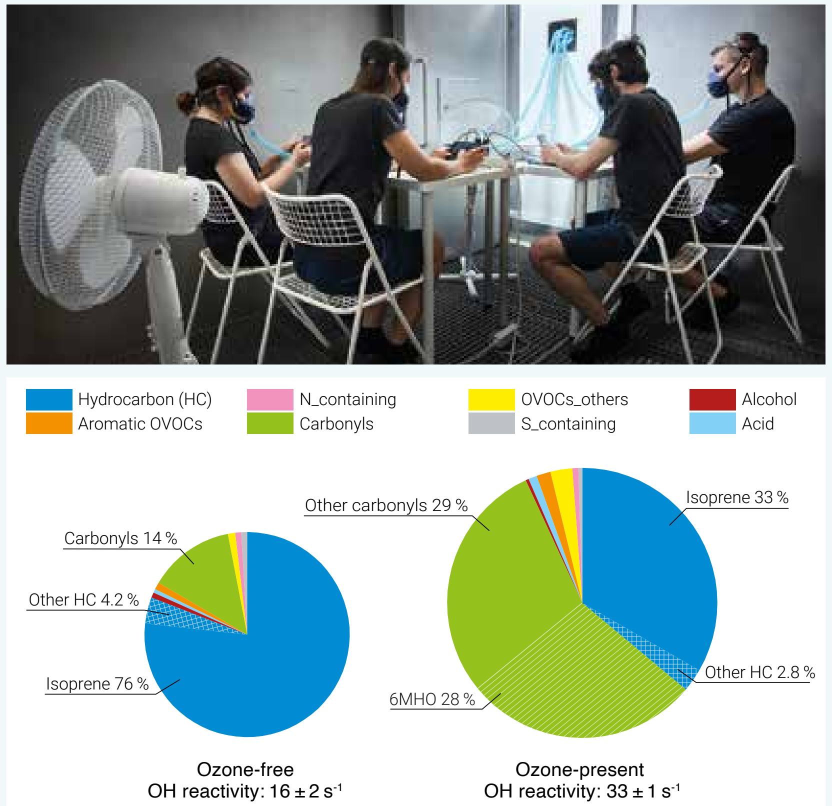


Figure 2: Human emissions from breath and skin measured separately in climate-controlled chambers. When exposed to ozone, human beings emit more compounds, more OH reactivity, and generate an associated OH field.

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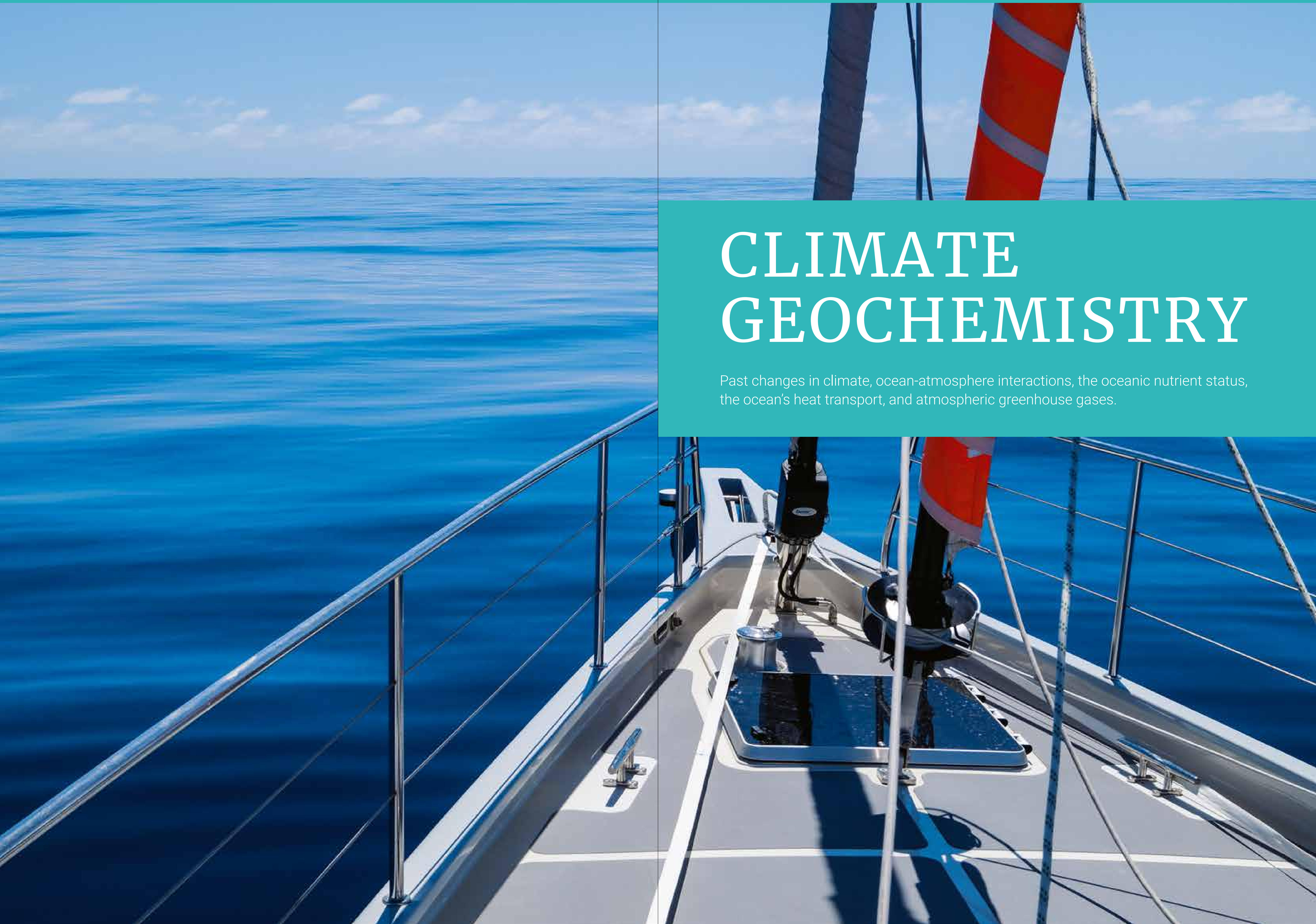

CLIMATE GEOCHEMISTRY

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

CLIMATE GEOCHEMISTRY DEPARTMENT

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 organized 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 paleo-proxies, both those measured at the 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 the Cariaco Basin off the coast of Venezuela, Lake Challa in the foothills of the Kilimanjaro, the Arabian Sea, the Dead Sea, and the maar lakes in the Eifel. We also investigate speleothems in Asia, Africa, and Central America and coral records in the tropical Pacific, amongst others.

Visit of Annalena Baerbock, the German Minister of Foreign Affairs, on the *S/Y Eugen Seibold*.

A second theme is 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 on 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.

The *S/Y Eugen Seibold*, donated by the Werner Siemens Foundation, is a technologically advanced research vessel that has been in full operation since May 2020. We have completed a full oceanographic transect in the North Atlantic, from Iceland to the equator between 2020–2022. Since March 2023, the *S/Y Eugen Seibold* has been operating in the equatorial Pacific to sample the upcoming/ongoing El Nino–La Nina oscillation. Given its design, 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. 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 with the organisms that produce them as they respond to in situ environmental conditions on a seasonal basis.

Since March 2020, Gerald Haug has been President of the German National Academy of Sciences Leopoldina. The Leopoldina has 1,650 members from more than 30 countries and almost all research areas, including 36 Nobel Laureates. The Leopoldina provides independent science-based advice to policy-makers and society on scientific and science policy matters. The Academy monitors, analyzes, and comments on scientific 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. 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 make recommendations for solving urgent global challenges to the participating heads of state and government in the run-up to each summit. The Leopoldina had the lead of the S7 meeting in 2022, where two topics related to this report have been in the focus: "Ocean and Cryosphere: The Need for Urgent International Action" and "Decarbonisation: The Case for Urgent International Action".

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DUST DELIVERY TO THE SOUTHERN OCEAN, MARINE PRODUCTIVITY AND CLIMATE FEEDBACKS

STEPHEN GALER – ISOTOPE BIOGEOCHEMISTRY GROUP

Figure 1: South America provides most long-range transported dust to the Atlantic sector of the Southern Ocean. The principal sources are glacial deposits in Patagonia (left) and the Altiplano Puna desert (right) based upon radiogenic isotope signatures.

> "We have to understand whether mineral dust input to the high-latitude oceans is a driver or a response to glacial-interglacial cycles."

We are looking at the millenial-scale effects of long-range South American dust deposition on fertilization of the HNLC (high nutrient low chlorophyll) Southern Ocean, to investigate whether dust input enhances marine productivity or merely responds to prevailing global climate conditions. This is a concerted effort to examine cause and effect and to test the Martin Hypothesis regarding micronutrient fertilization for ocean CO_2 drawdown, in a polar region setting of the world's oceans.

The main drivers and feedbacks for Southern Ocean productivity are (1) dust deposition (micronutrients; Martin highlighted iron in particular), (2) northward migration of the Southwesterlies during glacial periods (see our previous studies) – shifting the location of Southern Ocean fronts and enhancing regional upwelling (Ekman pumping) – along with (3) more general ocean circulation changes.

Dust inputs to the polar regions, delivering bioessential micronutrients, are potentially a major driver of marine productivity and were five-fold enhanced during glacials (Figure 2), but is this cause or effect?

In order to examine this question we have adopted a two-pronged approach. First, we want to determine where the dust is coming from, characterize its composition and track how these sources varied over time; for this we use Sr-Nd-Pb radiogenic isotope fingerprinting of sources and trace metal analysis. Second, we have been exploring the utility of barium stable isotope fractionation as a proxy for the abundance of organic matter in surface waters of the Southern Ocean to see the "effect" of dust on marine productivity.

We have analyzed an extensive suite of South American dust potential source areas – Sr-Nd-Pb radiogenic isotopes and trace metal signatures – to fingerprint where this long-range-transported dust originates: the samples were collected from a large number of Patagonian/Chilean glacial moraines as well as Argentinian loess deposits. The principal South American dust emissions originate from two regions: Patagonian glacial deposits

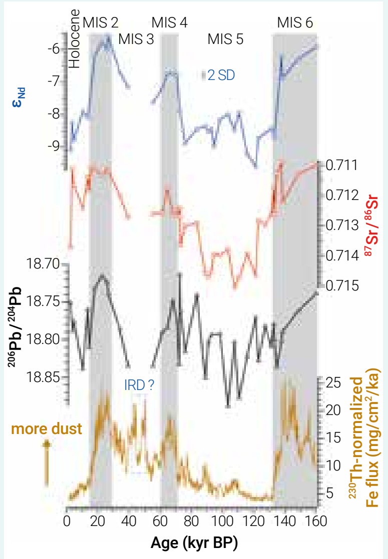

Figure 2: Dust fraction Nd-Sr-Pb radiogenic isotope record in Southern Ocean core ODP-1090 covering the last three glacial-interglacial cycles. Dust fluxes were up to five-fold higher during glacial periods (bottom, from Martínez-García et al. 2014) with an enhancement in Patagonian over Altiplano sources evident. IRD marks times of ice-rafted debris from Antarctica in the core.

and from the high-altitude Altiplano Puna region (Figure 1); we note that altitude is meteorologically favourable for long-range transport.

By analyzing dust fractions extracted from two cores from the Southern Ocean (e.g. ODP-1090, illustrated in Figure 2) we can show that during glacial periods, Patagonian dust sources were more predominant. This is a key observation, since it indicates that mechanical weathering is more significant than glacier or snow cover in enhancing net dust emission from glaciated regions, which is an important conclusion by itself.

To investigate the effects of dust on Southern Ocean marine productivity we use barium stable isotopic compositions, expressed in terms of the heavy-over-light isotope change $\delta^{138}/^{136}Ba$ in per-mil (‰). Barium is not a biologically-utilized element as far as it is known, but is depleted in surface seawaters which is thought to be due to in-situ precipitation of barite (barium sulphate) in oxygen-poor organic matter in surface waters.

We measured a surface transect and four depth profiles from the Southern Ocean along the Zero Meridian (Figure 3) from Polarstern cruise ANT XXIV/3 which show that the surface water depletion in barium can be related to the formation of barite in sinking organic matter. Further, the data follow a simple Rayleigh Law independent of whether they are in the Antarctic Circumpolar Current (ACC) or Weddell Gyre and are consistent with experimentally-derived isotope fractionation determined in the laboratory. Thus, we have a potential proxy in $\delta^{138}/^{136}Ba$

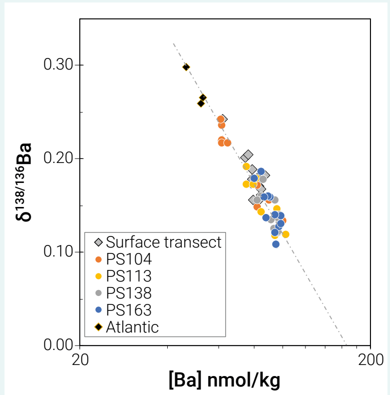

Figure 3: Barium isotopic compositions - expressed as $\delta^{138/136}Ba$ – from seawaters from the Southern Ocean along the Zero Meridian (cruise ANT XXIV/3) which includes surface waters from 47–67 °S along with four hydrocasts to the bottom from the ACC and Weddell Gyre. These data closely follow the Rayleigh Law with a solid/liquid fractionation factor of -0.2 ‰ $\Delta\delta^{138/136}Ba$, consistent with experiments of barite (barium sulphate) precipitation from seawater.

for the surface ocean sinking organic matter abundance (i.e. marine productivity), which can be related to the depletion of barium in seawater, archived in the barium isotope composition of barite in marine sedimentary cores. It is the latter that we intend to pursue in our further work to obtain Ba isotope paleo-proxy records of surface productivity that can potentially be relatable to dust input and atmospheric CO_2 sequestration over the past millenial climate cycles.

Lastly, we continue to exploit the potential of the *S/Y Eugen Seibold* underway air-filter sampling in determining the sources of West African dust outbreaks into the Eastern Atlantic Ocean.

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ENHANCED OCEAN OXYGENATION DURING PAST GEOLOGICAL WARM PERIODS

ALFREDO MARTÍNEZ-GARCÍA – ORGANIC ISOTOPE GEOCHEMISTRY GROUP

Figure 1: Dr. Alexandra Auderset analyzing the samples used to reconstruct the evolution of ODZs across the EECO and MMCO warm periods (left). Dr. Alan Foreman and Dr Nic Duprey collecting a coral core from Clipperton Atoll to reconstruct the variability of the ODZ over the past 100 years (center). Foraminifera samples used by Dr. Simone Moretti to reconstruct the response of ODZs to the PETM climate warming (right).

INTRODUCTION

Over the past three years, the Organic Isotope Geochemistry group has expanded the number of applications of a novel technique to measure the nitrogen isotopic composition of the trace amounts of organic material present within the mineral structure of different fossil types (e.g., foraminifera, diatoms, corals and tooth enamel). We have studied changes in ocean biogeochemistry in the past, with a particular focus on the reconstruction of the history of ocean oxygenation (see next section). In addition, we have pioneered the application of this technique to reconstruct the trophic structure of ancient ecosystems (see Lüdecke group), as well as to investigate the origins of photo-symbiosis in corals. Another important research line has been the combination of the analysis of organic biomarkers and inorganic tracers in speleothems to quantitatively reconstruct past climates (see Vonhof group).

RESULTS

Observations suggest that oxygen concentrations have been decreasing in coastal and open-ocean waters over the past five decades as a consequence of global warming, substantially expanding the volume of the ocean's Oxygen-Deficient Zones (ODZs). However, there is controversy as to the longer-term future of ODZs in response to prolonged climate warming, with both expansion and contraction having been predicted. We have contributed to this debate by studying the evolution of ODZs during warmer-than-modern periods of the geologic past.

In a first study we focused on two warm periods: the Middle Miocene Climatic Optimum (MMCO), when global temperatures where about 6 °C higher than today, and the Early Eocene Climatic Optimum (EECO), when temperatures were up to 13 °C warmer than today (Figure 2). We have shown that water-column denitrification in the eastern tropical North Pacific was greatly reduced during both the MMCO and the EECO (Auderset et al., 2022). Because denitrification is restricted to oxygen-poor waters, our results indicate that, in these two Cenozoic periods of sustained warmth, ODZs contracted. These results have been confirmed by recent studies using independent geochemical techniques (Hess et al., 2023; Wang et al., 2022).

In a more recent study, we investigated changes during the Paleocene–Eocene Thermal Maximum (PETM), which was the largest and fastest known pre-anthropogenic global warming event in the Cenozoic. While the rate of C emission was ~10 times slower than present, the amplitude of the reconstructed relative temperature change resembles the RCP 8.5 IPCC projections for future climate. For these reasons, the PETM may provide the most reliable geological evidence for the future state of ocean oxygenation. Our measurements of foraminifera-bound nitrogen isotopes indicate that the tropical North Pacific oxygen-deficient zone contracted rapidly during the PETM (Moretti et al., in review). Thus, our results from the study of warmer-than-modern periods of the past suggest that, contrary to most expectations, the ODZs of the ocean may eventually contract in response to protracted global warming.

"Evidence from past warm climates suggests that, contrary to most expectations, the oxygen-deficient zones of the ocean may contract in response to climate warming."

OUTLOOK

Following up on these results from the distant geologic past, we are now focussing on constraining the evolution of ODZs across the Anthropocene. Compilations of historical dissolved oxygen concentration measurements over the past century are very sparse and do not allow discrimination of oscillations from longer term (e.g., global warming-driven) trends. We have recently measured the nitrogen isotopic composition of a series of corals collected along the ODZ of the Equatorial Pacific (Figure1). Our preliminary results suggest no secular trend in ODZs over the past 80 years, but instead show strong decadal variations, indicating that the available direct instrumental observations, which are based on discontinuous data, are less robust than previously assumed (Duprey et al., in preparation). We are currently continuing this research by studying new coral cores collected in multiple new research campaigns that we have led over the past years.

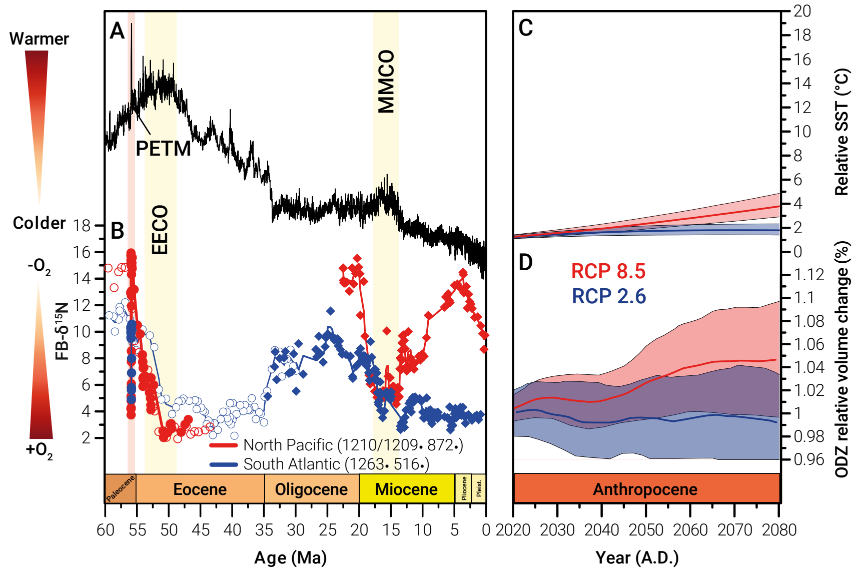

Figure 2: (A) Evolution of global temperature over the past 60 million years. (B) Foraminifera-bound $\delta^{15}N$ across the EECO, MMCO and the PETM (Auderset et al. 2022; Moretti et al., in review). Predicted evolution of global T (C) and ODZ relative volume change (D) over this century (IPCC Sixth Assessment Report, Climate Change 2021: The Physical Science Basis).

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PROBING THE OPEN OCEAN FOR CLIMATE GEOCHEMISTRY WITH THE EUGEN SEIBOLD RESEARCH SAILING YACHT

RALF SCHIEBEL – MICROPALEONTOLOGY GROUP

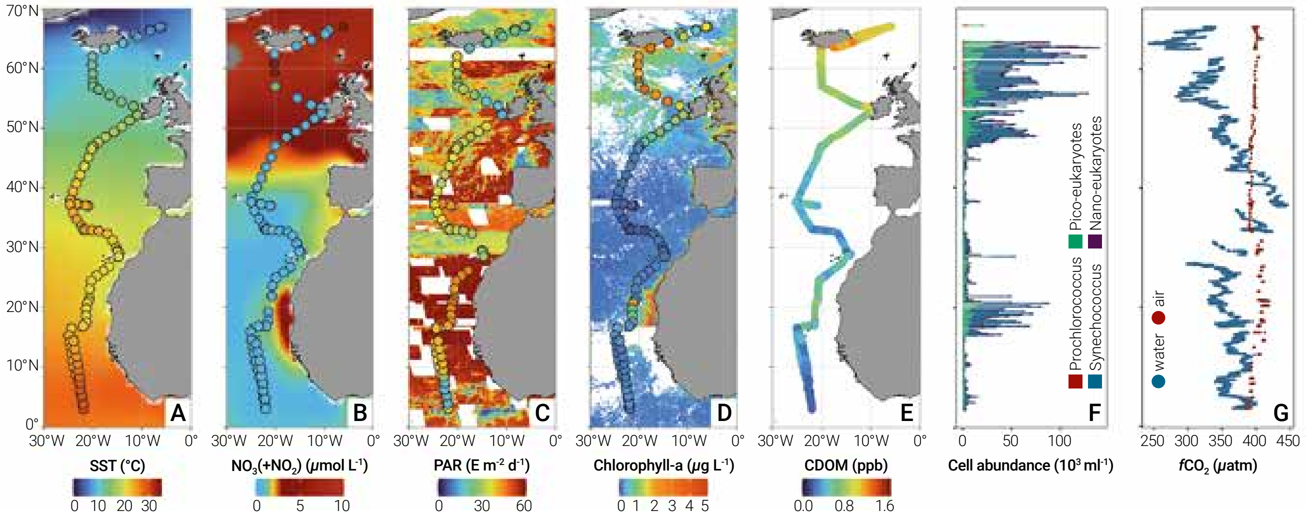

Figure 1: Data obtained with the *SYES* along a transect in the eastern North Atlantic in 2020 and 2021, in comparison to time-averaged datasets (background color in A to D). A) Sea surface temperature (SST), and B) $NO_3 + NO_2$ concentrations vs. annual average *World Ocean Atlas* SST and NO_3, respectively. C) Measured photosynthetically active radiation (PAR) and D) chlorophyll fluorescence in comparison to *AQUA MODIS* satellite data on irradiance (4 km res.) and chlorophyll *a* (8-day av.), respectively. E) Measured chromophoric dissolved organic matter (CDOM, *ECOtriplet* fluorometer), and F) total phytoplankton cells (*CytoSense* flow cytometer). G) CO_2 concentration in air (red) and surface water (blue). Deviations of measured data from the annual averages result from variations of conditions over the different time-scales (Aardema et al., submitted), Level-1 data in A, C, and D are at 1-Hz resolution and binned (100 bins) for visualization.

The first campaign of the *S/Y Eugen Seibold (SYES)* in the eastern North Atlantic (ENA) between Iceland and the equator, from 2019 to 2022, collected a wealth of biogeochemical data and samples from the atmosphere and surface ocean over the course of 15 expeditions and targeted projects (Figure 1). The different biomes of the ENA were sampled for seasonal variations of the biogeochemistry of the water column across the thermocline. Educational projects were undertaken with Swiss, German, and West African students at Mindelo, Cape Verde.

Expeditions were planned and conducted with the guidance of near-real time data supplied by satellite, which facilitated targeted sampling of small-to-mesoscale hydrological features such as eddies and provide a comprehensive context for the collected measurements and samples.

Quality-controlled data have been published on pangaea.de. Data and samples are analyzed in collaboration with, e.g., the Universities of Princeton, Las Palmas, and Oldenburg, the Max Planck Institute for Marine Microbiology (Bremen), Alfred Wegener Institute (AWI, Bremerhaven), Centre de Recherche et d'enseignement multidisciplinaire international (CEREGE, Aix-en-Provence), and the Smithsonian Tropical Research Institute (STRI, Panama). The entire suite of data is being applied to refine the calibration of paleoceanographic and paleoclimate proxies in terms of both upper ocean and atmospheric variables (Chaabane et al., 2023; Knecht et al., 2023; Repschläger et al., 2023).

Marine photosynthesis is the first step in energy capture in the ocean and is fundamental for global biogeochemical processes and ecosystem function. Thus, data on phytoplankton photophysiology were acquired. Data from fast repetition rate fluorometry (FRRf) and flow cytometry show that phytoplankton taxa are differentially affected by environmental conditions over diel cycles and sub-mesoscale hydrological features. Photophysiological effects explain the interplay between the phytoplankton community and its environment (Aardema et al., 2023).

Phytoplankton abundances at (sub-)micron size (≤ 20 µm) were analysed using semi-continuous flow cytometry. Across biomes and seasons, we observed distinctive patterns in cyanobacterial and nano-eukaryotic prevalence (Figure 1). Total phytoplankton abundances in the surface mixed layer ranged from < 10 * 10^3 cells mL^{-1} in the oligotrophic subtropical gyres to 150 * 10^3 cells mL^{-1} in the northern North Atlantic in spring, the Mauritanian upwelling, and the deep chlorophyll maximum (DCM), the last being dominated by cyanobacteria in the more oligotrophic waters.

Johann Wolfgang von Goethe, September 2, 1820, on climate observations: "It seems to me that the matter is of a large scale and difficult in many senses."

The combination of large-scale analyses of biologically active gases, microbial communities, and environmental data yield insights into the roles of the marine microbiota in CO_2 uptake and release, with implications for atmospheric CO_2. Data of unprecedented spatial and temporal resolution show the dynamics of both surface water and atmospheric CO_2 fugacity over a wide range of productivity regimes. Higher chlorophyll-*a* concentrations at more northern latitudes (July 2020) and the West African upwelling are associated with low surface water fCO_2 and elevated dissolved fCO_2, due to rates of net photosynthetic carbon fixation. In contrast, in the more oligotrophic tropics and subtropics, surface water fCO_2 is closer to and sometimes higher than atmospheric fCO_2. However, the high-resolution data show frequent deviations from this overall pattern and provide a more systematic understanding of upper ocean CO_2 turnover (Figure 2).

The *SYES* crossed the Atlantic and Caribbean Sea over New Year 2022/2023, sampling a zonal transect along 13 °N for Saharan dust and nutrient input, for the ground truthing of nitrogen and carbon isotope studies of past changes in the tropical Atlantic, and for studying phenomena such as the modern *Sargassum* bloom. In March 2023, the *SYES* arrived in the tropical Eastern Pacific (TEP) with the goal of capturing the biogeochemistry of an entire El Niño cycle. The campaign in the TEP is being realized in close cooperation with STRI and the Darwin Centre at Galapagos.

First ocean-atmosphere profiles across the TEP and the northern edge of the Peruvian–Ecuadorian upwelling were sampled in August 2023 for climate, hydrography, and biogeochemistry of the anticipated 2023/2024 El Niño. Seasonal expeditions to the upwelling system off Peru and Ecuador, in the Gulf of Papagayo, and Gulf of Panama regions influenced by mountain gap wind jets, will produce detailed information on the climate geochemistry of the El Niño Southern Oscillation (ENSO) and related ocean–atmosphere exchange processes.

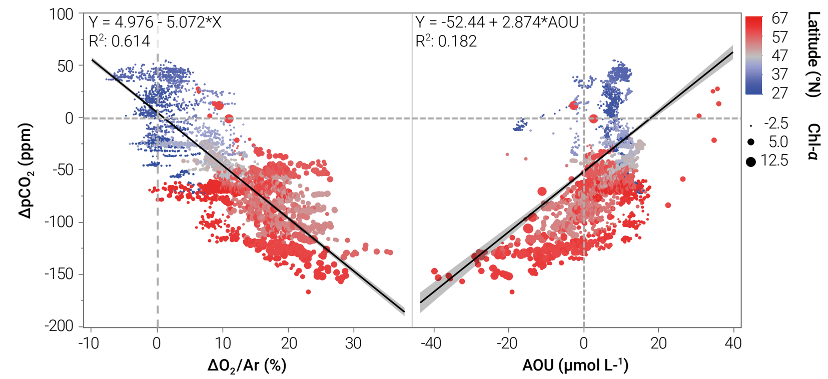

Figure 2: (A) Latitudinal changes in pCO_2, O_2, and apparent oxygen utilization (AOU) between the subpolar (red), temperate (gray), and subtropical (blue) eastern North Atlantic. At higher latitudes, higher chlorophyll-*α* (Chl-*α*, larger dots) concentrations, higher oxygen saturation (ΔO_2/Ar), and lower AOU result in an overall oceanic CO_2 sink, whereas the ocean is a CO_2 source at lower latitudes. Relative to the overall pattern (black regression lines), deviations are frequently captured by the high-resolution data produced with the *SYES*, providing insight into the rate of marine CO_2 turnover.

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ACKNOWLEDGEMENTS

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NOVEL ISOTOPIC MEASUREMENTS IN CARBONATES FOR CLIMATE RECONSTRUCTION

HUBERT VONHOF – INORGANIC GAS ISOTOPE GEOCHEMISTRY GROUP

Figure 1: Magnificent speleothem formations in the Caverna do Diabo (Brazil).

INTRODUCTION

Speleothems (stalagmites, stalactites, and flowstones) have become increasingly important for continental paleoclimate reconstruction. Speleothem calcite can be dated very precisely by uranium-series chronology, providing superior age control of speleothem paleoclimate records. While it has become clear that speleothems are sensitive recorders of paleoclimatic change, it has proven difficult to extract quantifiable proxy data from these records. This is illustrated, for example, in the many oxygen isotope ($\delta^{18}O$) records of speleothem calcite, as published over the past decades, that are generally interpreted to be influenced simultaneously by land surface temperature and by changes in $\delta^{18}O$ values of rainfall in the cave area. Without additional information, the classical proxy systems are unable to quantitatively deconvolve these signals.

RESEARCH OBJECTIVES AND RESULTS

The work in our group is dedicated to developing geochemical proxy systems that improve speleothem-based paleoclimate reconstructions so that parameters like land surface temperature or the isotope composition of paleo-rainfall can be reconstructed. We have done that by further refining our instrumentation for the stable isotope analysis of fluid inclusion water (microscopic amounts of rain water captured in speleothem calcite) and the optimization and calibration of the TEX_{86} paleotemperature proxy for speleothems (the latter in close collaboration with the group of Alfredo Martinez-Garcia). Further strategic collaboration with Goethe University Frankfurt (Germany) and the University of Bergen (Norway) provides access to the latest progress in clumped isotope paleothermometry (Wassenburg et al., 2021) and speleothem fluid inclusion microthermometry (Meckler et al., 2021).

In recent years, we have used these techniques to develop much-needed quantitative paleoclimate data in some key geographical areas that are currently experiencing accelerated anthropogenic climate change (Levy et al., 2023; Markowska et al., in revision; Wassenburg et al., 2021).

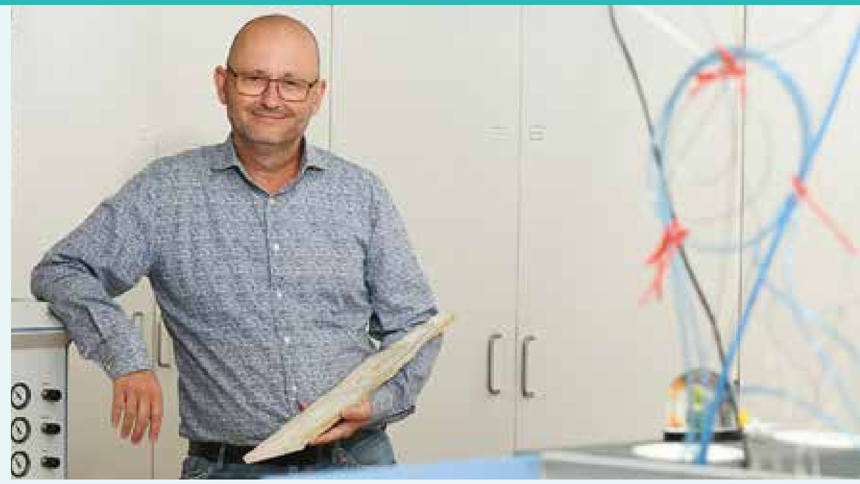
OUTLOOK

Our current research focus is on the evolution of monsoon systems as recorded in speleothem time series. In that context, we run field-based projects in relatively unexplored areas (e.g., Africa, and parts of Saudi Arabia) and maintain active collaboration with laboratories in South America and China. One new aspect that we are currently working towards, together with Johannes Gutenberg University Mainz and Goethe University Frankfurt, is the routine application of the U-Pb dating method, which will enable the study of much older speleothems than previously possible (Markowska et al., in revision; Figure 1).

FURTHER PROJECTS

Continental paleoclimate projects:
We run projects based on vertebrate (bone and teeth) isotope records to investigate paleoclimatological controls on animal diet. This is usually in close connection with novel nitrogen isotope work in the groups of Tina Lüdecke and Alfredo Martinez-Garcia (Lüdecke et al., 2022). In some of our projects we apply strontium isotope analysis to vertebrate fossils, and as such we also work in close collaboration with the group of Steve Galer at the institute.

Paleoceanographical projects:
In the context of the workflow around the *S/Y Eugen Seibold* research vessel, we carry out dissolved inorganic carbon isotope ($\delta^{13}C$) analysis of water samples routinely taken on board. We also provide corresponding $\delta^{13}C$ and $\delta^{18}O$ data for calcareous microplankton collected in the water column, in collaboration with the group of Ralf Schiebel. Further, we routinely perform $\delta^{13}C$ and $\delta^{18}O$ analysis of fossil marine biogenic carbonates, with a focus on very small (< 4 µg) $CaCO_3$ samples, enabling, for example, the routine analysis of a wide range of single-specimen planktonic foraminifera.



"Improving paleoclimate reconstructions from speleothem records through the development of new geochemical proxies."

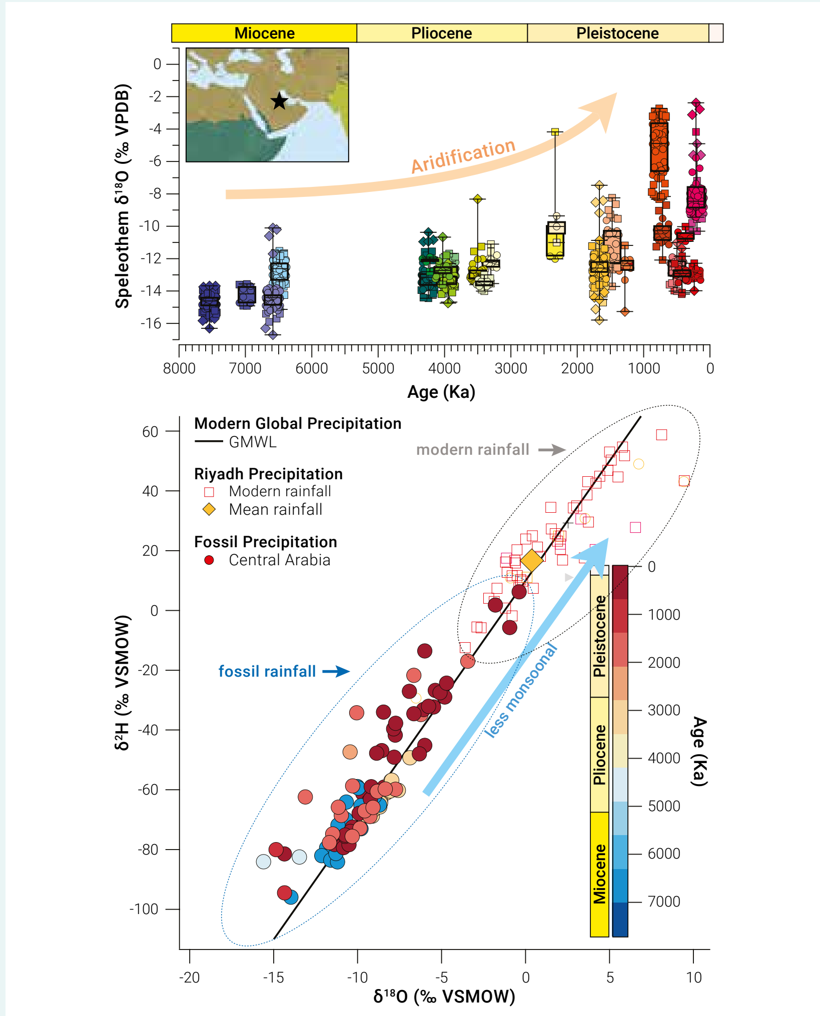


Figure 2: Markowska et al., *in revision*. Top panel: Speleothem $\delta^{18}O$ data from central Saudi Arabia record past humid episodes in this now hyper-arid desert. Bottom panel: Fluid inclusion isotope data of these speleothems detail decreasing monsoonal rainfall over time.

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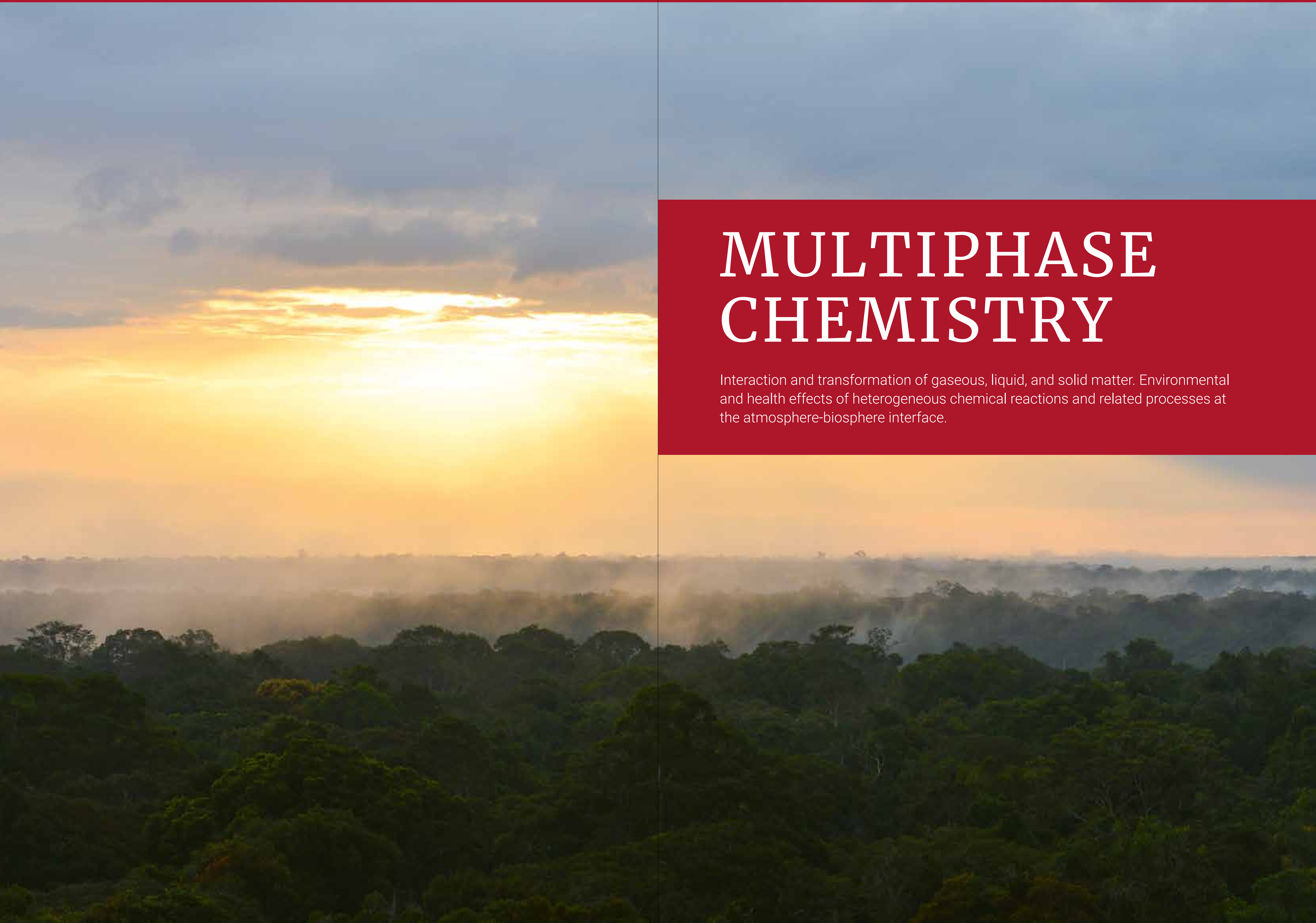

MULTIPHASE CHEMISTRY

Interaction and transformation of gaseous, liquid, and solid matter. Environmental and health effects of heterogeneous chemical reactions and related processes at the atmosphere-biosphere interface.

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 oxides, 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, i.e., in the present era of globally pervasive human influence on planet Earth. Key research topics addressed in the department include the transformation and environmental effects of primary biological and secondary biogenic aerosols as well as the chemical mechanisms, environmental causes, and mitigation of oxidative stress, allergies, and related inflammatory disorders.

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 bioassays and DNA analyses, microscopic and spectroscopic techniques, and kinetic process models.

The current main areas of research in the Multiphase Chemistry Department are broadly reflected by the research group names: Aerosol Analysis and Microscopy (*C. Pöhlker* et al.), Biomolecular Analyses and Interactions (*J. Fröhlich* et al.), Chemical Kinetics and Reaction Mechanisms (*T. Berkemeier* et al.), Inflammatory Processes (*K. Lucas* et al.), and Organic Pollutants and Exposure (*G. Lammel* et al.). Detailed information about recent results and ongoing research in each of these groups and subject areas is given in the individual reports on the following pages. We collaborate closely with other departments and research groups at the institute as well as alumni and research partners around the world, including former project team and research group leaders who recently moved on to new positions: *H. Su* at the Chinese Academy of Sciences, Institute of Atmospheric Physics in Beijing, *M. Pöhlker* at the Leibniz Tropospheric Research Institute in Leipzig, and *H. Tong* at the Helmholtz Center Hereon in Geesthacht.

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 project and group reports on the following pages. They comprise deep insights into the sources and interactions of aerosols in the Amazon rainforest; redox reactions, protein modifications, and oxidative stress in epithelial lining fluid; and chemical modulations of inflammatory immune responses.

In collaboration with international partners, we use and operate major research platforms for Earth system studies, such as the Amazon Tall Tower Observatory (ATTO), the German High Altitude and Long-Range Research Aircraft (HALO), and the *S/Y Eugen Seibold (SYES)* research yacht. Regional and global model simulations are performed in collaboration with the Atmospheric Chemistry Department (*J. Lelieveld* et al.) and with the independent Minerva Research Group (*Y. Cheng* et al.). During the COVID-19 pandemic, we also pursued scientific studies and outreach to help elucidate the transmission of SARS-CoV-2 by respiratory particles and mitigate their spread by protective measures as outlined on the following pages.

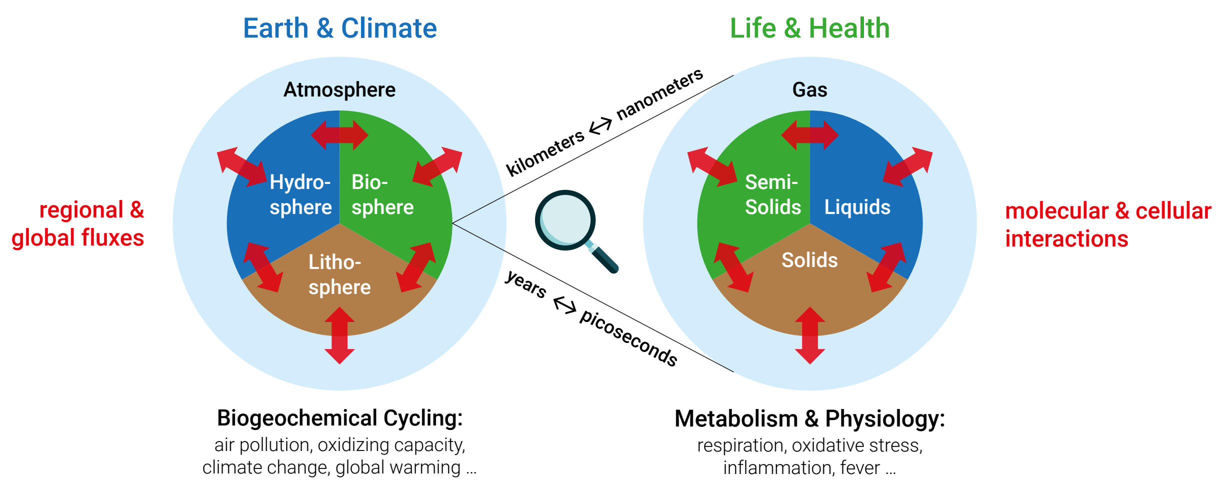

Figure 1: Multiphase processes influencing the Earth system, climate, life, and public health over a wide range of spatial and temporal scales: chemical reactions, mass transport, and phase transitions between gases, liquids, solids, and semisolid substances involved in molecular and cellular interactions as well as in regional and global fluxes of biogeochemical cycling.

ULRICH PÖSCHL

October 9, 1969 Born in Klagenfurt, Austria

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

1996–1997 Schrödinger fellow and postdoctoral researcher at the Massachusetts Institute of Technology, Cambridge, USA

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, Germany

2005–2012 Research group leader at the Max Planck Institute for Chemistry and lecturer at the Johannes Gutenberg University Mainz (JGU), Germany

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 Mainz (JGU)

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AEROSOL ANALYSIS AND MICROSCOPY

CHRISTOPHER PÖHLKER

"Atmospheric aerosols play a prime role in the hydrology and biogeochemistry of the rapidly changing rainforest ecosystem."

Figure 1: Scenes of clouds and fog recorded by a webcam on top of the ATTO tower.

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 with its prevailing biogenic aerosols represents a window into the pre-industrial and unpolluted past. We are applying a broad spectrum of techniques to shed light on the properties of these particles and their roles in atmospheric and biogeochemical cycles. One of our focal points has been to unravel the interplay of new particle formation in the upper troposphere followed by downward transport versus the direct emission of biogenic salts and microorganisms from the biosphere. During the contrasting dry season, smoke from mostly man-made forest and savanna fires overwhelm the biogenic aerosol. We found characteristically different signatures for smoke from Amazonian and African fires and determined that long-range transport of air masses from Africa has a marked influence on the Amazonian atmosphere. The continuous measurements at ATTO are complemented by 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 a core mission of the ATTO project. Through long-term aerosol measurements in combination with remote sensing of cloud properties, we have resolved the cloud microphysical response to changes in the aerosol population over a wide range of pollution states. Besides ATTO, we conduct aerosol sampling and observations on the *S/Y Eugen Seibold* research vessel and on the HALO research aircraft. The observed divergences between different environments and conditions provide deep insights into the effects of anthropogenic activities on air quality and climate in the Anthropocene.

ADVANCED MICROSPECTROSCOPY OF AEROSOL PARTICLES AND ENVIRONMENTAL SAMPLES

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. We also apply the novel x-ray ptychography technique to environmental samples, such as rock varnish, which can resolve nanoscale differences in the valence states of the key elements manganese and iron. During the COVID-19 pandemic, we used x-ray microspectroscopy for a nanoscale characterization of respiration aerosols that play a major role in airborne disease transmission.

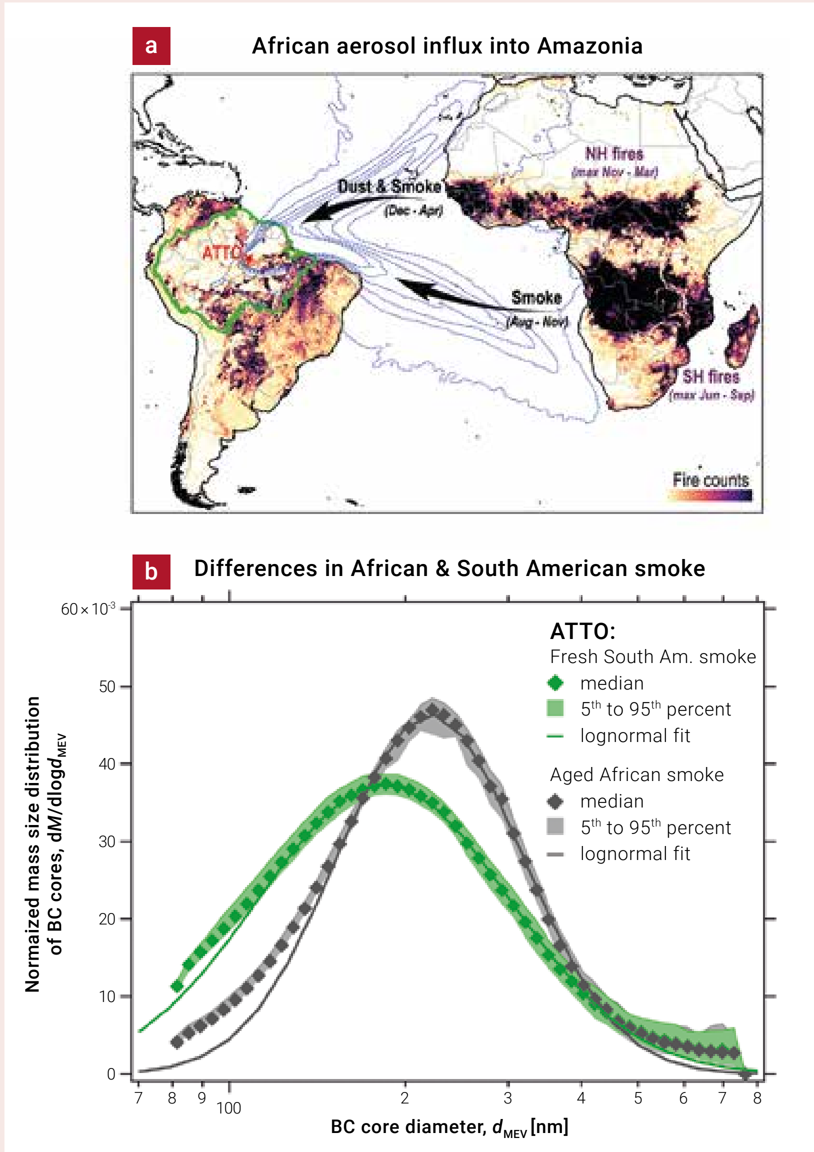

Figure 2: Transport of African smoke and characteristic black carbon mass size distributions. (a) Geography of transport smoke from African biomass burning across the Atlantic into the Amazon. The Atlantic trade winds north and south of the intertropical conversion zone are shown by means of a backward trajectory ensemble starting at ATTO. Biomass burning is represented by a map with the average density of satellite-detected fires. (b) Characteristic differences in the shape of refractory black carbon (rBC) mass size distributions of African vs South American smoke, measured at ATTO. Adapted from Holanda et al., 2023.

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BIOMOLECULAR ANALYSES AND INTERACTIONS

JANINE FRÖHLICH

> "We aim to understand the properties, interactions, and effects of biological aerosol particles and biomolecule interactions with air pollutants."

Figure 1: Release of grass pollen (left). Exposure of an allergen sample to a mixture of ozone and nitrogen dioxide gas (middle). Reaction mechanism of protein nitration and oligomerization upon exposure to ozone and nitrogen dioxide (Reinmuth-Selzle et al., 2017) (right).

INTRODUCTION

Biological aerosol particles and biomolecules are ubiquitous in our environment. Airborne bacteria, fungal spores, pollen, and other bioparticles play crucial roles in the spread of organisms and ecosystems, and they can act as allergens and pathogens or serve as ice nuclei (IN) and influence the formation of precipitation. In the atmosphere, bioparticles and biomolecules can undergo chemical and physical transformation, stress, and aging which changes their chemical, physical, and biological properties. For example, pollen can burst and release allergenic proteins into the atmosphere. The proteins can react with reactive oxygen and nitrogen species, either in the atmosphere or after inhalation in the respiratory tract, leading to chemical modification. These modifications can affect the allergenic and inflammatory potential of the proteins and may explain the increasing prevalence of allergic and inflammatory diseases that has been observed around the globe. The composition, abundance, impact, and multiphase chemical interactions of biological aerosols and components, however, are not yet well characterized and quantified. Thus, we investigate the chemical modification of allergenic proteins and its effects on immune responses; the molecular mechanisms of bacterial ice nucleation; and the diversity of biological aerosol particles and atmospheric ice nuclei.

RESULTS

In collaboration with the Lucas group, we found that the grass pollen allergen Phl p 5 elicited Toll-like receptor 4 (TLR4) activation in a reporter cell line. TLR4 is a pattern recognition receptor of the innate immune system and plays a central role in inflammatory processes. We also found that peroxynitrite, a physiological reactive species that is particularly important in oxidative stress and inflammation, causes significant protein nitration and oligomerization of Phl p 5. Moreover, the TLR4 activation increased when Phl p 5 was chemically modified with peroxynitrite. TLR4 activation may play a role in sensitization to the grass pollen allergen and may become particular important during oxidative stress and inflammation by creating positive feedback loops via TLR4 signaling.

Bacterial IN are among the most efficient biological IN, but their mechanism of action remains elusive. In collaboration with the Max Planck Institute for Polymer Research in Mainz, we have investigated the interactions of bacterial IN proteins with water molecules using sum-frequency generation spectroscopy. We found that the structural ordering of interfacial water molecules during cooling induced by heat-inactivated IN proteins is similar to that induced by active IN proteins. Thus, an intact three-dimensional protein structure – rather than water ordering alone – appears to be the essential factor for bacterial ice nucleation. Additionally, experiments with aqueous solutions of phospholipids and lipopolysaccharides showed that these membrane components are not part of the active nucleation site but rather enable protein assembly in an intact cell membrane. We also observed substantially improved ice nucleation when deuterated water was used, indicating stabilization of IN protein assemblies by the stronger hydrogen bonds of D_2O.

To study bioaerosol composition and ice nucleation activity of aerosol samples collected in a rural dryland on the eastern Mediterranean island of Cyprus we used shotgun metagenomic sequencing and freezing experiments. We found rainfall-related short-term changes in bioaerosol and IN composition, which may influence the hydrological cycle as well as public health. Particle washout and fungal spore discharge appear to play major roles in the observed composition changes.

OUTLOOK

In the next three years, we will continue to explore the reactions of proteins with reactive oxygen and nitrogen species and their roles in inflammation and allergy. We also intend to study the interactions of allergens with microbial components and particulate matter and the effects of these interactions on allergen modification and immune responses.

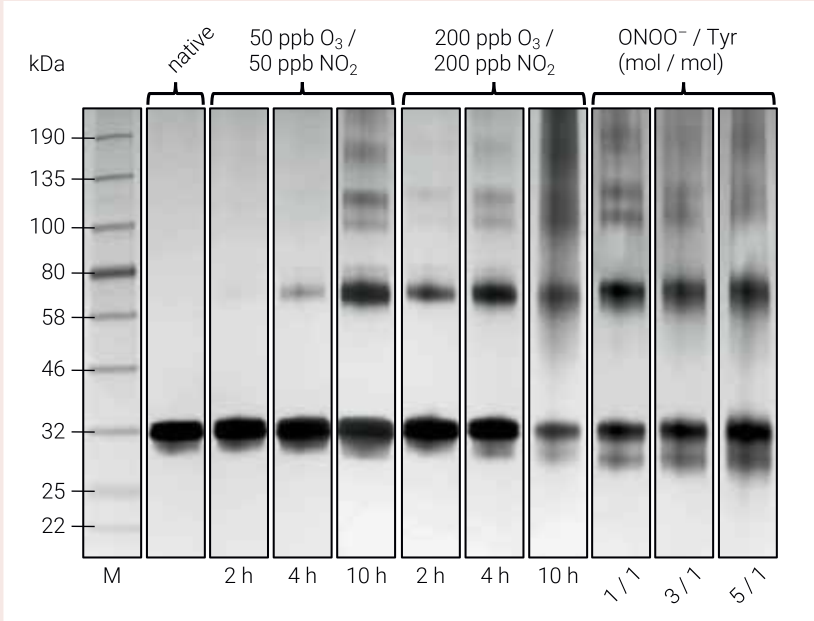

Figure 2: Silver-stained Sodium Dodecyl Sulfate – PolyAcrylamide Gel Electrophoresis (SDS-PAGE) of Phl p 5 before and after exposure to ozone and nitrogen dioxide (O_3/NO_2) and reaction with peroxynitrite (ONOO-) (Adapted from Backes et al., 2021). The native Phl p 5 consists of monomers (~ 32 kDa) and the modified Phl p 5 samples have monomers and different proportions of dimers and higher oligomers.

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CHEMICAL KINETICS AND REACTION MECHANISMS

THOMAS BERKEMEIER

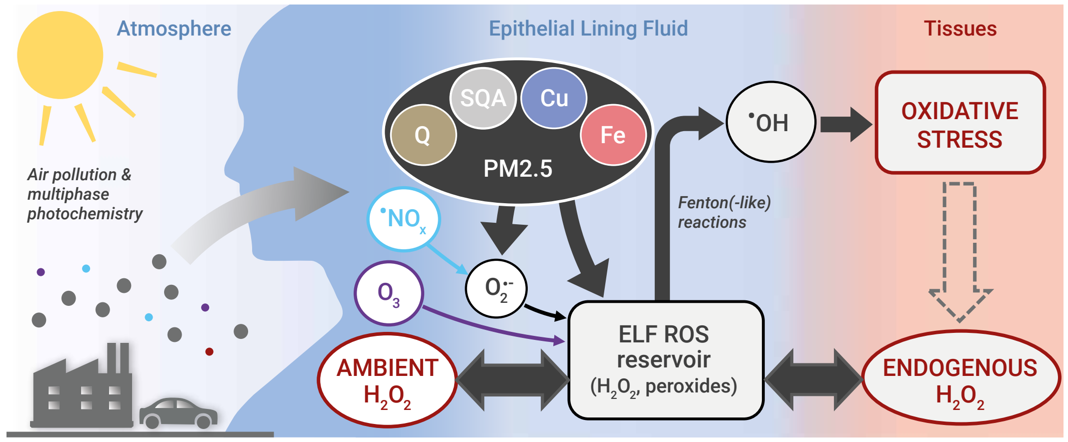


Figure 1: Health effects of atmospheric air pollution. Transition metal-mediated, catalytic conversion of peroxides leads to formation of the highly reactive OH radical that can trigger oxidative stress and, ultimately, cell death. Adapted from Dovrou et al. (2023).

Many processes in the atmosphere and in the human body occur at and across interfaces in multiphase systems consisting of gaseous, liquid, and solid phases. A detailed understanding and description of reaction kinetics in these systems is vital for predicting the rates at which oxidants are formed, compounds degrade, and surfaces evolve. We aim to resolve the processes and uncertainties governing atmospheric, physiological, and technical multiphase reaction systems at the molecular level. For this purpose, we develop and use advanced computer models and algorithms to design and analyze laboratory experiments and to understand the underlying reaction mechanisms.

KINETIC MULTILAYER MODELS, UNCERTAINTY QUANTIFICATION AND MACHINE LEARNING METHODS

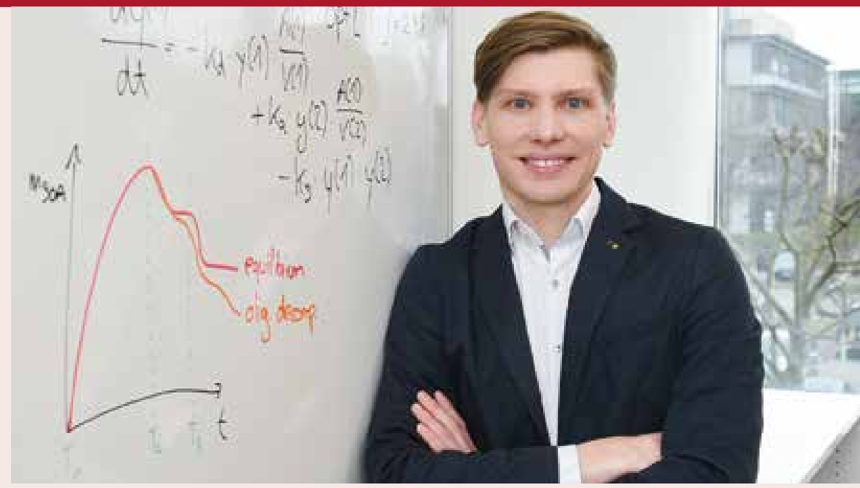
We use a Monte Carlo genetic algorithm (MCGA) for efficient, automated, and unbiased global optimization of model input parameters by simultaneous fitting to multiple experimental data sets. Recently, we have developed methods coupling global optimization with ensemble solutions to assess and control parametric uncertainty of kinetic model simulations. This approach facilitated a new computer method that helps to identify the optimal, i.e., most insightful experimental conditions for laboratory experiments, which we named 'kinetic compass'. For computationally expensive calculations, we developed machine learning methods that generate inexpensive surrogates of kinetic models, such as kinetic multilayer models of aerosol and cloud chemistry (KM-SUB, KM-GAP). We found neural networks to be highly accurate (R^2 = 0.998) and to operate at a fraction of the computational cost (< 0.1 %). We also used convolutional neural networks as quantitative structure-activity relationship (QSAR) models to predict the reduction potential of quinones from a large literature data set. The method enables efficient screening of new compounds for their relevance in atmospheric chemistry and public health.

CHEMICAL AGEING AND TRANSFORMATION OF ATMOSPHERIC AEROSOLS

The heterogeneous oxidation of oleic acid particles by ozone is one of the most frequently investigated model systems for the oxidative processing of atmospheric aerosols. Yet, existing kinetic and mechanistic analyses revealed systematic differences and inconsistencies that have been a matter of ongoing debate. We were able to reconcile most experimental data available in the literature with consistent sets of multiphase chemical kinetic parameters. We concluded that secondary chemistry involving Criegee intermediates is crucial for resolving the discrepancies in earlier studies.

AIR POLLUTION HEALTH EFFECTS AND OXIDATIVE STRESS

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 investigate how the composition of fine particulate matter (PM2.5) and gaseous air pollution are linked to their negative health outcomes. Inhalation of air pollution contributes to production of reactive oxygen species (ROS) in the epithelial lining fluid (ELF) of the human lung and causes oxidative stress (Figure 1). We have developed a computer model, KM-SUB-ELF 2.0, that couples the chemistry of air pollutants in ELF with chemical and biological processes in tissues and blood vessels. The model is able to simulate molecular modification and damage to proteins resulting from air pollution. We could show that ROS and oxidant concentrations in the ELF (Figure 2a) may be primarily determined by the release of endogenous ROS and the inhalation of ambient gas-phase H_2O_2 (Figure 2b), as chemical production from inhaled PM2.5 only accounted for a minor fraction of total ROS (~ 1 %). In contrast, the production of highly noxious OH radicals in the ELF (Figure 2c) is determined (> 90 %) by chemical reactions involving the air pollutants PM2.5 and nitrogen dioxide (NO_2) in the current model. Hence, our findings suggest that the adverse health effects of PM2.5 may not be primarily related to direct chemical production of ROS, but rather to the conversion of peroxides into more reactive species. We also found that traffic-related air pollutants, PM2.5 and NO_2, act synergistically in the formation of nitrotyrosine, a common biomarker of oxidative stress (Figure 2d).



"We combine experiments and models to understand the multiphase chemical kinetics and health effects of atmospheric air pollutants."

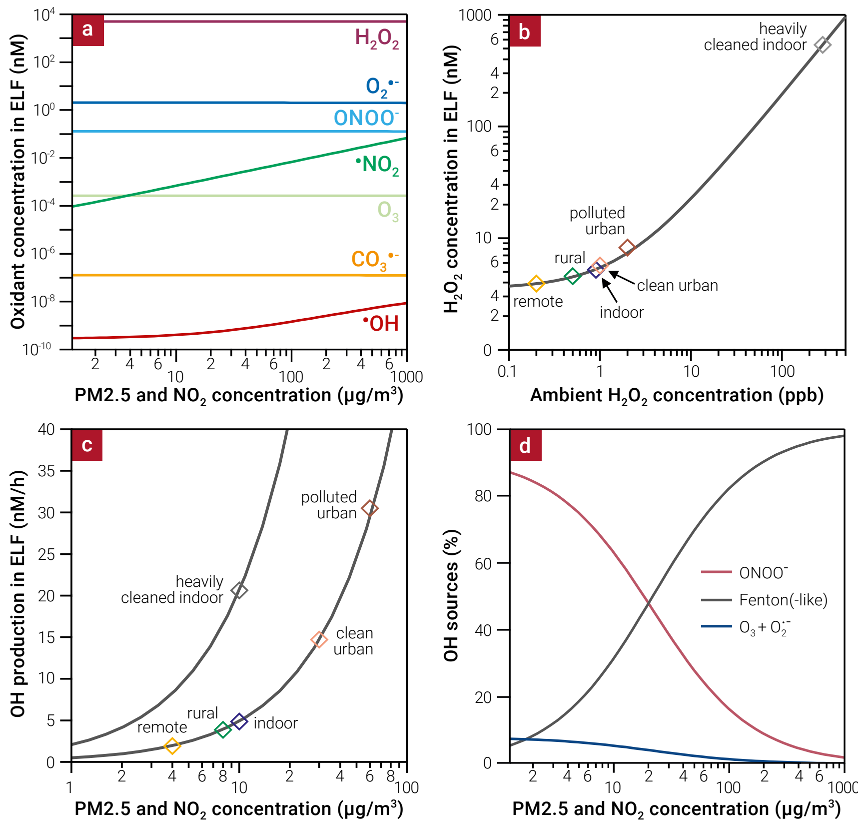


Figure 2: Model results of epithelial lining fluid composition and chemistry after exposure to air pollution in KM-SUB-ELF 2.0. (a) Reactive oxygen species, (b) hydrogen peroxide (H_2O_2), (c) hydroxyl radicals (OH), and (d) sources of OH under different pollution scenarios. Adapted from Dovrou et al. (2023) and Mishra et al. (2023).

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INFLAMMATORY PROCESSES

KURT LUCAS

“Insights into the chemical mechanisms of inflammatory processes are opening up new perspectives for diagnosis and treatment of diseases.”

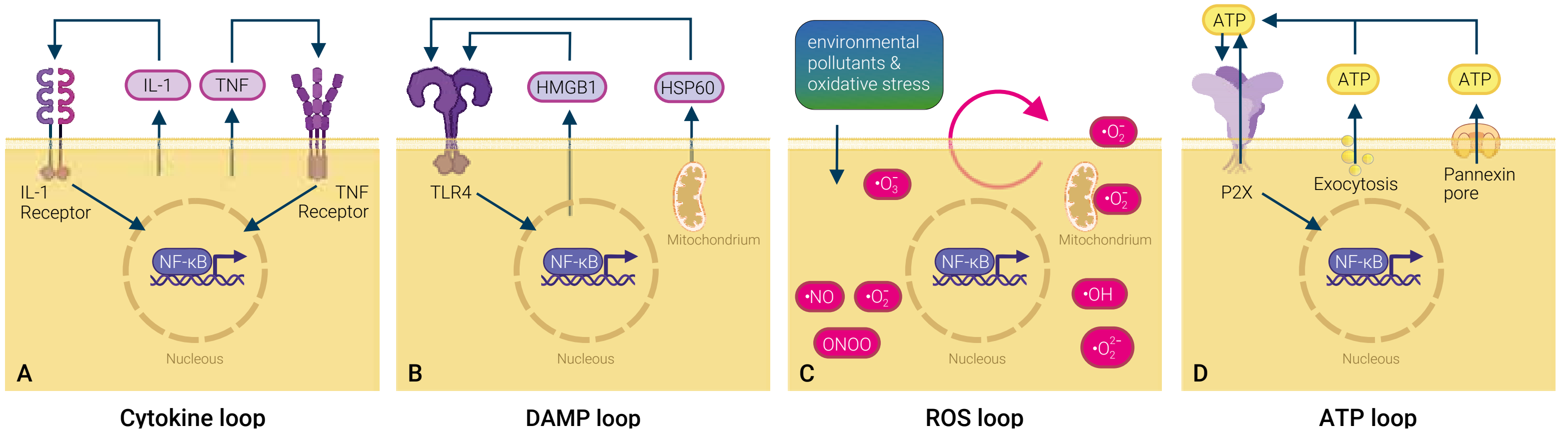

Figure 1: Recursive molecular processes (feedback loops) that drive inflammation via NF-κB activation. The cytokines interleukin-1 (IL-1) and tumor necrosis factor (TNF) activate NF-κB via their specific receptors. Toll-like receptor 4 TLR4 engages in a DAMP loop with high mobility group box 1 (HMGB1) and heat shock proteins (HSPs). Oxidative stress induces the generation of more ROS/RNS and can activate NF-κB (ROS loop). Extracellular ATP is a potent mediator of NF-κB activation and is sensed via purinergic receptors such as those from the P2X family. As a result, more ATP is released from cells, creating an ATP-dependent loop.

Inflammatory processes play an essential role in the human immune system, but the underlying chemical mechanisms are not fully understood. Our studies focus on recursive molecular loops that can amplify inflammation. We are also investigating how substances such as plant extracts and molecular hydrogen can effectively attenuate inflammation in acute and chronic diseases, including allergies, chronic fatigue syndrome (CFS), and long COVID. In addition, we study 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 increased activation of pattern recognition receptors (PRRs) and inflammatory responses. Our research is carried out in close cooperation with the Fröhlich group, the University Medical Center, and the Institute of Pharmacy of the Johannes Gutenberg University Mainz (JGU) as well as other collaborators from the biomedical sciences.

Inflammatory processes are a response to infection or injury, and their function is to fight pathogens and repair damaged tissue. Molecular signaling during inflammation is complex and dynamic. Interleukin-1 (IL-1) and tumor necrosis factor (TNF) activate the transcription factor NF-κB, which controls the expression of about 250 mostly proinflammatory genes, including IL-1 and TNF. This feedback can form a loop, here termed cytokine loop (Figure 1A). NF-kB also activates the transcription of IL-6, IL-8, and many others. Unregulated NF-κB activation can result in a cytokine storm, which is often fatal.

A second loop that activates NF-κB results from damage-associated molecular patterns such as heat shock proteins (HSPs) and high mobility group box 1 (HMGB1). They are released during inflammation and sensed by PRRs such as Toll-like Receptor 4 (TLR4) (Figure 1B). We are exploring herbal compounds that can block TLR2 or TLR4, e.g., Ceylon cinnamon extract and specifically cinnamaldehyde.

A third loop of NF-κB activation is the overproduction of ROS/RNS (Figure 1C). Such reactive species can be of environmental or physiological origin. In principle, the ingestion of molecular hydrogen induces the production of the antioxidants thioredoxin and glutathione, and, thus, molecular hydrogen can mitigate ROS/RNS during inflammation. In collaboration with the JGU Institute of Pharmacy, an effervescent tablet was developed to produce hydrogen-enriched water.

In addition, we found a fourth loop in inflammation signaling that is triggered by adenosine triphosphate (ATP) (Figure 1D). Outside the cell, ATP is a potent pro-inflammatory stimulant. Extracellular ATP is sensed by purinergic receptors such as P2X4 and P2X7. In concert with the channel protein pannexin, more ATP is released. We hypothesize that the ATP loop may be causal for long COVID and we suggest that the four recursive loops of inflammation (cytokine, DAMP, ROS/RNS and ATP) occur simultaneously and interact in an autocrine and paracrine manner (Figure 2). If the hypothesis can be confirmed, it may pave the way for better diagnostics and treatment of long COVID.

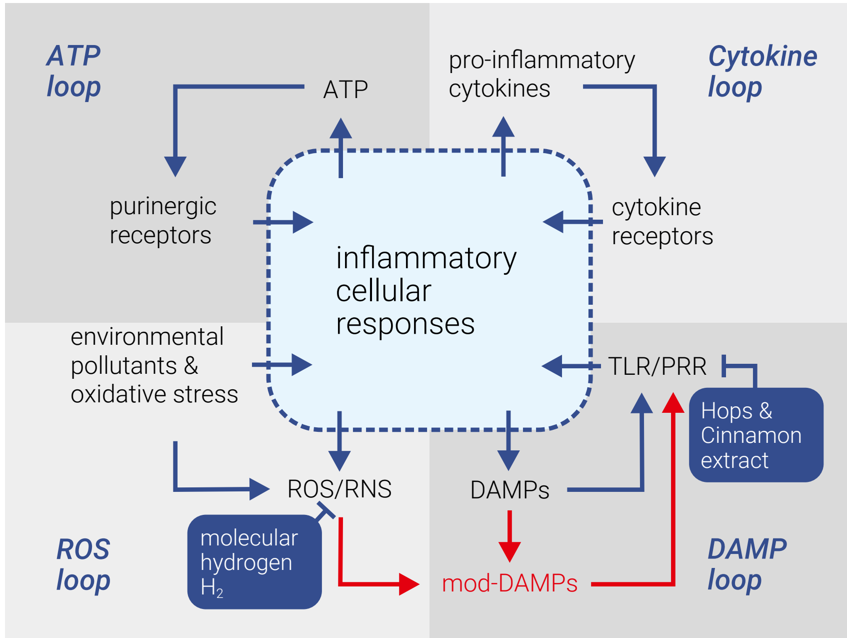

Figure 2: Amplification of inflammatory processes and innate immune responses during inflammation. The four feedback loops are interrelated and can be triggered by environmental pollutants, oxidative stress, injury, or infection.

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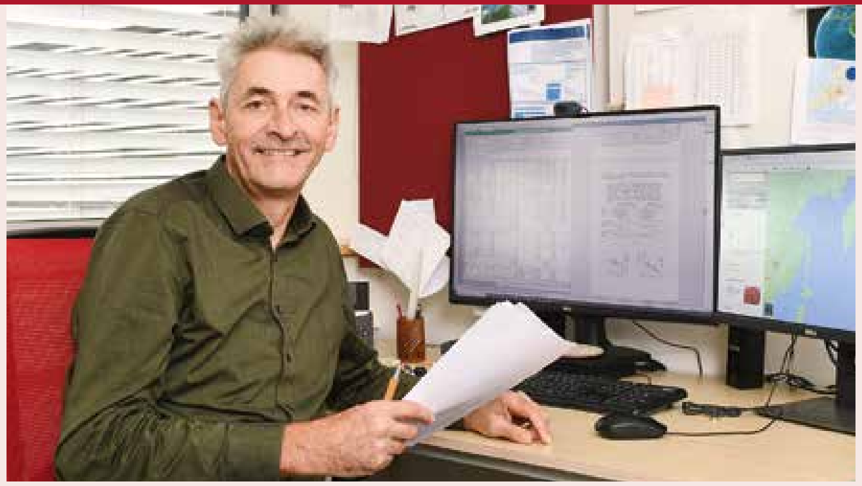
ORGANIC POLLUTANTS AND EXPOSURE

GERHARD LAMMEL



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

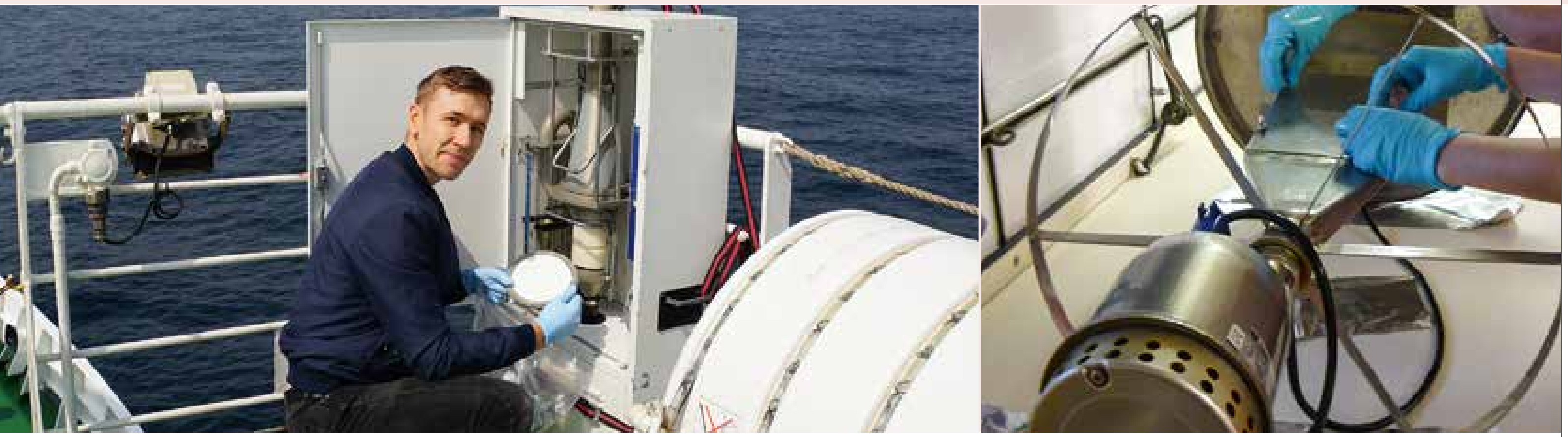


Figure 1: Sampling atmospheric trace gases and aerosol particles (left) and surface seawater (right) on board research vessels.

INTRODUCTION

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 they 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 vastly exceeds the atmospheric residence time. The latter depends strongly on partitioning in the aerosol.

Also, many long-lived organic pollutants are detrimental to human health upon chronic exposure. Apart from inhalation, uptake as food is a dominant exposure path, which is relevant for lipophilic pollutants that bio-accumulate in food webs.

RESULTS

Endosulfan is an organochlorine insecticide which was applied mostly in subtropical and tropical agriculture, largely as a substitute for DDT, which had been banned since the 1970s. It is thought that endosulfan is now distributed globally, including in oceans and the Arctic. It was banned in 2013, but remains stored in soils, water bodies and also in the atmosphere and continues to circulate in the Earth system. The substance's fate is not fully understood, as the pollutant's distribution and its degradability in soils, seawater and in the atmosphere are insufficiently characterized.

For the first time, we determined the levels of endosulfan in air and ocean surface water of the Atlantic Ocean, based on air and water samples collected on board research vessels (RV Meteor and *S/Y Eugen Seibold*) and at coastal sites, from southern mid latitudes to the Arctic, and subsequent trace analysis. This project is part of the collaborative research with the RECETOX Centre of the Masaryk University, Brno, Czech Republic.

Unlike other organochlorine pesticides, the concentrations of endosulfan in seawater are found to be particularly high in the western South Atlantic, clearly influenced by the historically high emissions from South American countries. The observations suggest that historical reversion of the vertical flow – from atmospheric deposition to re-volatilization to the marine atmosphere – started in this sea region.

In order to quantify degradability of endosulfan in air, we determined $k_{OH} = 5.8 \times 10^{-11} \exp(-1960\ K/T)\ cm^3\ s^{-1}$ as the reaction rate coefficient with the hydroxyl radical by means of pulsed vacuum UV flash photolysis and time-resolved resonance fluorescence. This value suggests photochemical atmospheric half-lives between 2 and 6 months in low and mid latitudes and even longer in high latitudes. The new value is more than one order of magnitude below the model prediction (QSAR: EPIsuite/AOPwin, USEPA), which was previously used for the pesticide's environmental risk assessment. The observed trend of the pollutant's concentration in the environment following the ban suggests that degradation in soils and waters might have been overestimated, too.

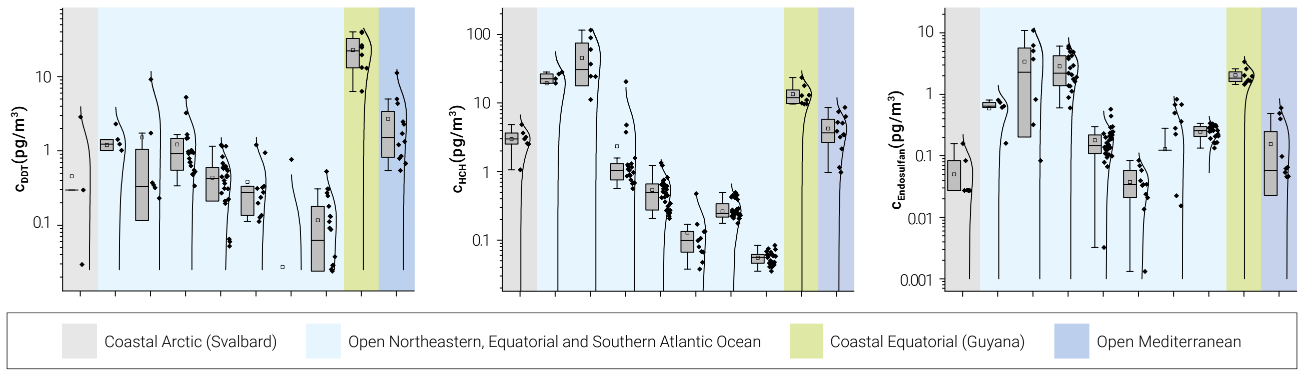


Figure 2: Distributions of the organochlorine pesticides DDT (left), hexachlorocyclohexane (center) and endosulfan (right) in marine air (sum of isomers and metabolites, sampled on board ships and at coastal sites, various seasons).

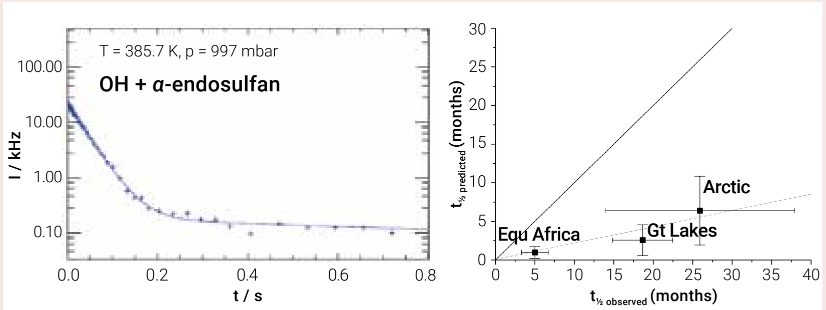


Figure 3: Endosulfan: decay kinetics in air (left) and comparison of model-predicted (multimedia model) and observed (air monitoring networks) total environmental half-lives of endosulfan illustrating the existence of unknown sinks in soil or water.

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MULTIDISCIPLINARY EXCHANGE AND COLLABORATION

ULRICH PÖSCHL

"Multidisciplinary exchange, collaboration, and open science are essential for a prosperous Anthropocene."

1

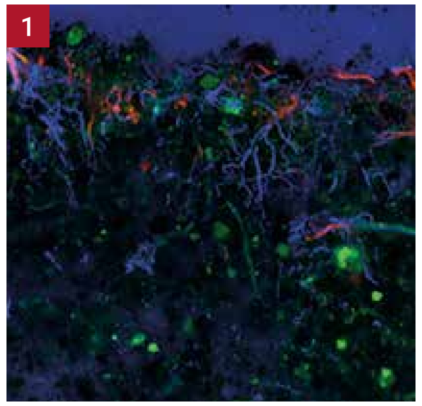

Figure 1: Fluorescence micrographs of cyanobacteria-dominated biocrust with photoautotrophic organisms in red, sand grains in green, and polysaccharides in blue (scale bar 0.6 mm; Kratz et al., 2022).

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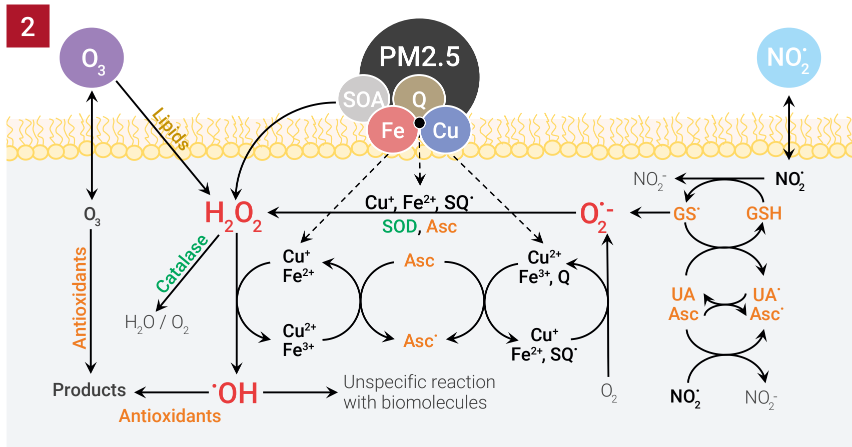

Figure 2: Production, interconversion, and scavenging of reactive oxygen species (ROS) by air pollutants and endogenous molecules in the epithelial lining fluid (ELF; Lelieveld et al., 2021).

The Anthropocene, i.e., the present era of globally pervasive human influence on planet Earth, is characterized by a widespread increase in air pollutants including combustion- or traffic-related aerosol particles, nitrogen oxides, and ozone. These pollutants can have a strong influence on atmospheric chemistry and physics, climate, and public health, but their actual interactions and effects remain to be fully unraveled and quantified. Among the key questions and challenges are the active interplay, coupling, and mutual interference of different types of anthropogenic and biogenic traces gases, particles, and their exchange across the atmosphere–biosphere interface.

A molecular understanding of heterogeneous or multiphase chemical reactions between gas molecules and viscous liquid, semi-solid, or glassy organic substrates depends on the description and quantification of the kinetics of accommodation at the surface, transfer across the gas–substrate interface, and further transport into the bulk of the substrate (adsorption vs. absorption). For this purpose, we have introduced a novel kinetic parameter: an effective mass accommodation coefficient that depends on penetration depth and is a function of surface accommodation coefficient, volatility, bulk diffusivity, and the condensed phase reaction rate coefficient. The new approach can be combined with the traditional Fuchs–Sutugin approximation of mass-transport kinetics. It resolves apparent discrepancies of several orders of magnitude between mass accommodation coefficients derived in earlier studies from experimental data or from molecular dynamics simulations of gas–particle partitioning in secondary organic aerosols, ranging between unity and 10^{-2}.

In a series of collaborative studies involving biologists, chemists, and geoscientists across and beyond the institute, we found that biological soil crusts and other cryptogamic covers have a major impact on the biogeochemical cycling and atmospheric abundance of carbon, nitrogen, and mineral dust. Recent investigations showed how the emissions of reactive nitrogen gases like HONO and NO biological soil crusts depend on the microbial composition, heterogeneity, water content, and activation of different genes. Moreover, we investigated the effects of biocrusts on regional and global dust cycling. A first estimate based on a combination of experimental data and model calculations revealed that biocrusts reduce the global atmospheric dust emissions by ~ 60 %, preventing the release of ~ 0.7 Pg dust per year. Overall, the results show that biocrust effects should be taken into account in the modelling, mitigation, and management of global change.

With regard to water uptake and activation of aerosol particles serving as cloud condensation nuclei (CCN), we compiled a large data set of globally distributed field measurements that were performed over the past two decades and cover a wide range of conditions from pristine rainforest to polluted megacity air. From these measurement data, we have derived global average values for the effective hygroscopicity of fine aerosol mass fractions of organic particulate matter and inorganic ions (κ_{org} = 0.12 ± 0.02, κ_{inorg} = 0.63 ± 0.01). Model calculations suggest that the sensitivity of global climate forcing to changes in κ_{org} and κ_{inorg} is small and that the global average parameter values provide a robust approximation and constraint for an important aspect of global climate modelling.

Collaborative studies with biomedical researchers provide insights into the mechanisms and interactions by which air pollutants and other environmental stressors impact human health. Kinetic model studies revealed how different types of pollutants influence the production and interconversion of reactive oxygen species (ROS) in the epithelial lining fluid of the human respiratory tract, whereby the formation of hydroxyl radicals may be most relevant for the generation of oxidative stress and adverse physiological effects. Experimental investigations showed that co-exposure to air pollution and traffic-related noise can lead to synergistic effects that may contribute substantially to the burden of disease in urban and industrial settings.

With regard to the COVID-19 pandemic, we collaborated with partners across and beyond the institute to assess indoor infection risks and elucidate the efficacy and limitations of face masks. Moreover, we investigated the effectiveness, energy efficiency, and sustainability of different ventilation methods. We showed that continuous natural ventilation through partially opened windows, optionally supported by simple technical devices like exhaust fans (mechanical extract ventilation), is a simple and highly effective way to ventilate classrooms and similar indoor environments in an energy-saving, resource-efficient, and climate-friendly manner – also beyond the pandemic (www.ventilation-mainz.de; Klimach et al. 2022; Helleis et al. 2023, https://zenodo.org/record/8382177).

OPEN SCIENCE

Experiences at the science-policy interface related to the pandemic, air quality, climate, and human health confirmed that open science is essential for efficient multi- and transdisciplinary exchange. As stated in the opening remarks of the Berlin Open Access Conference 2023 (oa2020.org/b16-conference/agenda), transparent forms of quality assurance that can be followed, reproduced, and refined by everybody around the world are among the main reasons why full and immediate open access to scholarly research publications is needed. In times of growing irrationality, alternative facts, postfactual discussions, and fake news, it seems ever more important to demonstrate the effectiveness of the scientific discourse as a reference for societal decision making. Thus, open access, open peer review, and interactive public discussion are important steps on the way to an epistemic web that documents the scientific discourse in accordance with critical rationalism – openly telling the world not only what we know, but also how well we know it, and where the limitations are (www.mpic.de/5438504/poeschl-agu-fellow).

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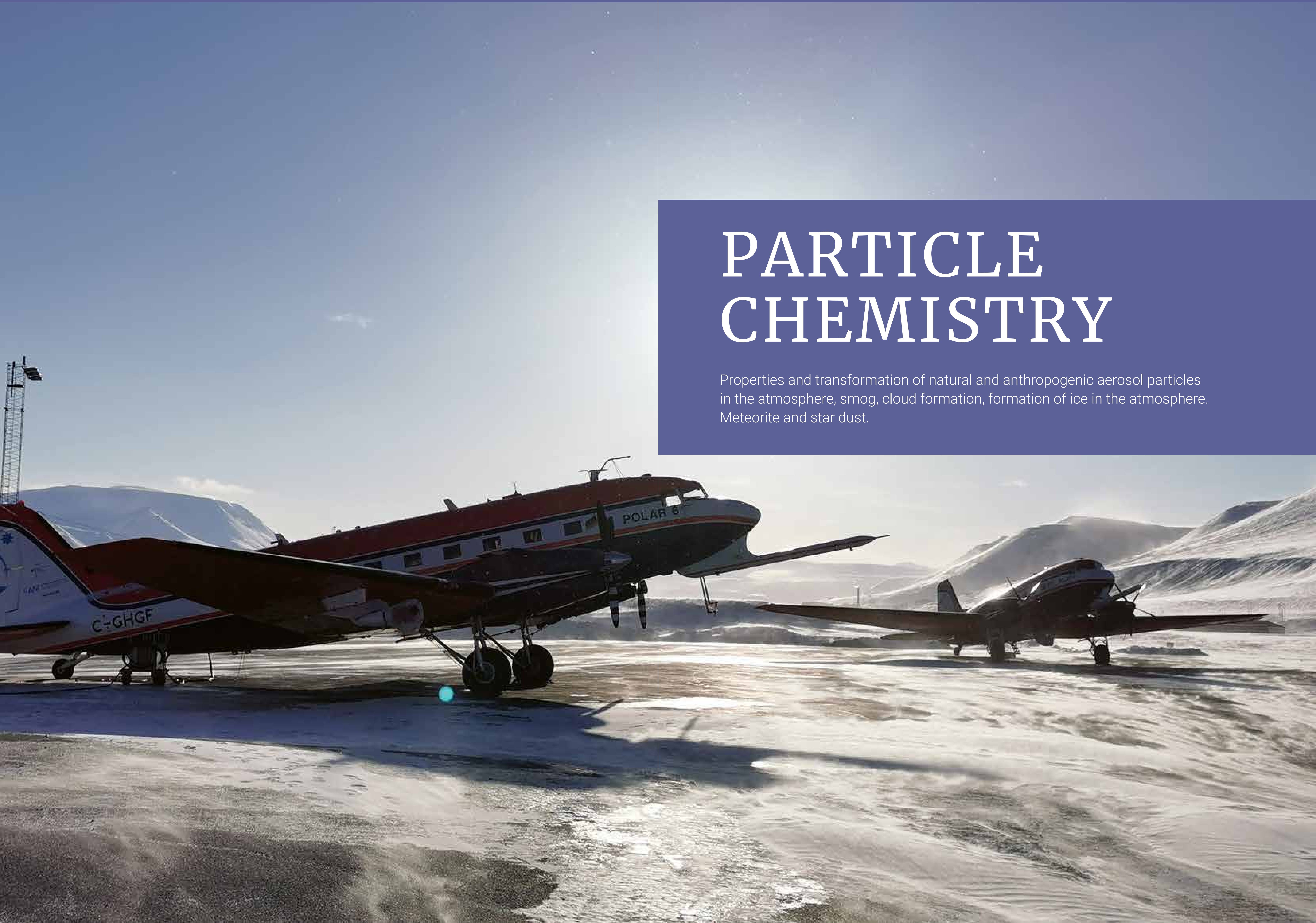


PARTICLE CHEMISTRY

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

This is the last report for the Particle Chemistry Department (PCD) as its Director, Prof. Stephan Borrmann, will retire in spring 2025. Since 2000/2001, the PCD has been a joint structure between the Institute for Physics of the Atmosphere (IPA) at the Johannes Gutenberg University Mainz (JGU), where S. Borrmann holds a full professor position (C4) and MPIC, where he has a formal part-time appointment as director.

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/JGU), (4) Physics and Chemistry of the UTLS Aerosol (Franziska Köllner at IPA/JGU and Stephan Borrmann), and (5) Nano- and Microparticle Research (NAMIP, PD Peter Hoppe).

RESEARCH FOCUS

In the past 23 years, the experimental research of the PCD has focused on the processes and the physical and chemical properties of atmospheric aerosols, clouds, large hydrometeors, sources of air pollution, as well as particulate matter of extraterrestrial origin.

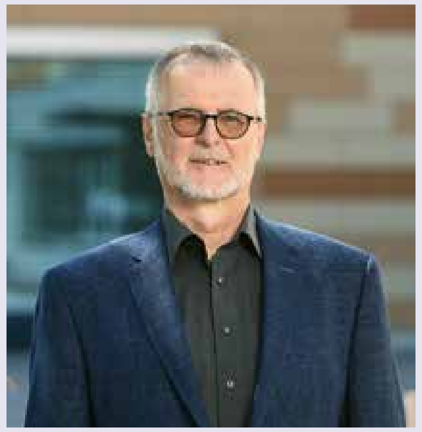
EXPERIMENTAL FOCUS

The adopted methodologies encompass techniques for ground-based, mobile, and aircraft-borne field measurements as well as intricate laboratory experiments. This includes the development of cutting-edge instrumentation. Within our department we maintain facilities like the Mainz Vertical Wind Tunnel (at IPA/JGU; see report by M. Szakáll), the Mobile Laboratory for Atmospheric Research (Mola; see report by F. Drewnick), and the NanoSIMS laboratory (see report by P. Hoppe). We operate six advanced aerosol mass spectrometers for field research, five of which have been utilized on ten research aircraft from five different countries. Examples are the German DLR HALO, the DLR Falcon, IAGOS-CARIBIC, the AWI Polar P6, the British BAe 146 FAAM, the NASA DC-8, the NSF/UCAR HIAPER GV (see reports by J. Schneider, F. Köllner/S. Borrmann), the French ATR, and the Russian M-55 "Geophysica" high altitude research aircraft. Several instruments were developed in-house, including the Aircraft-based Laser Ablation Aerosol Mass Spectrometer (ALABAMA), the unique ERICA particle mass spectrometer (ERc Instrument for Chemical Composition of Aerosols), the HALOHOLO holographic cloud particle imaging probe, and parts of Mola. Since 2001, PCD instrumentation and Mola have been deployed in 103 national and international field campaigns. These field projects and the instrument developments, as well as our laboratory research, were supported by roughly 10 million Euro from external grants (e.g., from DFG, EU, BMBF, etc.), which includes ≈ 20 % contribution from industry contracts, as well as by internal funding from the Max-Planck Society.

TEACHING AND EDUCATION

Established as a common structure of JGU and MPIC, the primary mission of the PCD extends beyond research to encompass a strong focus on formal education. This includes Ph.D. programs and academic curricula tailored for undergraduate and graduate students of meteorology, physics, and chemistry. Since 2000, in our department 61 Ph.D. theses, 12 M.Sc. theses, 40 "Diplom" theses, and 18 B.Sc. theses were completed, or are currently underway. Of these 131 graduates, ≈ 44 % are female. After the successful habilitations (i.e., qualification as a postdoctoral lecturer, i.e., a "Privatdozent", PD) of J. Schneider and M. Szakáll at JGU, A. Theis will finish his habilitation in 2024. Besides these three higher qualifications, our leadership formation efforts also include seven former members (five female) from our department have become professors at universities in five different countries. Several members of the department – including PD J. Schneider, PD M. Szakáll, A. Theis, F. Köllner, and S. Borrmann – are engaged in course teaching for the Meteorology curriculum at JGU. The total number of peer-reviewed scientific publications including authors from PCD since 2000 is 485 (including 25 in high-ranking journals). Five examples from the current reporting period are listed here.

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 Johannes Gutenberg University Mainz (JGU)

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., Germany

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

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

SELECTED PUBLICATIONS

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EXPORT OF AEROSOL FROM THE ASIAN SUMMER MONSOON INTO THE NORTHERN LATITUDE UTLS

FRANZISKA KÖLLNER AND STEPHAN BORRMANN – PHYSICS AND CHEMISTRY OF THE UTLS AEROSOL GROUP

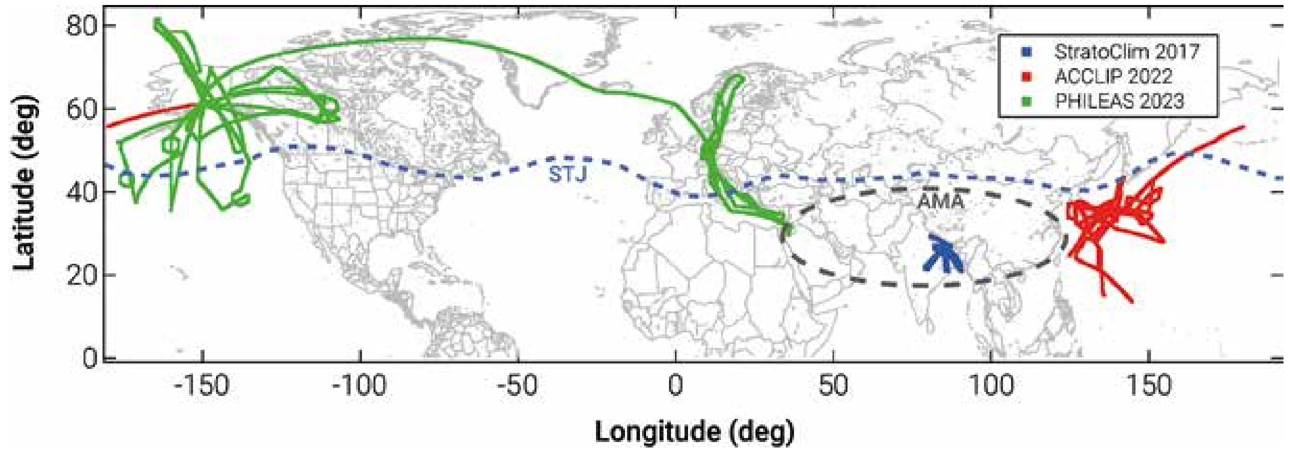

Figure 1: Paths of the research flights conducted during StratoClim 2017 in the center of the AMA, ACCLIP 2022 in the western Pacific south of the STJ and PHILEAS 2023 in the northern Pacific and Europe.

The Asian summer monsoon (ASM) circulation connects fast convective transport of boundary layer emissions with anticyclonic motion in upper levels, in this way influencing the physicochemical characteristics of aerosol in the upper troposphere and lower stratosphere (UTLS). In the past decade, the chemical nature of the so-called Asian tropopause aerosol layer (ATAL) has been the subject of debate. The first *in situ* measurements up to 20 km altitude were conducted with our aerosol mass spectrometer ERICA onboard the M-55 Geophysica high-altitude research aircraft during the 2017 StratoClim mission (Figure 1). The unique, novel ERICA instrument (Hünig et al., 2022; Dragoneas et al., 2022; Molleker et al., 2020) combines laser desorption ionization mass spectrometry and thermal desorption with subsequent electron impact ionization technique. This allows measurements of refractory and non-refractory aerosol components for sub-micron-sized particles. Figure 2a shows mass concentrations of particulate organics, nitrate, and ammonium as a function of potential transport from inside the ASM over the Himalayas. Our analysis suggests that ammonium nitrate and organics are the dominant aerosol species within the ATAL. The organic aerosol was exposed to photochemical aging while being slowly lifted above the ASM. Also, we found that the ATAL is largely controlled by secondary aerosol formation, as evident from the presence – up to 70 % – of particles containing solely non-refractory aerosol components (Appel et al., 2022). In contrast to the secondary particle type, a non-negligible fraction of the particles includes refractory components. Together with concurrently in situ collected impactor samples that were analyzed offline by means of electron microscopy and X-ray microanalysis, silicates were identified as a prominent refractory particle type (Ebert et al., 2023).

The ASM-influenced air becomes distributed in the Northern hemispheric UTLS, preferentially via east- and westward eddy shedding. We focused on *in situ* aerosol composition measurements of this export of ASM air within the framework of the NASA Asian summer monsoon Chemical & CLimate Impact Project (ACCLIP, summer 2022; Osan, South Korea), and the TPchange PHILEAS project (Probing HIgh Latitude Export of air from the Asian Summer monsoon, summer/autumn 2023; Oberpfaffenhofen, Germany, and Anchorage, Alaska). Here, our ERICA instrument was also successfully operated on the US NSF/NCAR HIAPER and on the German HALO research aircraft, after its initial deployment on the M-55 Geophysica within the ASM center in 2017. We thus collected with the same instrument a unique data set covering ASM-influenced air in a broad geographical range from the center of the anticyclonic system to the eastern Mediterranean Sea as well as in the western and northeastern Pacific (Figure 1). Figure 2b shows mass concentrations of nitrate summarized in a potential temperature-latitude space plot with data from these three missions. We observed the quasi-horizontal transport of Asian monsoon anticyclone (AMA)-trapped aerosol into the western Pacific and even in the extratropical lower stratosphere across the subtropical jet (STJ). The air masses are characterized by processed aerosol with enhanced ammonium nitrate (Figure 2) and organic loadings. Regarding the single-particle mass spectral analyses, we were able to re-sample the secondary aerosol particle type, providing evidence that nitrate-rich single particles from the ATAL were transported into the extratropical stratosphere. Particularly from the ACCLIP mission, we have first indications that the organic aerosol is more photochemically aged within the filaments over the western Pacific, compared to aerosol measured within the ATAL. During the 43 research flights of the three missions, we collected the world's most extensive data set for ATAL- and ASM-derived aerosols, which should allow us to better understand the effect of the ASM on the aerosol chemical composition at higher altitudes.

“After successfully probing the Asian Tropopause Aerosol Layer, we now aim to document changes of the aerosol properties in air masses resulting from eddy shedding off the Asian Monsoon anticyclone.”

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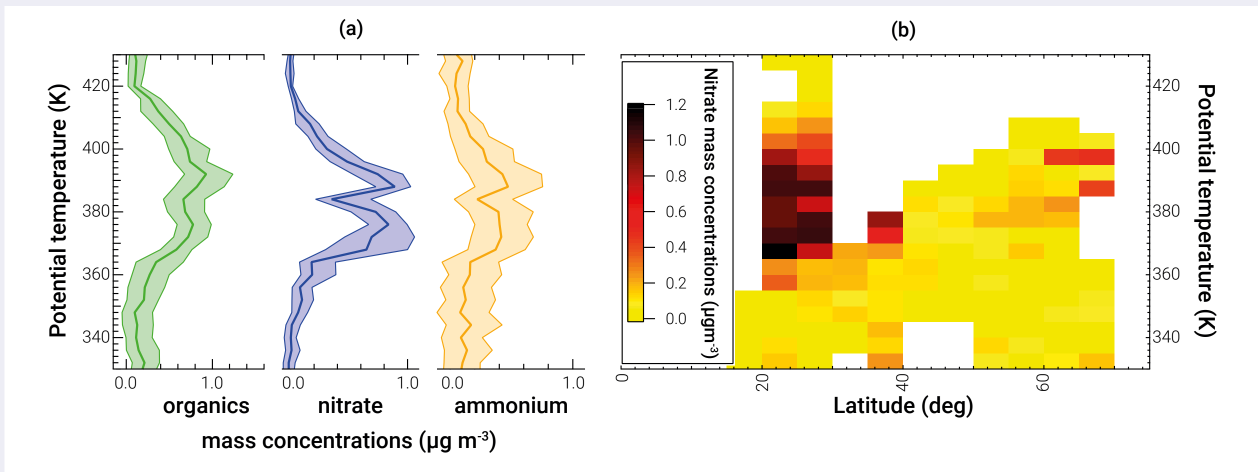

Figure 2: (a) Mass concentrations of particulate organics, nitrate, and ammonium as a function of potential temperature altitude. The thick lines and the shaded areas represent the medians and 25th/75th percentiles of the StratoClim mission in 2017. (b) Nitrate mass concentrations (75th percentiles) as a function of potential temperature and latitude. The data include the missions StratoClim 2017, ACCLIP 2022, and PHILEAS 2023 (except flights from Oberpfaffenhofen).

VERTICAL DISTRIBUTION OF AEROSOLS – HOW WELL DO GROUND-BASED MEASUREMENTS REPRESENT THE LOWER BOUNDARY LAYER?

FRANK DREWNICK – INSTRUMENTAL AEROSOL ANALYTICS GROUP

"To obtain a representative picture of the lower boundary layer, we must include the altitude dependence of multiple variables in ground-based measurements."

Figure 1: Combined measurements of the mobile laboratory MoLa and the measurement drone FLab during a field campaign on the Swabian Jura.

The vast majority of atmospheric measurements is performed within a few meters above the ground and often based on the assumption that the lower boundary layer is well-mixed and that these measurements are representative for this lowermost part of the atmosphere. Rarely, large vertical structures, like towers or tall buildings, are used to probe the atmosphere at different altitudes or to investigate vertical fluxes of air components. However, such measurements are extremely costly and limited to the location of the respective facility.

Also sampling with the mobile aerosol research laboratory MoLa is limited to a few meters above ground level. MoLa was developed in our group at the MPIC and allows for state-of-the-art *in situ* measurements of aerosol and trace gas variables with high spatial flexibility. To extend its measurement capabilities several hundred meters upwards into the boundary layer, we developed the flying laboratory FLab.

FLab is based on a hexacopter that can carry a payload of up to 6 kg over 15 minutes and up to altitudes reaching 500 m above ground. Within these constraints, we designed the instrumental setup of the drone to allow for the discrimination of different aerosol types – which especially close to emission sources might represent individual plumes – from the background with high temporal resolution. This includes on-line measurements of particle number concentration and size distribution, black carbon concentration, mixing ratios of CO_2, ozone and water vapor as well as basic meteorological quantities. For efficient field application, FLab is equipped with on-board data acquisition with direct radio transmission to the ground station.

To thus connect MoLa measurements to those from higher up, intercomparison phases of FLab at the MoLa inlet height are included in all flights. Dedicated test flights for optimization of on-board aerosol sampling and measurement flight patterns were performed, which showed that for hovering situations at the MoLa inlet height, results from both platforms agree reasonably well. Especially the combination of continuous MoLa data with those from repeated FLab flights provides valuable synergies that go beyond the findings of both types of experiments on their own.

The first combined field application of MoLa and FLab took place in Summer 2023 on the Swabian Jura in southern Germany (Figure 1). This expedition, which also served as a proof-of-concept for this instrument development, was part of the Collaborative Research Center "TPChange" and was executed jointly with partners from the Universities of Mainz and Darmstadt. The main purpose of this field campaign was the investigation of the vertical transport of trace matter from the boundary layer into the upper troposphere/lower stratosphere (UTLS) region under strong convective situations. To achieve this, continuous MoLa measurements were combined with frequent FLab flights to explore the lower boundary layer composition and homogeneity, while partners investigated the upward transport into the UTLS.

Vertical profiles of meteorological and aerosol-related variables just before and just after the passing of a thunderstorm show significant differences. Further, these variables are also heavily dependent on measurement altitude (Figure 2). These first results already indicate that measurements performed exclusively at ground level might not provide a full picture of the lower boundary layer under all atmospheric conditions.

In addition to such applications, where the homogeneity of this part of the boundary layer and the representativeness of ground-based measurements are determined, FLab will also be used to investigate source-related fingerprints in the atmosphere. This includes, for example, the quantitative analysis of fugitive emissions, for which the concentration distribution and the cross-sectional area of the plume must be known, or direct capture of aging and dilution processes with quasi-Lagrangian measurements in the evolving plume.

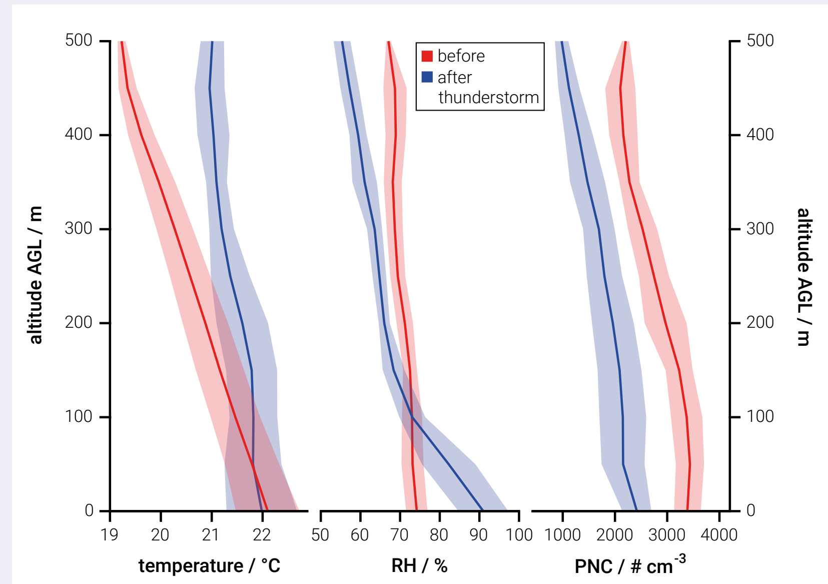

Figure 2: Vertical profiles of ambient temperature and relative humidity as well as particle number concentration (PNC) in the lower boundary layer, measured with FLab shortly before and after a thunderstorm passing the field site.

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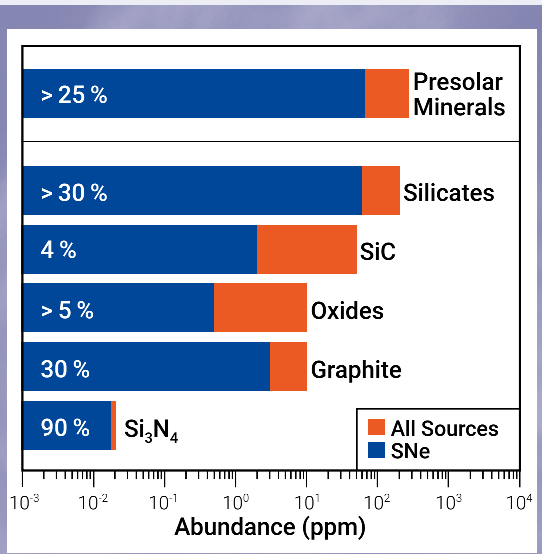
NANO- AND MICROANALYTICAL STUDIES OF MATTER FROM SPACE AND EARTH

PETER HOPPE – NANO- AND MICROPARTICLE RESEARCH GROUP



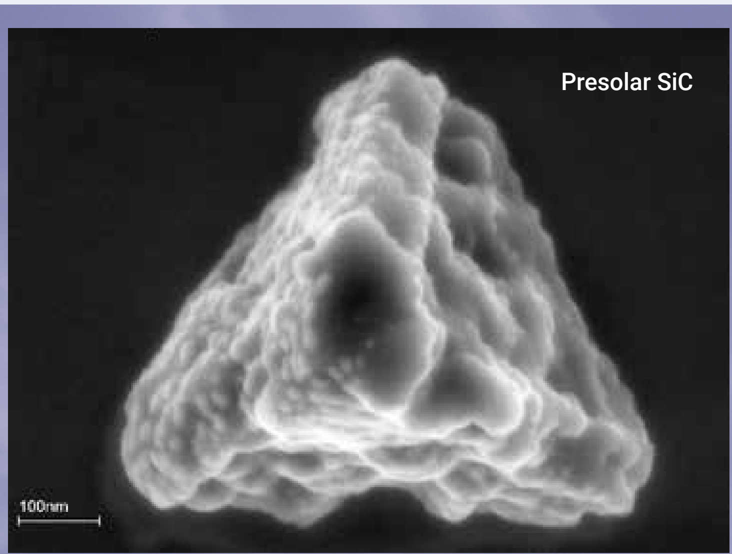


Figure 1: Abundances in parts per million (ppm) of presolar grains in the matrix of primitive meteorites. Orange bars indicate abundances from all potential stellar sources and blue bars those from supernovae and their progenitors. From Hoppe et al. (2022).

INTRODUCTION

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

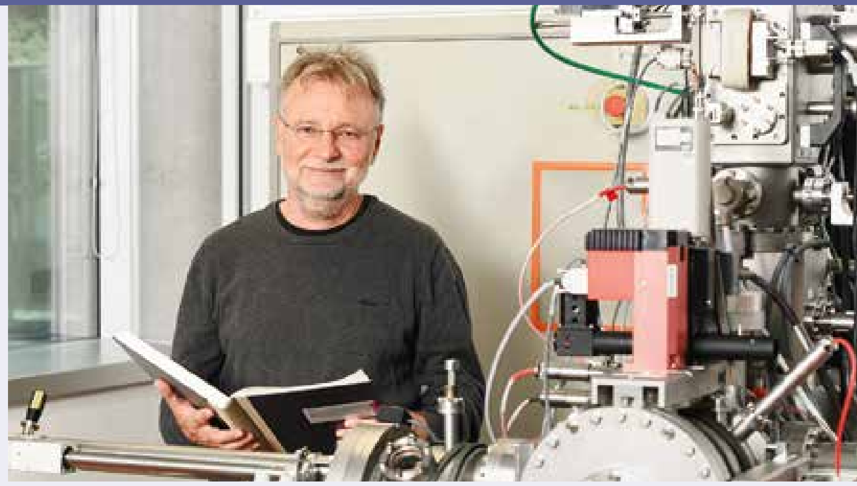
Major scientific themes addressed during the last three years included (i) the origins of the solid matter that went into the making of our Solar System, (ii) planetary bodies in the early Solar System, and (iii) foraminifera shells as proxies for paleoclimate reconstruction (in cooperation with the Climate Geochemistry Department).

RESULTS

By studying isotopic compositions of 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. Our results of Mg isotope studies suggest that more than 30 % of presolar silicates, the most abundant type of presolar grains, are from massive stars that eventually exploded as supernovae (Figure 1; Hoppe et al., 2022). This implies that supernovae and their progenitor stars contributed much more dust to the molecular gas and dust cloud from which our Solar System formed than previously thought. Furthermore, we showed that presolar SiC grains from supernovae carry large amounts of (now extinct) radioactive ^{26}Al (Hoppe et al., 2023), whose decay is considered the most important heat source for planetary melting and differentiation in the early Solar System.

Besides ^{26}Al, radioactive ^{60}Fe could have been an important heat source for planetary melting and differentiation. We applied an improved analysis setup to get a better understanding of the causes of the large variability of estimated ^{60}Fe abundances in the literature. Our *in situ* studies of troilite and chondrule silicate in primitive meteorites indicated only a low level of ^{60}Fe in the early Solar System, in line with studies of meteoritic bulk samples by MC-ICP-MS, but at odds with previous *in situ* studies by SIMS (Figure 2; Kodolányi et al., 2022).

Our group was part of the initial analysis team that studied matter returned from the C-type asteroid Ryugu to Earth in 2020 by JAXA's Hayabusa2 mission.



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

These studies showed that the samples are mainly composed of materials similar to those of carbonaceous chondrite meteorites, particularly the CI (Ivuna-type) group. Compared to other natural samples, the samples of Ryugu have a chemical composition that more closely resembles that of the Sun's photosphere (Yokoyama et al., 2023).

We investigated the applicability of foraminiferal Mn/Ca ratios as proxies of environmental conditions, in correlation with trace element data obtained by fs LA-ICP-MS. High-lateral resolution measurements with the NanoSIMS allowed us to discern between Mn incorporated into the shell carbonate and Mn-bearing coatings on top of the shells (Öğretmen et al., 2022). In addition, we continued the characterization of standard materials to improve the suitability of the NanoSIMS for paleoclimate proxy investigations.

OUTLOOK

We will continue our nano- and microanalytical studies (NanoSIMS, RIMS, FIB/TEM) of different types of extraterrestrial and terrestrial materials. Of particular interest will be isotope studies of yet largely unexplored astrophysically diagnostic elements in presolar silicates (DFG-funded project of Dr. Jan Leitner) and of high-resolution elemental abundance studies of microfossils for paleoclimate reconstruction. Following the retirement of Dr. Peter Hoppe in spring 2025 it is planned that the NanoSIMS group will be integrated under a new leadership into the Climate Geochemistry Department.

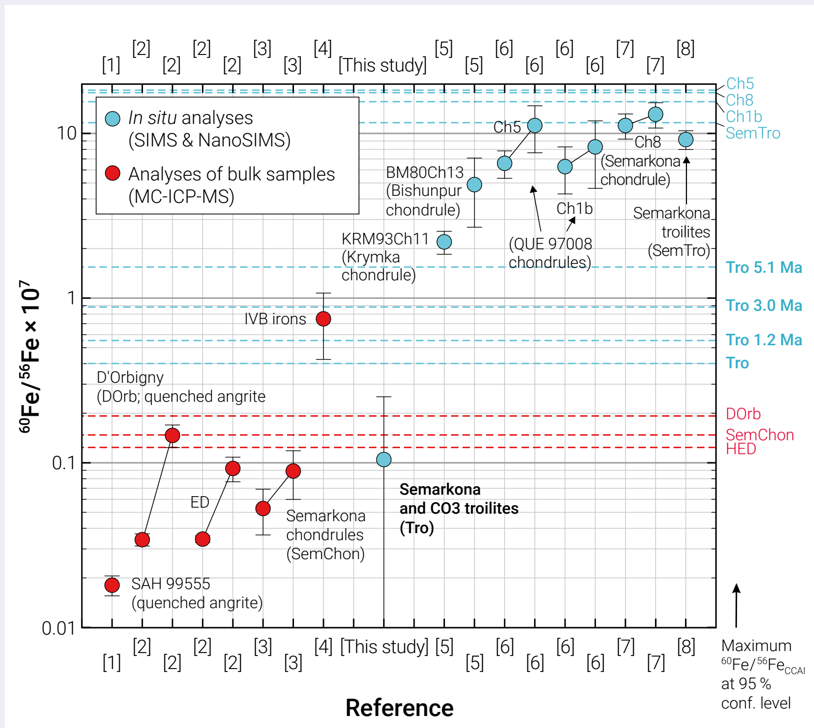


Figure 2: Inferred initial ^{60}Fe/^{56}Fe ratios of Solar System objects. Our in situ analyses of meteoritic troilites suggest a low level of ^{60}Fe in the early Solar System, in line with data obtained by MC-ICP-MS for bulk meteorites. From Kodolányi et al. (2022).

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METEORIC MATERIAL IN LOWER-STRATOSPHERIC AEROSOL PARTICLES

JOHANNES SCHNEIDER – AEROSOL AND CLOUD CHEMISTRY GROUP

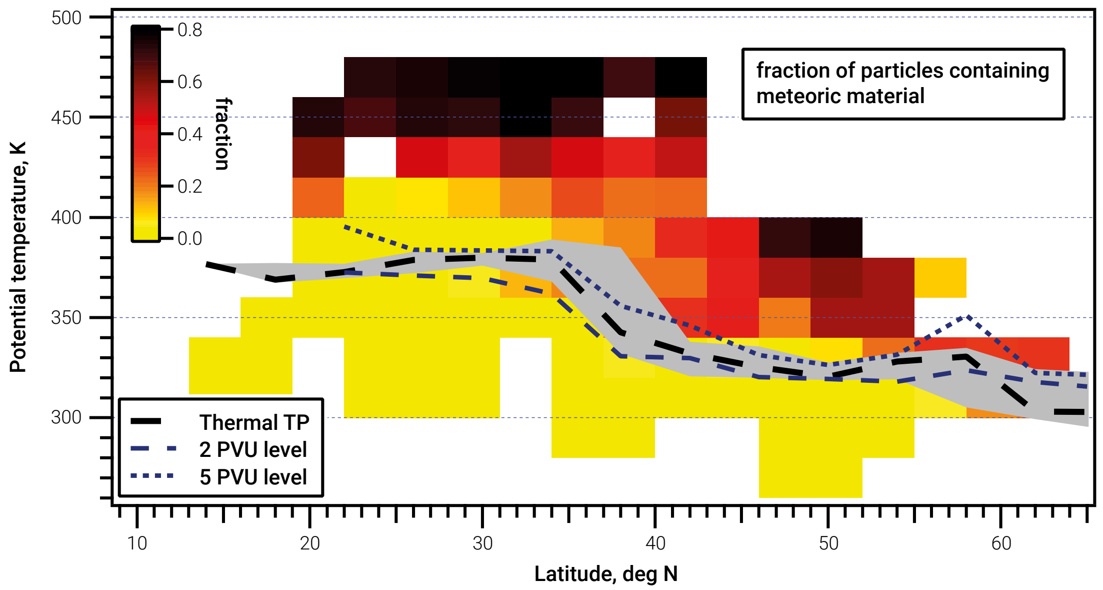

Figure 1: Fractional abundance of particles containing meteoric material as a function of potential temperature and latitude. Also shown is the median thermal tropopause (from ECMWF; TP) along with interquartile range (gray shading) and two dynamic tropopause levels (2 and 5 PVU) (Schneider et al., 2021).

Aerosol particles in the upper troposphere and lower stratosphere (UTLS) play an important role in the Earth system: firstly, by direct scattering of sunlight back to space, secondly, by influencing homogeneous and heterogeneous cirrus cloud formation in the upper troposphere, and thirdly, by providing surfaces for heterogeneous chemical reactions. An important natural source of atmospheric particles is the continuous meteoric particle import of extraterrestrial origin. After sedimentation into the lower stratosphere, the meteoric material, mainly iron, magnesium, and silicon, is dissolved in the sulfuric acid droplets of the stratospheric background aerosol.

Our findings come from a variety of aircraft-based field experiments in the UTLS: The HALO missions ML-CIRRUS (2014) and CAFE-AFRICA (2018), the mission StratoClim (2016 and 2017) on the high-altitude research aircraft Geophysica, and ND-MAX (2018) using NASA's DC-8. These aircraft missions covered different altitudes, latitudes, and seasons: Western Europe for spring and summer, the Mediterranean, tropics and subtropics for summer, as well as North America and the North Atlantic for winter. The data were obtained with two different aerosol mass spectrometers: The ALABAMA (Aircraft-based Laser Ablation Aerosol Mass Spectrometer; Clemen et al., 2020; Köllner et al., 2021) and the ERICA (ERC Instrument for Composition of Aerosols, Dragoneas et al., 2022; Hünig et al., 2022). Both the ALABAMA and the ERICA are single-particle analysis instruments that use laser ablation and ionization, followed by ion detection in a bipolar time-of-flight mass spectrometer. The ERICA additionally features a thermal desorption unit for quantitative analysis of non-refractory aerosol compounds. In all datasets we observed a distinct particle type in the lower stratosphere that is interpreted as particles containing meteoric material dissolved in sulfuric acid.

Figure 1 shows that the fraction of the meteoric particles increases in high and middle latitudes very close to the tropopause but not in the tropics. In theta-latitude space, the particle fraction remains as low as in the troposphere between the tropopause (around 370–380 K) and 400 K at latitudes south of 30° N. This observation indicates that the source for this particle type must be above the tropopause, because otherwise the upwelling air masses in the tropics would contain this particle type also at lower potential temperatures.

"Particles containing meteoric material represent a significant component of the lower stratospheric aerosol and are therefore important for cloud formation and atmospheric chemistry."

As an example, cross-tropopause mixing is visualized by means of tracer–tracer correlation between O_3 and H_2O in Figure 2 for ML-CIRRUS. Panel a) shows all data from the O_3 and H_2O measurements, color-coded by equivalent latitude, revealing a clear separation between air masses of mid-latitude and tropical origin. Mixing between extratropical stratospheric and tropospheric air is indicated by mixing lines with equivalent latitudes > 30° N, connecting regions of elevated extratropical and low stratospheric H_2O values. The green-colored data points that correspond to tropical air masses (equivalent latitude < 30° N) do not show such mixing. Panel b) shows the H_2O and O_3 data for all sampled particles (grey) and for all meteoric particles (black). The density of black data points is highest in the stratospheric branch of the tracer–tracer correlation, but downward mixing along the mixing lines in the extratropics is also evident.

These data demonstrate the widespread presence of meteoric material in stratospheric aerosol particles. Using the particles containing meteoric material as a tracer for stratospheric transport, our observations confirm the upward motion of air masses over the Asian monsoon anticyclone and the associated transport into the stratosphere, the exchange between the stratosphere and troposphere in the extratropics, and the efficient isentropic mixing between high and low latitudes above 440 K potential temperature.

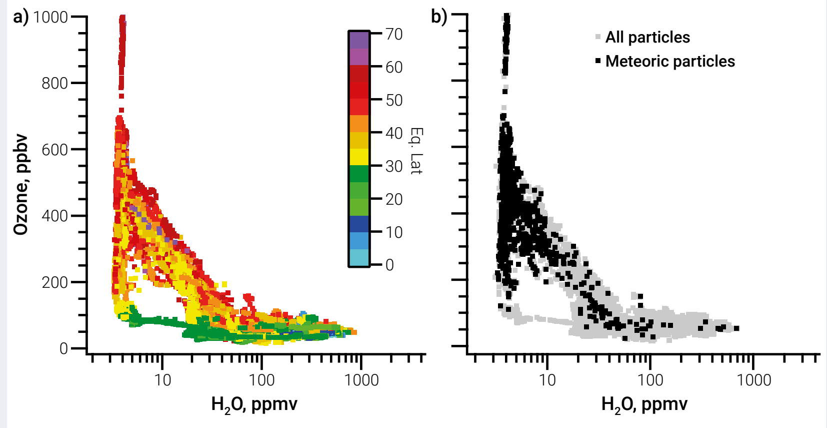

Figure 2: Mixing diagrams (O_3 versus H_2O) for the ML-CIRRUS campaign, color-coded a) by equivalent latitude, b) by occurrence of meteoric particles. Meteoric particles are mixed downwards from the stratosphere along the mixing lines connecting the stratospheric and tropospheric branch. Air masses with tropical origin (equiv. latitude < 30°) in the troposphere contain no meteoric particles, because no downward mixing occurs in the tropics (Schneider et al., 2021).

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LABORATORY INVESTIGATIONS INTO THE MELTING OF HAILSTONES

MIKLÓS SZAKÁLL – ATMOSPHERICAL HYDROMETEORS GROUP

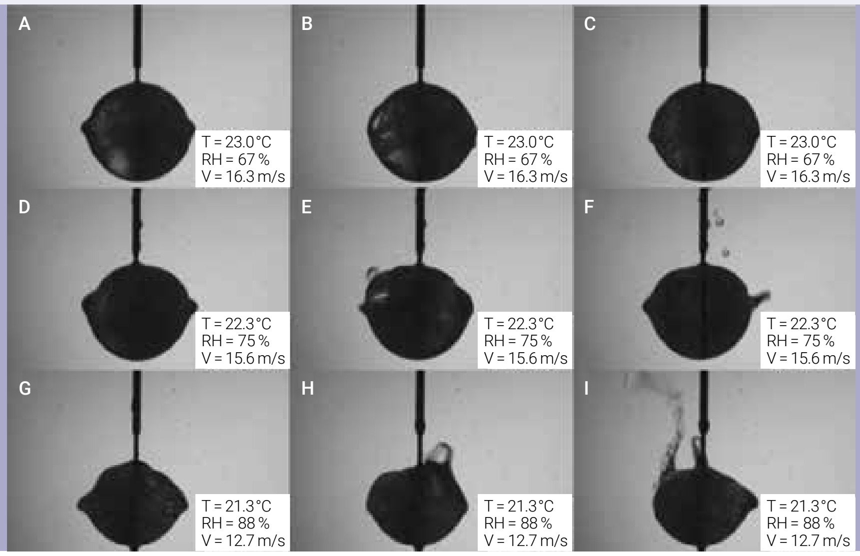


Figure 1: Images of a melting hailstone (initially 2 cm in diameter) in the wind tunnel taken at frame rates corresponding to 10 Hz. (Source: A. Theis, IPA/JGU)

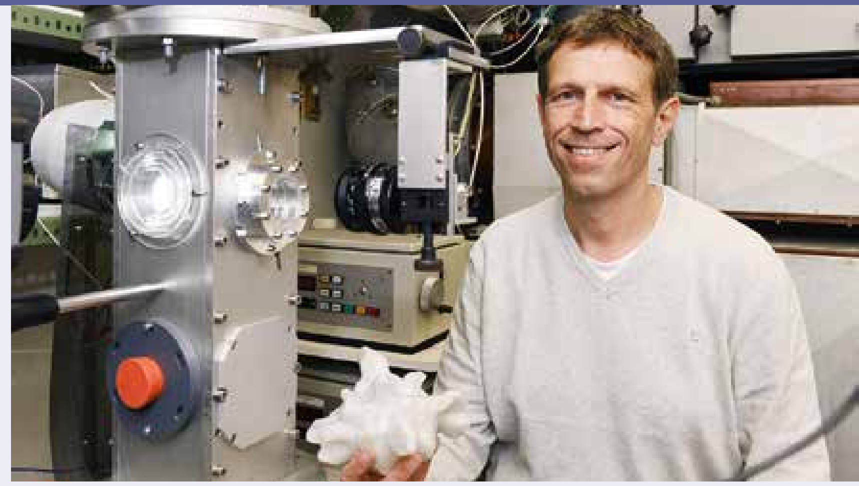
INTRODUCTION

Severe weather events including heavy rain and hail that cause damage and fatalities are increasing in number every year. These precipitation types are mostly initiated via the ice phase through melting, a process that has remained insufficiently investigated so far. Hailstones, the largest particles in the global precipitation system, may reach sizes of up to 15 cm. When falling through the atmospheric melting layer, they pass several stages during which their shapes, densities, and terminal velocities change and during which the melt water behavior, including internal mixture and droplet shedding, shows important variations. In wind tunnel experiments, we have thoroughly determined these microphysical parameters, which are of great importance in cloud models and radar meteorology, in particular the size distributions of drops that are shed from melting hailstones. These significantly influence the development of drop sizes and precipitation in clouds.

WIND TUNNEL STUDIES

Experiments to investigate the melting of hailstones were performed at the Mainz vertical wind tunnel laboratory. Hailstones were represented by solid ice spheres with diameters of 10 to 20 mm and densities of 0.9 g/cm^3, which were tethered in the observation section. Their terminal velocities were precisely adjusted and maintained during melting. The initial ambient temperature of -2 °C was linearly increased, generating heating rates between 0.03 and 0.16 °C/s (corresponding to ambient lapse rates from 0.1 to 2.71 °C per 100 m). The relative humidity was kept almost constant at defined values between 15 and 90 %. Various cameras recorded the hailstones during the entire melting process and tracked the temporal development of several parameters. In post-processing, we determined the onset of melting, melting rates, shedding rates, shed drop size distributions, variations in the axis ratios, and equilibrium masses of liquid water. Variations in terminal velocities and total melting times were directly measured. During melting of hailstones, the melt water accumulates on the surface of the solid ice sphere until it starts to shed droplets (Figure 1).

This shedding was observed by an in-line digital holographic imaging system that we developed in our laboratory based on the design of the HALOHOLO aircraft instrument from our department. From the holograms, we obtained information about the shed droplet spectra as shown in Figure 2. The solid line represents a lognormal fit to the data, indicating a bimodal character of the size distribution. Continuous shedding started at a melt water fraction of 15 %. The melt water torus on the hailstone surface (Figure 1) became unstable and released drops of 1 mm in diameter, which are visible in the second broader mode of the drop size distribution. Later, when the melt water fraction exceeded 20 %, shedding occurred less frequently but more water was shed per event so that filaments containing large volumes of water erupted from the hailstone surface (Figure 1). When these teared off, they produced drops with diameters between 3 and 4 mm that sometimes burst into smaller (≈ 100 μm) drops. These events are attributed to the first, smaller mode of the drop size distribution. A theoretical background for modeling and predicting these effects for inclusion in precipitation forecast models is still missing.



“For the purpose of realistic radar retrievals and numerical cloud simulations, it is essential to characterize the microphysical parameters of ice particles during the transition from the ice to the liquid phase.”

OUTLOOK

Another important process that affects the development of drop sizes and precipitation in clouds is the breakup of drops. We are currently investigating two breakup processes in our wind tunnel laboratory within the framework of a DFG-funded project. The first is the spontaneous breakup of drops reaching a size where they become unstable due to strong oscillations; the second is the breakup after collision with other drops. The Mainz vertical wind tunnel allows the study of single events of individual large drops that are ready for spontaneous breakup as well as collisions of two drops of different sizes followed by coalescence or breakup. The breakup efficiencies are determined in dependence on the drop sizes and the drop size distributions. Based on the new measurements and literature data, model simulations are performed to estimate the impact of drop breakup on the development of the cloud drop size spectrum and precipitation. The results improve the accuracy of precipitation forecasting, which is of increasing importance as extreme precipitaion events become more frequent and severe due to climate change.

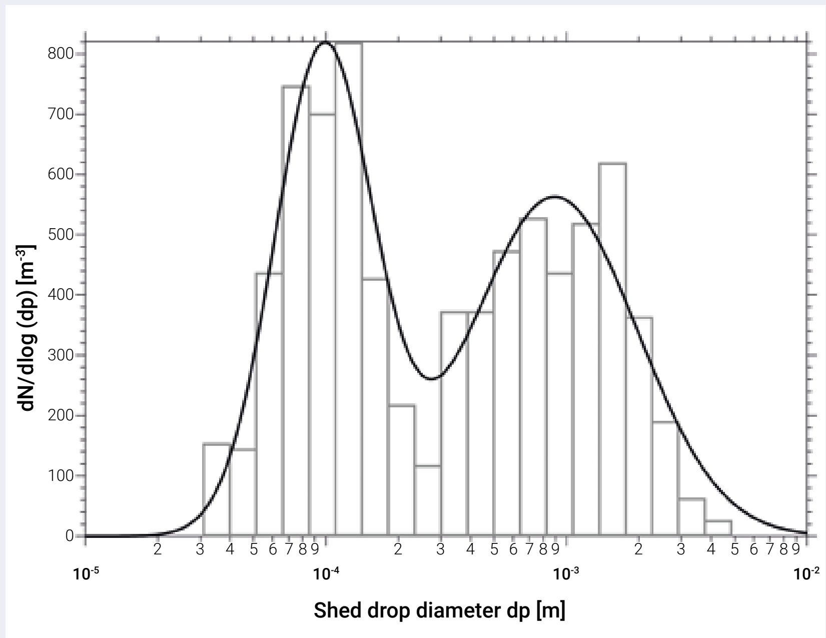


Figure 2: Size distribution of shed droplets that is representative for a melting hailstone with an initial diameter of 20 mm falling at 27 % RH and 21 °C. The terminal settling velocity of the hail varied between 20 and 13 m/s depending on its state of melting.

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INDEPENDENT RESEARCH GROUPS

Aerosols and regional air quality, hominin meat consumption, high pressure chemistry and physics, and satellite remote sensing.

AEROSOLS, AIR QUALITY AND CLIMATE

YAFANG CHENG – AEROSOLS, AIR QUALITY AND CLIMATE GROUP

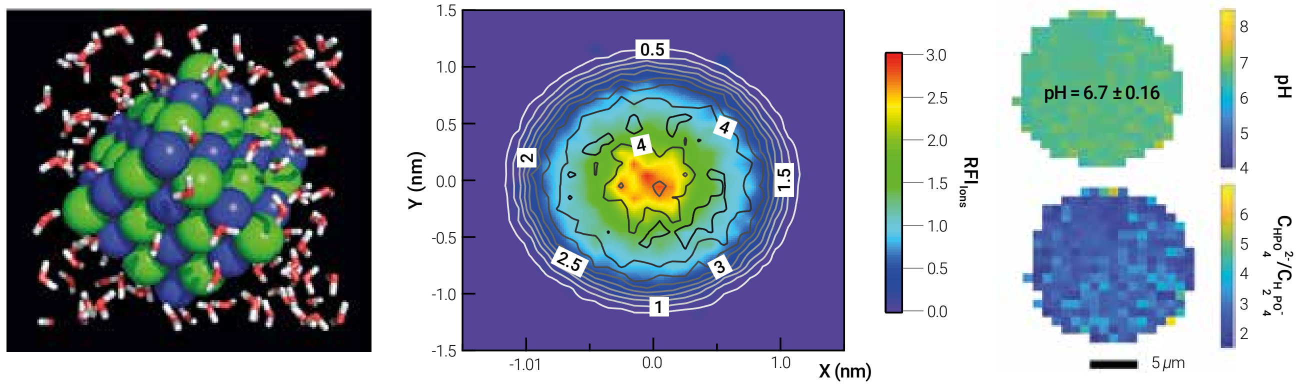


Figure 1: Molecular dynamics simulations (Chen et al., Faraday Discussion 2023; molecular structure plotted with VMD) and advanced Raman techniques (Li et al., Chem 2023) to study the physical chemical properties of aerosol nanoparticles and microdroplets.

Due to their diverse sources and properties, complex life cycles, and tight coupling with the hydrological cycle and atmospheric circulation, aerosol processes are a major source of uncertainty in assessing climate change on regional and global scales. To address the challenge, our group is taking a multiscale integration approach by combining laboratory and field experiments, scientific instrument development, numerical model simulations as well as machine learning techniques. Our research is focused on the following key areas: aerosol nanoparticles and microdroplets, atmospheric aerosol and haze chemistry, and aerosol-radiation-cloud interactions and climate impact. Recent research highlights are summarized below.

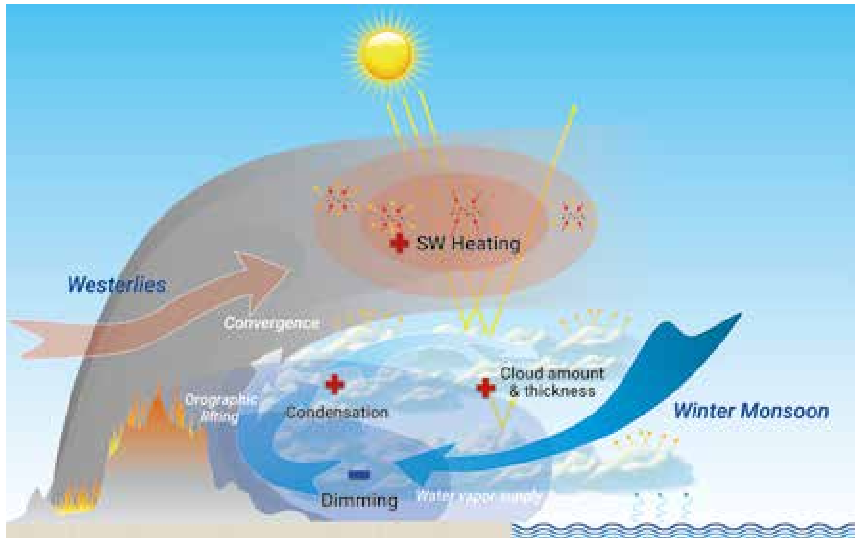


Figure 2: Synergetic feedback of smoke aerosol–cloud–boundary-layer interaction coupling with the monsoon in subtropical southeastern Asia (Ding et al., Nature Communications 2021).

NEW MEASUREMENT TECHNIQUES AND THEORY OF AEROSOL ACIDITY

Acidity plays a key role in aerosol formation and strongly influences aerosol effects on air quality, climate, and the ecosystem. Using advanced single-particle and hyperspectral Raman microscopies, we directly measure the pH distribution in microdroplets (Li et al., Chem 2023) (Figure 1). A similar approach was applied to determine ion activities in aqueous droplets under highly supersaturated conditions (Li et al., EST 2022). In terms of the driver of aerosol pH at regional/global scales, with our newly developed aerosol buffer theory (Zheng et al., Science 2020), we show that, in general, aerosol acidity is primarily buffered by NH_3, with a negligible contribution from CO_2, despite a 10^4 to 10^7 higher abundance of CO_2 in the atmosphere (Zheng et al., EST 2023). This is because the aerosol pH is at the very far end of the CO_2 buffering range in atmospheric aerosol systems. These findings provide new experimental techniques, theories, and insights to advance our understanding of aerosol acidity and associated chemistry in aerosol droplets.

"The overall goal of our research is a fundamental and predictive understanding of the origins, interactions, and impacts of aerosols in the Earth system, to resolve aerosol effects on regional air quality and climate, and to increase the reliability of global change projections."

CLIMATE EFFECTS OF BLACK CARBON AND WILDFIRES

Black carbon (BC) and brown carbon (BrC) aerosols are among the most important short-lived climate warming agents. However, Cappa et al. (Science 2012) found a negligible enhancement of BC's light absorption by coating, challenging the applicability of classical Mie theory to atmospheric aerosols and leading to debate on BC's climate impact. With advanced instrument and experimental design, we show that the Mie theory still holds for atmospheric aerosols. The previous discrepancies can be attributed to the extremely low volatile (eLV) organics, which account for 5 %–100 % of the total BC coatings (Zhang et al., One Earth 2023). We also discovered that BC surface chemistry represents a previously unknown pathway producing substantial amounts of highly oxygenated eLV organic aerosols (Li et al., Chem 2022).

Regarding the interactions of BC with atmospheric dynamics, we show that BC can trigger a "tipping point" of planetary boundary layer (PBL) development (Wang et al., One Earth 2023). When exceeding a critical threshold of aerosol optical depth, due to a BC-induced decoupling of mixing zones, the daily maximum PBL height decreases abruptly, which largely reduces the dilution leading to persistent pollution. At meso- or synoptic scale, we found strong radiative forcing of wildfire BC and BrC over the remote arctic region (Yue et al., One Earth 2022). Wildfire aerosols can also strongly enhance low cloud coverage over both land and ocean in subtropical southeastern Asia, through the synergetic effect of aerosol–cloud–boundary layer interactions with the Asian monsoon (Ding et al., Nature Communications 2021) (Figure 2).

UNDERSTANDING EFFICACY OF PREVENTIVE MEASURES AGAINST THE TRANSMISSION OF SARS-COV-2

Transmission by droplets and aerosols is important for the spread of respiratory viruses like SARS-CoV-2 and influenza. We showed that variations in mask efficacy can be explained by different regimes of virus abundance and are related to population average infection probability and reproduction number (Cheng et al., Science 2021). For SARS-CoV-2, the viral load of infectious individuals can vary by orders of magnitude, but we found that most environments and contacts are under conditions of low virus abundance (virus-limited), where masks are effective at preventing virus spread (Figure 3). Because of the non-linear dependence of mask efficacy on the viral load, masks are particularly effective in combination with other preventive measures like ventilation and distancing.

SELECTED PUBLICATIONS

Zheng et al: Multiphase buffer theory explains contrasts in atmospheric aerosol acidity, Science (2020).

Cheng et al.: Face masks effectively limit the probability of SARS-CoV-2 transmission, Science (2021).

Ding et al: Aerosol-boundary-layer-monsoon interactions amplify semi-direct effect of biomass smoke on low cloud formation in Southeast Asia, Nature Communications (2021).

Wang et al.: Black carbon-induced regime transition of boundary layer development strongly amplifies severe haze, One Earth (2023).

Li et al.: Spatial homogeneity of pH in aerosol microdroplets, Chem (2023).

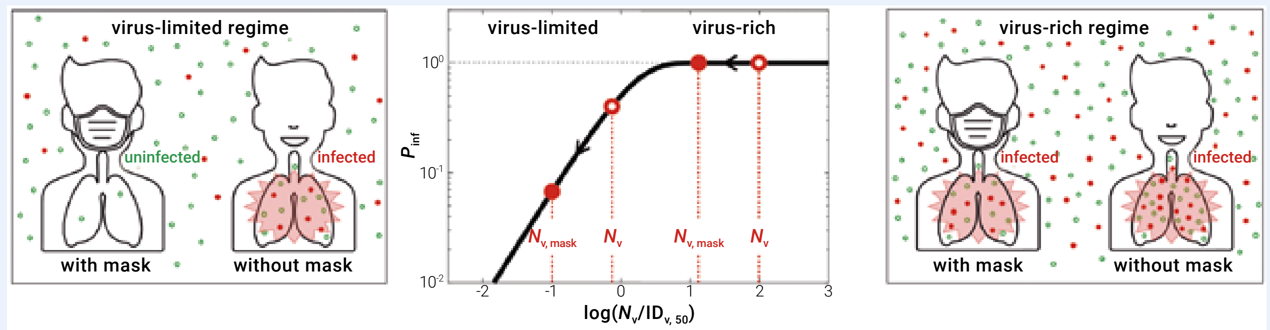


Figure 3: Schematic illustration of different regimes of abundance of respiratory particles and viruses (Cheng et al., Science 2021).

SEARCH FOR NEAR-ROOM-TEMPERATURE SUPERCONDUCTIVITY AT HIGH PRESSURES

MIKHAIL EREMETS – HIGH PRESSURE CHEMISTRY AND PHYSICS GROUP

Figure 1: Preparing diamond anvils for high-pressure diamond anvil cells. This device is used to generate pressures exceeding one million bars between two conically cut diamonds. Substances rich in hydrogen, such as hydrogen sulfide, lanthanum or yttrium hydrides, are tested to determine their superconducting properties.

INTRODUCTION

Following our discovery of superconductivity (SC) with a critical temperature (T_c) of 203 K in hydrogen sulfide H_3S compressed to approximately 150 GPa, a new family of superconductors, hydrogen-rich superconductors (superhydrides), has emerged. LaH_{10} holds the current record T_c of approximately 250 K. New superconductors with even higher T_cs close to room temperature appear to be within reach, given the predictions of numerous promising phases in the binary Mg-H, La-H, Ce-H, and ternary Li-Mg-H systems. We have made substantial progress in synthesizing novel phases with preliminary calculated T_cs exceeding 290 K. In addition to the search for new high-temperature superconductors, in recent years we have continued to characterize the superconducting state in superhydrides under extreme high-pressure conditions. The primary technique involves four-probe electrical transport measurements, which provide T_c and detect the zero-resistance state below T_c. We have also made significant strides in developing magnetic susceptibility measurements, which give us a wealth of information about a superconductor, including T_c, lower critical field H_{c1}, London penetration depth λ_L, vortex creep, critical current density, and other parameters. In particular, the trapped flux method is highly effective when combined with a diamond anvil cell (DAC), as it eliminates background from the DAC. This is achievable because the signal is measured in a nominally zero-applied magnetic field. Finally, we have estimated the superconducting gap in H_3S by infrared spectroscopy. Currently, we are developing a tunneling spectroscopy technique under high-pressure conditions as a direct probe for the superconducting gap.

It is important to note that SC in hydrogen-rich compounds, such as H_3S, LaH_{10}, YH_9 and YH_6, CaH_6, CeH_9, and CeH_{10}, has been successfully reproduced and confirmed by several independent research groups. Importantly, the crystal structure of the heavy atom sublattice for these compounds has been thoroughly characterised, ensuring reliable comparisons of results between different research teams.

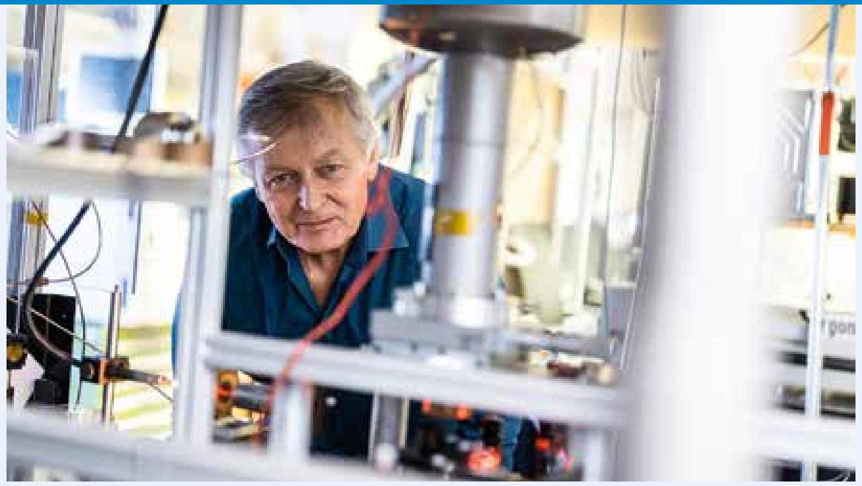
The field of new superconductors has evolved from studying binary systems at high pressures to the recent exploration of more complex superconductors at moderate and ambient pressures (Figure 2). The numerous predictions of superconductors with a T_c above 80 K at ambient pressure are highly promising for practical applications.

RESULTS AND OUTLOOK

In addition to the extensive studies of the electrical and magnetic properties of hydrides mentioned earlier, we are pursuing the ambitious and important goal of achieving room-temperature superconductivity (RTSC) at high pressures. We have conducted studies on the yttrium–hydrogen system, where a T_c of 306–325 K was predicted for the YH_{10} compound. However, we discovered that the highest hydrogen content reached at 410 GPa is YH_9, which exhibited a T_c of 243 K at 200 GPa. We are continuing to study other promising candidates for RTSC, such as MgH_6, LaH_{18}, CeH_{18}, and LuH_{10}. We conducted preliminary screening of the phase diagrams for these systems using the X-ray diffraction technique and are currently performing electrical transport measurements.

Additionally, we are continuing our research on metallic hydrogen. We have successfully demonstrated the transformation of hydrogen into a semi-metallic state at pressures above 300 GPa. Hydrogen transitions from a poor metal to a normal metal at higher pressures. Our current focus is on the next challenge: achieving superconducting hydrogen, which is predicted to occur at pressures above approximately 450 GPa. This goal is realistic, given that we have already attained pressures of 410 GPa for hydrogen samples and 477 GPa for gold samples. By utilizing the correlation between lattice parameters of gold samples and the shift of the diamond Raman edge in stressed diamond anvils, we have developed a new pressure scale that enables for reliable determination of pressures abave 300 GPa. This also facilitates the comparison of results between different research groups

Furthermore, we are in the midst of the search for new superconductors at atmospheric pressure or at pressures below 10 GPa. The discovery of technologically friendly superconductors that operate at temperatures above that of liquid nitrogen could potentially trigger a technological revolution.



"Our goal is to achieve superconductivity at room temperature under high pressure and above liquid nitrogen temperatures under ambient pressure."

SELECTED PUBLICATIONS

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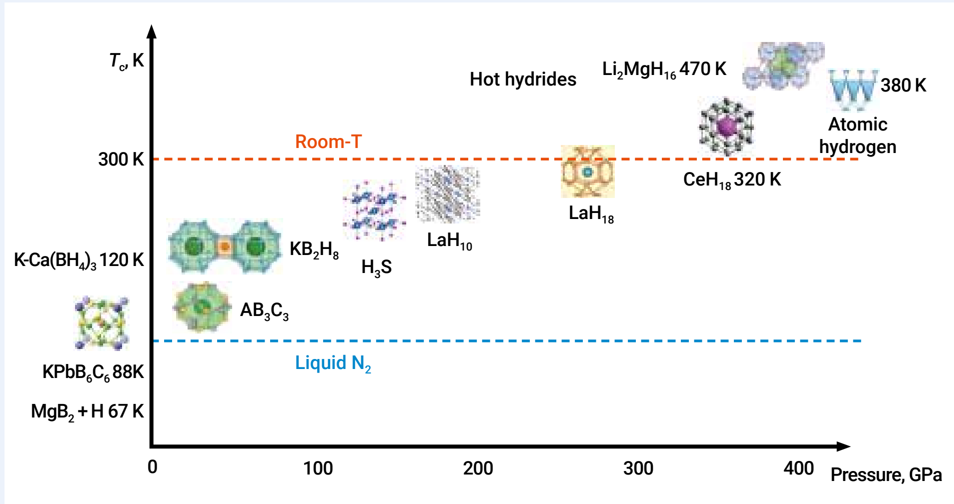

Figure 2: Diagram showing representative high-temperature conventional superconductors. The compounds are indicated by their chemical formula and structural units, placed on the diagram at their range of stability and critical temperatures. Compounds to the left of the diagram are ambient-pressure superconductors. The horizontal blue line corresponds to liquid nitrogen temperature, and the red line corresponds to room temperature.

THE ONSET AND EVOLUTION OF EARLY HOMININ MEAT CONSUMPTION

TINA LÜDECKE – HOMININ MEAT CONSUMPTION GROUP

Figure 1: Excavation of fossils in Gorongosa National Park, Mozambique (left), dentition of a baboon (*Papio ursinus*), an omnivore that constitutes as a prime analogous model for early hominin evolution (middle), and a cross-section of a *Homo erectus* molar (right).

INTRODUCTION

The main goal of the Emmy Noether Group for Hominin Meat Consumption (HoMeCo) is to investigate when meat entered the diet of our human ancestors and how its consumption developed. The incorporation of animal-based foods into the diets of our early ancestors has been hypothesized to be a major catalyst in human evolution and is thought to have contributed to brain expansion and tool use, among others. However, direct evidence for the trophic behavior of our hominin ancestors remains elusive. The earliest signs of meat consumption include ca. 3 Ma-old stone tools and cut marks on fossil bones, but their origin is still debated.

Nitrogen isotopes ($\delta^{15}N$) measured in collagen from ancient bone and dentin provide key insights into the dietary behavior of species in modern ecosystems and the recent geological past (<120,000 years ago). However, due to diagenetic alteration, such analyses have been limited to sites with exceptional preservation. Unlike bone or dentin, organic matter in tooth enamel is protected by its highly mineralized structure, potentially preserving isotopic signals over millions of years. However, the low organic matter content in enamel has so far prevented $\delta^{15}N$ analysis.

In the last two years, our HoMeCo team and colleagues have developed a novel application of the oxidation-denitrification method that allows measurements of the isotopic composition of mineral-bound nitrogen in small amounts of tooth enamel ($\delta^{15}N_{enamel}$). We established that $\delta^{15}N_{enamel}$ records the isotopic composition of diet and preserves a trophic signal in both a feeding experiment and in natural ecosystems. We then applied it to the study of early hominin tooth enamel. Below, we summarize some of our most relevant findings.

RESULTS

In a controlled feeding experiment with rodents, we showed that nitrogen concentration in tooth enamel is sufficient for $\delta^{15}N_{enamel}$ analyses and that $\delta^{15}N_{enamel}$ differs significantly between dietary groups. As only small samples are required (< 5 mg enamel), analyses of size-limited, diagenetically robust tooth enamel are possible, and, as such, this approach represents a promising new dietary proxy for reconstructing food webs and investigating the trophic ecology of extant and extinct taxa.

As a proof of concept, we analyzed $\delta^{15}N$ values in the bone collagen and enamel of modern carnivores and herbivores from several African localities. The $\delta^{15}N_{enamel}$ of these wild mammals showed a several permille-increase between herbivores and carnivores. Moreover, there is a strong positive correlation between $\delta^{15}N$ of the enamel and the bone collagen from the same individuals. Additionally, we analyzed modern fauna from Gorongosa National Park (Mozambique) for enamel $\delta^{13}C$, $\delta^{15}N$, and $\delta^{18}O$ data, which allowed us to reconstruct an isotopic food web for a well-constrained ecosystem. Again, we found a statistically significant difference between herbivore and carnivore $\delta^{15}N_{enamel}$ values.

This modern African mammalian fauna served as a comparative dataset for our first fossil $\delta^{15}N_{enamel}$ study. We reconstructed the position of southern African *Australopithecus* in its paleo-food web to evaluate the consumption of animal versus plant resources in this taxon. We first analyzed the mammalian fauna at Sterkfontein cave, Member 4 (~ 3.5 Ma, South Africa) to establish a $\delta^{15}N_{enamel}$ baseline for contextualizing hominin values. We then analyzed tooth enamel of seven *Australopithecus* sp. individuals. Our results represent the first $\delta^{15}N_{enamel}$ dataset for early Pleistocene hominins and reveal large variation between *Australopithecus* individuals, suggesting a high degree of dietary flexibility. *Australopithecus* $\delta^{15}N_{enamel}$ values do not overlap with the ones of carnivores, indicating that these early hominins had a predominantly plant-based diet.

“Using nitrogen isotopes of fossil tooth enamel, our group will reconstruct the incorporation of animal resources into the diets of our early ancestors, which is considered a key event in human evolution.”

OUTLOOK

While it appears that the Pliocene australopithecines from Sterkfontein had not transitioned to intensive meat consumption, questions remain about the behavior and diets of other early hominin taxa. We plan to generate $\delta^{15}N_{enamel}$ data to reconstruct the onset and evolution of meat consumption of Plio-Pleistocene hominins, including species of *Australopithecus*, *Kenyanthropus*, *Paranthropus*, and *Homo*. We will target key localities in the East African Rift System and the South African Cradle of Humankind. These sites span from 4.2 to 1.4 Ma, a critical period of climate-induced environmental change and hominin adaptation. This unprecedented $\delta^{15}N_{enamel}$ dataset will contribute significantly to our understanding of regional, temporal, and taxonomic variation in the dietary behavior of our early ancestors. Our group will evaluate the onset, evolution, and importance of animal resource consumption, as well as the role of dietary flexibility in the extinction and adaptive radiation of early hominin taxa.

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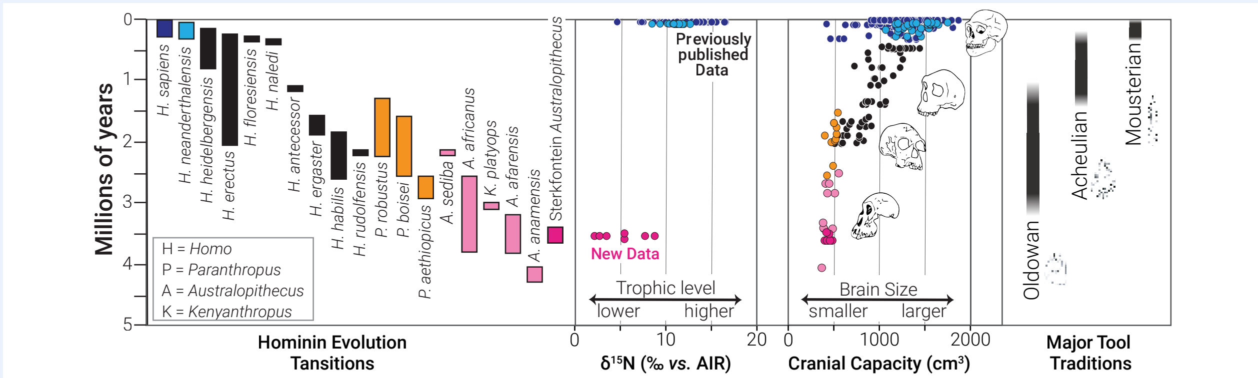

Figure 2: Temporal relationships between hominin evolution, nitrogen isotope values ($\delta^{15}N$), hominin cranial capacity, and major tool traditions. Sterkfontein Member 4 Australopithecus data represent the first $\delta^{15}N$ measurements of an early hominin. Their low $\delta^{15}N$ values point to a largely plant-based diet. Adapted from Lüdecke et al. (under review).

IDENTIFYING VOLCANIC PROPERTIES FROM SPACE

THOMAS WAGNER – SATELLITE REMOTE SENSING GROUP

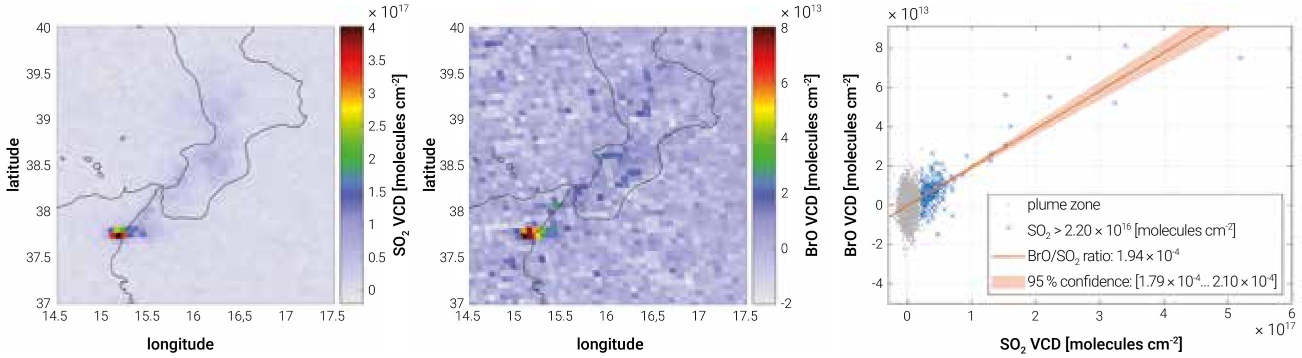

Figure 1: Maps of the vertical column densities of SO_2 (left) and BrO (center) with enhanced values in the plume of Mount Etna on January 29, 2019. Analysis of the spatial correlation of the two trace gases (right).

INTRODUCTION

The research activities of the Satellite Remote Sensing Group focus on the exploitation of the spectral information gathered from ultraviolet/visible satellite instruments, which allow us to quantify important atmospheric (trace) gases such as, e.g., NO_2, H_2O, SO_2, or BrO. Our most recent work exploits the unprecedented spatial resolution provided by the TROPOMI sensor onboard the Sentinel-5 Precursor satellite (S-5P).

Besides their occasionally hazardous impact on human populations, volcanoes can play an important role in atmospheric chemistry and climate. They emit mainly CO_2, H_2O, and SO_2, but their plumes contain many more trace gases, in particular halogen compounds.

The early UV/vis satellite instruments had "footprints" that were much larger than typical volcanic plumes. Thus, locally enhanced trace gas absorptions within the large ground pixels were strongly diluted and typically fell below the detection limits. As a consequence, using early satellite instruments, volcanic trace gases could only be detected for strong volcanic eruptions. The TROPOMI instrument, launched in 2017, has a markedly improved spatial resolution. Its footprint of 3.5 x 5.5 km² is similar to the extension of typical volcanic plumes, leading to a much weaker dilution effect and thus facilitating also the detection of weakly absorbing trace gases inside small volcanic plumes (Wagner et al., 2023).

RESULTS

Ground-based remote sensing observations have identified the BrO to SO_2 ratio to be an important volcanic parameter whose strong inter-volcano variation suggests a link to the volcano magmatic composition and therefore the type of volcano. Similar studies from space are highly desirable in order to establish a global and consistent catalogue of the BrO to SO_2 ratios of volcanic plumes. To achieve this aim, the largest challenge is improving and adapting existing BrO analysis algorithms for TROPOMI observations of volcanic plumes. BrO is a weak atmospheric absorber with optical depths typically below 1×10^{-3}. Spectral interferences with atmospheric absorptions of O_3 and HCHO and the absorption of a varying stratospheric BrO background further complicate the BrO analysis. Finally, the presence of clouds systematically affects the retrieved BrO signal. In comprehensive sensitivity studies, we studied these different effects separately. We quantified and minimised their impacts (Warnach et al., 2023), and compared to previous studies, we were able to lower the BrO detection limit by up to a factor of 5, allowing for the derivation of a large catalogue of 1,500 volcanic plumes over four years (2018–2021). This catalogue increased the number of volcanoes with successful BrO detections from satellite from 11 to 43 and encompassed also plumes from weak eruptions, which makes it much more representative for the entirety of volcanic emission compared to previous studies.

Figure 1 (left and center) shows an example of the simultaneous detection of SO_2 and BrO in a plume from Mount Etna. A fairly linear correlation of both trace gases is found (right). Figure 2 shows a summary of our global catalogue of BrO to SO_2 ratios. One striking finding is that in spite of the large variability of the BrO to SO_2 ratios, clear systematic differences are found for different types of volcanoes. This demonstrates the potential of our new method for the classification of volcanic properties from space. Part of the remaining variability of the BrO to SO_2 ratios can be attributed to different activity states of individual volcanoes or different atmospheric conditions.

"We are most challenged by the weak signals"

OUTLOOK

Especially for horizontally extended plumes of large volcanic eruptions, atmospheric chemistry can strongly affect the plume composition as it is transported from the volcano. Such plumes constitute ideal natural laboratories for the study of the chemical evolution of halogen compounds and the mixing of the plume with surrounding air and will be the subject of further studies. Our new algorithm will also be applied to other satellite instruments, especially the new suite of geostationary instruments.

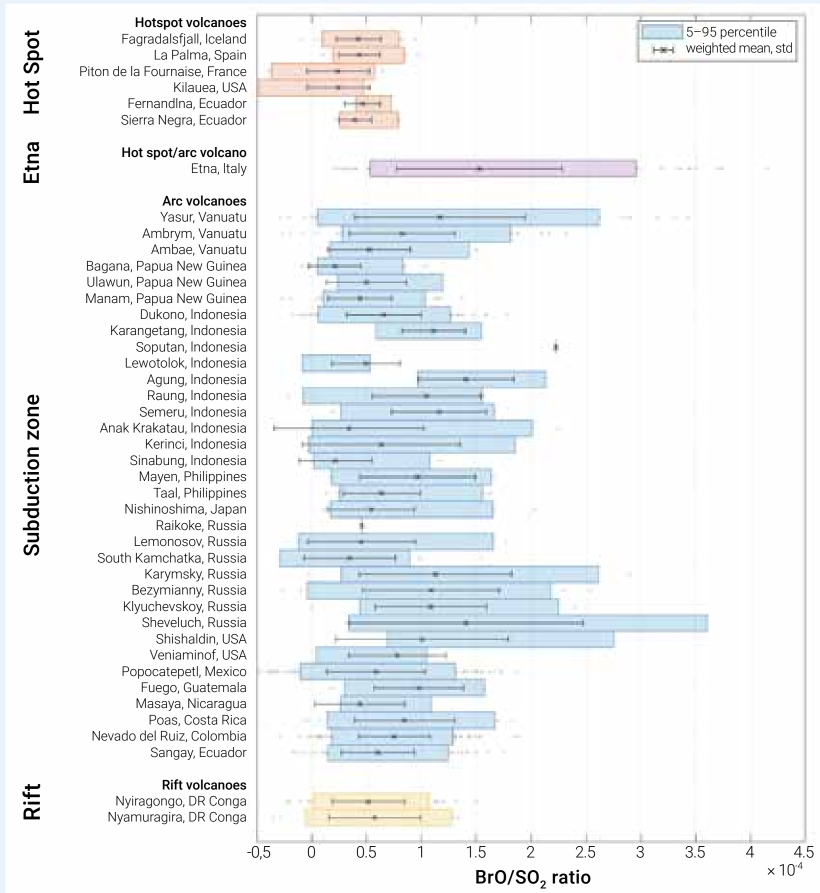

Figure 2: Mean BrO/SO_2 ratios of the 43 volcanoes in our global catalogue. The shaded areas indicate the 5 to 95 percentiles; the mean and the standard deviation are represented by the x and error bars. Colors indicate different types of volcanoes.

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ACKNOWLEDGEMENTS

TROPOMI NO_2 data is provided by the European Space Agency (ESA) and KNMI.

CENTRAL SERVICES

Administration, export control and shipping, information technology, instrument development and electronics, mechanical workshop, facility management, apprenticeship, and communications.

ASSIST AND MAINTAIN

The Central Services at the Max Planck Institute for Chemistry encompass administration, export control and shipping, information technologies (IT), instrument development and electronical workshop, mechanical workshops, facility management, researchers support, and communications. Researchers support is addressed on page 24. These support functions play a vital role in facilitating the daily operations of the MPIC's scientific research departments and groups, as they are responsible for maintaining the institute's infrastructure and managing its external connections.

ADMINISTRATION

The administration offers economic, legal, and organizational backing to facilitate research. This encompasses the management of approximately 300 staff members, oversight of procurement policies, execution of administrative tasks related to projects and external funding, financial record-keeping, budget management, and handling travel expenses. The administration is structured into three core areas: Human Resources, Purchasing, and Finances. Additionally, all support facilities, including facility management and Building Coordination, are interconnected with the institute's administration.

EXPORT CONTROL AND SHIPPING

Conducting scientific campaigns typically involves shipping a large number of measuring instruments, laboratory equipment, and accessories abroad. Many within the institute also send goods, equipment, samples, and information to collaboration partners, outside agencies for technical support or repair, sample analysis centers, and more.

Export Control governs not just the transfer of Dual-Use items, support & assistance, information, data, & software, there is also a requirement to be aware of the export permissions needed for specific types of chemicals which, due to their specific natures, may be used as precursors in the manufacture of explosives or drugs for example. Navigating all these regulations can in many cases be a labor intensive and mentally taxing affair, which is why the institute has established a Shipping and Export Control group to relieve the scientific groups of their need to take on this burden alone. A main aim of the export control group is to ensure the correct export restriction information and points of order are brough to the attention of the scientist for each type of export or transfer which is required to leave the institute.

The group can also be of assistance when navigating the requirements of export documentation for customs, whether the goods being exported are to be exported permanently or only temporarily, and for providing general advice and guidance when dealing with customs for shipping or passenger air travel.

FACILITY MANAGEMENT

The facility management oversees the maintenance of the institute's infrastructure and manage all building equipment, including advanced ventilation and temperature control systems designed for laboratories and clean rooms. Working collaboratively, the team is dedicated to creating and sustaining a conducive work environment. The responsibilities extend from general caretaker services to the thorough inspection of all electrical equipment. Furthermore, the unit manages the reception desk and handles the receipt of goods.

INFORMATION TECHNOLOGIES (IT)

The IT group ensures the smooth operation of the institute's IT infrastructure and manages associated facilities such as the Global Fire Monitoring Center in Freiburg, HALO Aircraft, ATTO Tower and the *S/Y Eugen Seibold*. The IT group consists of seven people and supports all employees with their more than 1,000 network-enabled end devices and a variety of operating systems. The team also manages all servers and the network, without which working at MPIC would no longer be possible.

Among the most important projects of the last three years is the introduction of a new high-performance file server. This involved the coordinated migration of many hundreds of terabytes of data. We also rebuilt the institute's network. In addition, the server room was completely rewired and converted to 100Gb/s. All switches were replaced, all sub-distributions were rewired and our WLAN was upgraded to the brand new Wifi7.

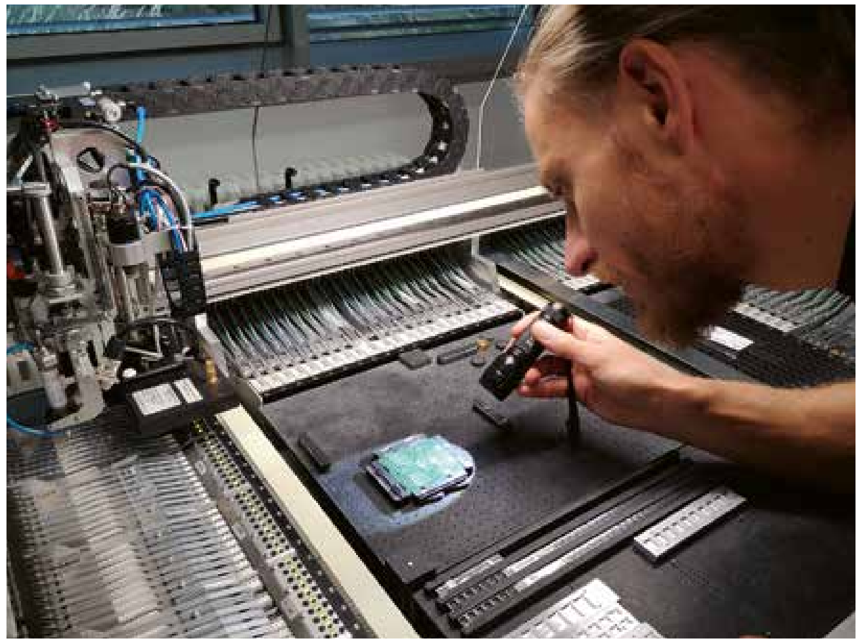
A special focus was and still is on increasing IT security through a variety of measures such as introducing a mail gateway with sandbox, replacing the central institute firewall, switching to new anti-virus software, installing a network access only for MPIC service devices (LAN, WLAN and VPN), and introducing certificate-based VPN tunnels.

The IT team is also regularly on site during campaigns and provides necessary services. In 2022, for example, it supported MPIC scientists during the CAFE-BRAZIL aircraft mission in Brazil.

The group has also been operating the IT infrastructure at the Amazon Tall Tower Observatory (ATTO) in the Brazilian rainforest. In 2022, an air-conditioned container has been set-up exclusively for IT. Thus, a lot of hardware had to be moved under adverse conditions in a short period of time. In 2023, major reconstructions were carried out in the network of the ATTO site. These are aimed at increasing operational reliability and availability as environmental influences, such as lightning strikes, regularly cause network problems. But also incorrectly configured measuring devices can negatively influence the network. Thus, the measures such as converting partial routes to fiber optics for lightning protection reasons, especially at the towers and installing redundant radio links to increase fail-safety were implemented.

The IT group is also responsible for maintaining also maintains the IT structure of the research yacht *S/Y Eugen Seibold*. They were involved in the renewal of the satellite system and enabled a faster and more stable transfer of research data from the ship.

INSTRUMENT DEVELOPMENT AND ELECTRONICS



Studies in Earth System science, be it in the laboratory, on research platforms such as HALO, ATTO and *S/Y Eugen Seibold*, or during scientific campaigns, often require instrumentation that are typically commercially not available or has to be modified to meet environmental operational needs. Often these instruments also have to fulfill stringent compliance requirements for usage on board of aircraft or ships.

A team of five staff members, along with two to four trainees in the Instrument Development and Electronics group offers consulting, design, manufacturing, programming, calibration, deployment and automated data acquisition and evaluation in various programming languages. Almost all electronic hard- and software components are created using off the shelf or custom-made process controllers and component-based visualization software. This accelerates the design process considerably. The campaign support includes online, remote and in-person activities and contributions, including repair of expensive hi-tech lab equipment, which helps reduce service costs.

The service unit's unique infrastructure comprises for instance a fully automated surface mount dispense-, pick-and-place-system, a 5-axis CNC milling machine, micro spot welder, sheet metal processing equipment and an anechoic electromagnetic interference (EMI) testing chamber for pre-compliance testing. This setup allows to efficiently produce customized electronic, mechanical, and electro-mechanical systems.

Over the past three year, the group worked on a wide range of projects, such as

- developing impactor boxes for automated pH-measurement of aerosol particles;
- developing control hard- and software, and designing mechanical parts for an automated elevator platform for vertical gradient measurements at the ATTO tower (RoLi);
- revising the ERICA instrument from GEOPHYISCA for use on DC8/HIAPER/HALO;
- improving gas and aerosol inlet systems for airborne aerosol and chemical ionization mass spectrometers (AMS, ALABAMA, PTR-TOF).

Additionally, during the COVID-19 pandemic, the group carried out extensive measurement and modelling studies on air quality and infection risk in indoor environments.

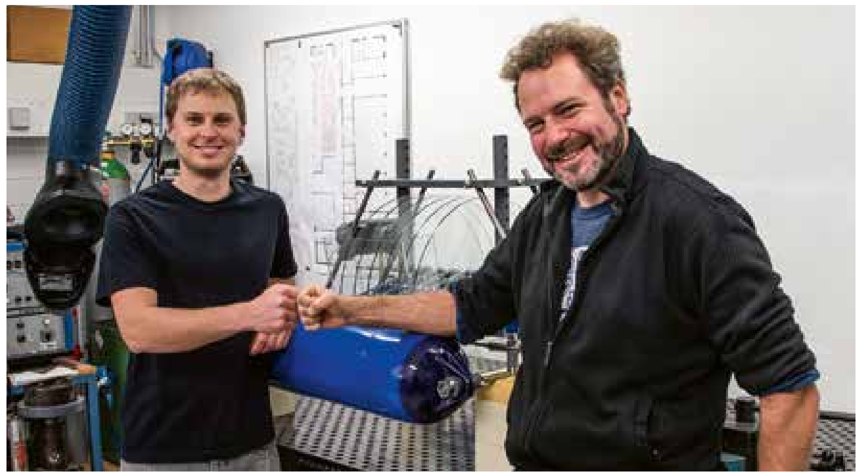
MECHANICAL WORKSHOP

A team of 14 skilled employees in the Mechanical Workshop handles a wide range of operations, such as welding high-quality materials, working with special metals and electroplating. the colleagues contribute to developing scientific instruments and maintaining the institute's infrastructure, closely collaborating with researchers, the instrument development and electronics group, and the facilities management.

In recent years the workshop team collaborated, for instance, in manufacturing mechanical parts for the automatic measuring robot "RoLi" and related experimental setups.

The workshop team also repaired and installed research devices in and on the *S/Y Eugen Seibold* during the boat's overhaul in Bremerhaven in 2023. Special spare parts for the drive train of *S/Y Eugen Seibold*, such as an intermediate shaft and pulleys, were produced at the MPIC workshop to enable the vessel to continue its voyage to Panama.

New technologies such as 3D printers are being used for additive production of light and high-complexity workpieces that cannot be realized with conventional machinery. In 2022, a new CNC turning-milling machine with 2 X 5 axis machining has thus been purchased. Installing this large-dimension machine required a fundamental restructuring of the workshop space. Since spring 2023 workshop staff are trained on the machine.



APPRENTICESHIPS

Apprenticeships are an integral part of the German vocational system, typically lasting three years and taking place in two locations: the practical component in a company and the theoretical part at a vocational school. It is, therefore called dual education system (Duales Ausbildungssystem).

The institute has been training apprentices since 1949. On average, approximately 15 individuals in the professions of precision mechanic and electronics technician for devices and systems are being trained. The young people 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. To ensure training on modern machines, a new CNC milling machine was purchased specifically for the training workshop.

In 2021, the MPIC was honored with an award for being an exceptional training center within the MPS. The recognition was attributed to the high standard of training, characterized by its interdisciplinary, well-founded, broad, and practice-oriented approach.

COMMUNICATIONS

The Communications and Outreach team at the institute promotes and supports the broader research mission of MPIC. The group of seven takes on multiple responsibilities beyond just managing **public and media relations**. It also offers a range of internal services to enhance the institute's research activities. For instance, the **graphics office** contributes to the creation of scientific illustrations and provides a variety of photos and animations. The **library** aids in conducting literature searches, while the **international office** provides onboarding support to incoming scientists and their families, helping them navigate tasks like applying for residence permits and settling into life in Germany. Additionally, the group assists in organizing seminars and events.

Outreach initiatives at MPIC are dedicated to engaging both the media and the general public equitably. This is accomplished through the distribution of press releases and digital content on various social platforms (LinkedIn, X, Facebook, and YouTube), as well as direct interactions with the public during exhibitions at local events.

Regarding media outreach, spanning from 2020 to the present day, the institute issued more than 80 press releases. In terms of public outreach, it consistently shares its research with a diverse audience, encompassing the residents of Mainz and its adjacent regions. Researchers also actively participate in outreach activities of the Mainzer Wissenschaftsallianz (Mainz Research Alliance), which is dedicated to enhancing Mainz's status as a hub for scientific engagement. However, as a result of the COVID-19 pandemic, several events had to be canceled, or in some cases, transitioned to an online format, often leading to lower attendance.

As of 2023, MPIC has returned to hosting various visitor groups and providing internships for secondary school students. Furthermore, it participates in nationwide events like Girls' Day, which seeks to inspire young girls to explore scientific and technical career paths. In July 2023, the institute collaborated with the nearby MPI for Polymer Research to offer an open day, attracting a remarkable 1,300 visitors exclusively to MPIC.

In 2021, of MPIC and the International Centre for Sustainable Development of the Bonn-Rhein-Sieg University of Applied Sciences stated the joint venture KLUGER Transfer. The project focuses on bridging the gap between scientific advancements in climate, environment, and health and their dissemination. Funded for three years by the German Federal Ministry of Education and Research, KLUGER Transfer accelerates interdisciplinary collaboration and knowledge sharing. Subprojects like Teaching, Citizen Science, and Local Governance and Business engage specific audiences, while "Tandem Talks" facilitate scientific discussions. Further, a transfer study analyzes the attitudes of scientific staff in non-university research institutions. Outreach activities aim to connect with the media and the public. By enhancing knowledge transfer, KLUGER aims to contribute to a more informed and engaged society.

Furthermore, the institute is a part of two associations actively engaged 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, with the aim of enhancing understanding of climate change.

STAFF AND BUDGET

In December 2022, a total of about 300 persons were employed at the institute, among them 100 scientists, 47 PhD students and 10 technical trainees. 39,5 % of the staff were female, 60,5 % male.

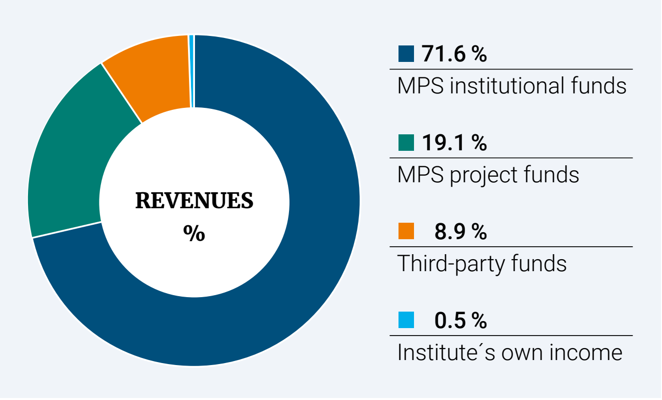
242 staff members were paid from institutional funds, 22 scientists received payment from third-party project funding, 13 from scholarships and 13 by graduate schools.

The annual budget of the institute is approximately € 24 million. A major fraction derives from MPS institutional funds provided by federal and state governments. An overview of revenues and expenditures is given on the right.

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. It offers family-friendly working conditions for both men and women.

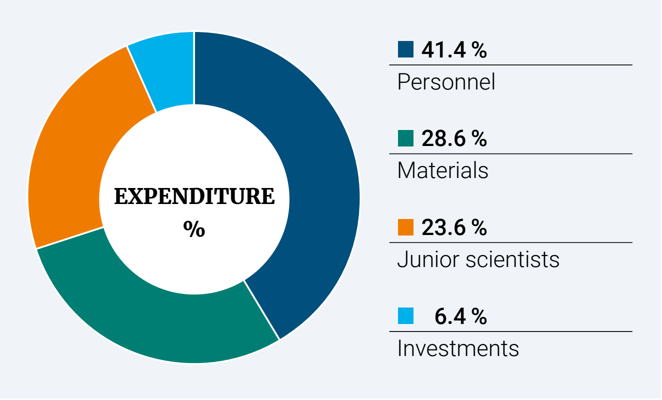
REVENUES 2022

Percentage distribution excluding construction activities.



EXPENDITURES 2022

Percentage distribution excluding construction activities.



GLOSSARY

ACC
Antarctic Circumpolar Current

ACCLIP
Asian Summer Monsoon Chemical and Climate Impact Project

ACP
Atmospheric Chemistry and Physics, a Copernicus OA journal

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)

ALABAMA
Aircraft-based Laser ABlation Aerosol MAss spectrometer

AMA
Asian Monsoon Anticyclone

AMOC
Atlantic Meridional Overturning Circulation

AMS
Aerosol mass spectrometer

AMT
Atmospheric Measurement Techniques, a Copernicus OA journal

AOU
Apparent Oxygen Utilization

AQABA
Air Quality and climate change in the Arabian Basin

AQUA
A NASA scientific research satellite

ASM
Asian summer monsoon

ATAL
Asian Tropopause Aerosol Layer

ATTO
Amazon Tall Tower Observatory

AWG
Anthropocene Working Group

AWI
Alfred Wegener Institute, Bremerhaven

BCO
Barbados Cloud Observatory

BG
Biogeosciences, a Copernicus OA journal

BIOSPHERE
American Earth system science research facility

BLUESKY
Measurement campaign to assess the impact of COVID-19 lockdowns on the environment

BMBF
Federal Ministry of Education and Research

Br-CIMS
Bromide Chemical Ionization Mass Spectrometry

CAFE
Chemistry of the Atmosphere Field Experiment

CAFE-AFRICA
Chemistry of the Atmosphere Field Experiment – Africa

CAFE-BRAZIL
Chemistry of the Atmosphere Field Experiment – Brazil

CARE-C
Climate and Atmosphere Research Center, Nicosia, Cyprus

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

CCN
Cloud Condensation Nuclei

CDOM
Colored dissolved organic matter

CEA
French Commissariat à l'Energie Atomique

CEREGE
European Research and Teaching Center for Environmental Geosciences, Aix-en-Provence

CERN
European Council for Nuclear Research

CFS
Chronic Fatigue Syndrome

CIRRUS-HL
Formation, Lifetime, Properties and Radiative Impact of High-Latitude Cirrus Clouds

CLOUD
Cosmic Leaving Outdoor Droplets

CNC
Computer numerical control, the automated control of machining tools by computer

COVID-19
Coronavirus disease 2019

CPT section
Chemistry, Physics and Technology Section of the MPS

DACs
Diamonds anvil cells

DAMPs
Damage-associated molecular patterns

DC8
Douglas DC-8 jetliner

DCM
Deep Chlorophyll Maximum

DEAL
Project DEAL, consortium that negotiates transformative open access agreements on behalf of its fellow members, the German academic institutions

DFG
German Research Foundation

DKK
German Climate Consortium

DKRZ
German Climate Computing Center

DLR
German Aerospace Center, Cologne

DTU
Danish Technical University, Lyngby

ECMWF
European Centre for Medium-Range Weather Forecasts

EECO
Early Eocene Climatic Optimum

EGU
European Geosciences Union

ELF
Epithelial lining fluid

EMAC
ECHAM/MESSy for Atmospheric Chemistry

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

EMI
Electromagnetic interference

EMME
Eastern Mediterranean and the Middle East

EMME-CARE
Eastern Mediterranean Middle East – Climate and Atmosphere Research Center

ENA
Eastern North Atlantic

ENSO
El Niño–Southern Oscillation

EPA
Environmental Protection Agency, USA

EPIsuite
Estimation Program Interface

ERICA
ERc Instrument for Chemical composition of Aerosols

ESA
European Space Agency

ESRP
Earth System Research Partnership

ETH Zürich
Eidgenössische Technische Hochschule Zürich

EUREC4A
Elucidating the role of clouds-circulation coupling in climate

FIB/TEM
Focused ion beam / transmission electron microscope

FLab
Flying Laboratory

FRRf
Fast Repetition Rate Fluorometry

Geophysica
The Myasishchev M-55 research aircraft

GFZ
German Research Centre for Geosciences in Potsdam

GMD
Geoscientific Model Development, a Copernicus OA journal

Gorongosa NP
Gorongosa National Park Mozambique

HALO
High Altitude and Long Range Research Aircraft

HALO-(AC)^3
Mission to provide a better understanding of the processes behind the drastic climate changes in the Arctic

HALOHOLO
Instrument for cloud particle holography developed for installation on HALO

Hayabusa2 Mission
"Peregrine Falcon 2": Japanese asteroid sample-return mission

HIAPER
High-performance Instrumented Airborne Platform for Environmental Research

HMGB1
High-mobility-group box 1 protein

HNLC
High nutrient low chlorophyll

HoMeCo
Hominin Meat Consumption (Emmy Noether Group for)

HOOVER
HO_x OVer Europe

HSP60
Heat Shock Protein 60

IAGOSCARIBIC
In-service aircraft for a global observing system - Civil Aircraft for the Regular Investigation of the Atmosphere Based on an Instrument Container, Munich based

IN
Ice nuclei

INPA
Instituto Nacional de Pesquisas da Amazonia, Manaus, Brazil

IPA
Institute of Atmospheric Physics

IPCC
Intergovernmental Panel on Climate Change

IUPAC
International Union of Pure and Applied Chemistry

JAXA
Japanese Aerospace Exploration Agency

JGU
Johannes Gutenberg University Mainz

JPL
Jet Propulsion Laboratory, NASA

KLUGER Transfer
Joint project KLUGER (Climate - Environment - Health) Transfer – together with Bonn-Rhein-Sieg University of Applied Sciences

KM-GAP
Kinetic multi-layer model of gas-particle interactions in aerosols and clouds

KM-SUB
Kinetic multi-layer model of aerosol surface and bulk chemistry

KNMI
Royal Dutch Meteorological Institute

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

London penetration depth
Distance to which a magnetic field penetrates into a superconductor

MAX-DOAS
Multi-AXial Differential Optical Absorption Spectroscopy

McFAN
Multiphase chemistry experiment in Fogs and Aerosols in the North China plain

MCGA
Monte Carlo genetic algorithm

MC-ICP-MS
Multicollector - inductively coupled plasma - mass spectrometry

MIT
Massachusetts Institute of Technology

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

MMCO
Middle Miocene Climatic Optimum

MODIS
Moderate-Resolution Imaging Spectroradiometer

MoLa
Mobile Laboratory

MOSAiC
Mass spectrometer measurements on clouds and aerosols for a better understanding of the Arctic climate. Central Arctic

MPGC
Max Planck Graduate Center

MPIC
Max Planck Institute for Chemistry

MPIP
Max Planck Institute for Polymer Research

MPS
Max Planck Society

NAMIP
Nano- and Microparticle Research

NanoSIMS
Secondary ion mass spectrometer with <100 nm spatial resolution

NCAR
National Center for Atmospheric Research

ND-MAX
NASA/DLR-Multidisciplinary Airborne eXperiments

NF-kB
Nuclear factor kappa-light-chain-enhancer of activated B cells

NSF/NCAR
National Science Foundation/National Center for Atmospheric Research

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

OA
Open Access

OA2020
Global initiative that aims to transform existing scholarly journals from subscription to OA

ODP-1090
Site 1090 from the Ocean Drilling Program

ODZ
Oxygen Deficient Zone

OMO
Oxidation Mechanism Observations

PBL
Planetary boundary layer

PCD
Particle Chemistry Department

PCGS
Paul Crutzen Graduate School

PD
Private lecturer

PETM
Paleocene-Eocene Thermal Maximum

PHILEAS
Probing HIgh Latitude Export of air from the Asian Summer monsoon

Phl p 5
Major grass pollen allergen (Phleum pratense)

PM2.5
Particulate matter with diameters smaller than 2.5 µm

PM10
Particulate matter with diameters smaller than 10 µm

PNC
Particle number concentration

POPs
Persistent organic pollutants

ppbv
Parts per billion by volume

PRR
Pattern recognition receptors

PTR-TOF
Chemical ionization mass spectrometer

PVU
Potential vorticity unit

QSAR
Quantitative structure-activity relationship

rBC
Refractory black carbon

RECETOX
Research Centre for Toxic Compounds in the Environment

RH
Relative humidity

RoLi
Automatic measuring robot

RTSC
Room-temperature superconductivity

S-5P
Sentinel 5 Precursor satellite

S/Y Eugen Seibold
Sailing yacht Eugen Seibold

SARS-CoV-2
Severe acute respiratory syndrome coronavirus 2

SC
Superconductivity

SDS-PAGE
Sodium Dodecyl Sulfate – PolyAcrylamid Gel Electrophoresis

SOA
Secondary organic aerosol

SST
Sea surface temperature

StratoClim
Stratospheric and upper tropospheric processes for better climate predictions

STRI
Smithsonian Tropical Research Institute, Panama

STJ
Subtropical jet

SYES
Sailing Yacht (S/Y) Eugen Seibold

TAC
Thesis Advisory Committee

TEP
Tropical Eastern Pacific

TerraClime
DFG funded project funded

TEX_{86}
TEX_{86} paleotemperature proxy; an organic paleothermometer based upon the membrane lipids of mesophilic marine Nitrososphaerota

TLR4
Toll-like receptor 4

TNF
Tumor Necrosis Factor

TP
Thermal tropopause

TPChange
DFG funded Transregional Collaborative Research Center

TROPOMI
TROPOspheric Monitoring Instrument

UBC
University of British Columbia in Vancouver

UFP
Ultrafine Particle Concentrations

UTLS
Upper troposphere and lower stratosphere

UTOPIHAN
Upper tropospheric ozone: processes involving HO_x and NO_x

UV/vis
Ultraviolet/visible

Vortex creep
Vortices arise when the magnetic field starts to penetrate the materials in the form of quantized flux

ZOTTO
Zotino Tall Tower Observatory in the Siberian taiga

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

δ^{18O}
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

^{60}Fe
Iron isotope, radioactive

ATP
Adenosine triphosphate

BC
Black carbon

BrC
Brown carbon

CH_3
Methyl group

CH_3CN
Acetonitrile

CH_3O_2
Methyl peroxy radical

CH_4
Methane

Cl radicals
Chloride radicals

CO_2
Carbon dioxide

D_2O
Deuterium oxide

DDT
Dichlorodiphenyltrichloroethane

H_2O
Water

H_2O_2
Hydrogen peroxide

H_2SO_4
Sulfuric acid

HCHO
Formaldehyde

HNO_3
Nitric acid

HONO
Nitrous acid

IL-1
Interleukin-1

LaH_{10}
Lanthanum hydride

Mg
Magnesium

N
Nitrogen

N_2
Nitrogen (molecular)

NH_3
Ammonia

NM VOC
Non-methane volatile organic compounds

NO
Nitric oxide

NO_2
Nitrogen dioxide

NO_3
Nitrate radical

NO_X
Nitrogen oxides;
$= NO + NO_2$

O_2
Oxygen

O_3
Ozone

OH
Hydroxyl

PAA
Polyacrylic Acid

PAHs
Polycyclic aromatic hydrocarbons

PAN
Peroxyacyl nitrate

RNS
Reactive nitrogen species

RO_2
Organic peroxy radicals

ROS
Reactive oxygen species

SO_2
Sulfur dioxide

VOCs
Volatile organic compounds

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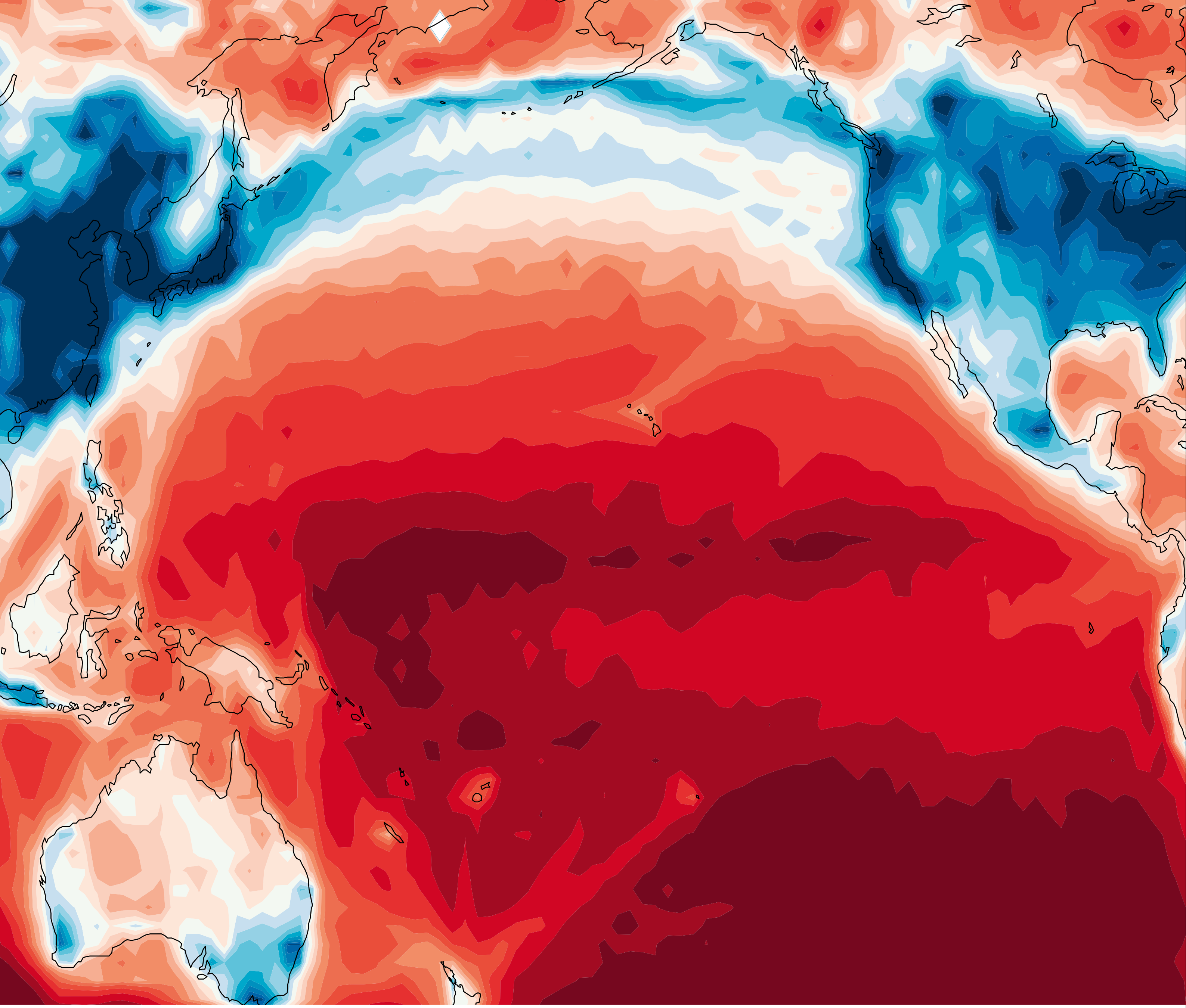

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