



第9届中法大气环境国际研讨会

9TH Sino-French Joint Workshop on Atmospheric Environment

Book of Abstracts

Harnessing Artificial Intelligence for Air Pollution
Prevention in a Changing Climate:
Beyond Anthropogenic Origins

HANGZHOU - CHINA
April 8-11, 2026

Contents

| | |
|---|----|
| Advances in remote sensing techniques for atmospheric trace gases in China .. | 1 |
| Rapid HCl Production from Chlorine Oxidation Sustains Coastal Atmospheric Chlorine Cycling | 2 |
| Global air-pollution policy effectiveness for curbing major ozone precursor emissions over two decades | 3 |
| The Nitrogen Oxides Chemistry in Polar Urban Environment Revealed by N and O stable isotopes | 4 |
| Tire Antioxidants and their Quinone Derivatives in Aerosol, Clouds | 5 |
| Molecular-scale Study of Molecules of Atmospheric Interest Using Cryogenic Matrices | 6 |
| Source Apportionment of PM ₁₀ in Nouméa and Health Risk Assessment: Influence of the Nickel Smelter on Air Quality at Griscelli School | 7 |
| Online molecular composition and processing of aqueous secondary organic aerosol in clouds at a mountain site in southeastern China | 8 |
| Cloud chemical composition: pesticides in water droplets | 9 |
| The reactions of ozone with alkenes and subsequent chemistry | 10 |
| Molecular Characteristics, Origins and Atmospheric Reaction Behavior of Atmospheric Amines in Four Chinese Cities | 11 |
| Selfreaction of peroxy radicals re-investigated by laser photolysis / cw Cavity Ring Down Spectroscopy | 12 |

| | |
|--|-----------|
| Development of Green Methanol in Shipping and Methanol-SCR Denitration Technology | 13 |
| Tackling Seasonal Smog: Breaking Crop Residue Buringing’ s Grip | 14 |
| Electronically Engineered Hierarchical Heterojunction Catalysts for Low-Concentration NO Photocatalytic Purification | 15 |
| Arctic Air Pollution: New Insights and Future Perspectives | 16 |
| AI-based Probabilistic Air Quality Forecasting | 17 |
| Characterization of secondary organic aerosol from the ozonolysis of α-pinene using laser trapping and Raman spectroscopy | 18 |
| Exposure Studies of Living/biological Organisms: how can smog chambers revolutionize such exposure studies? Illustration: how the PolluRisk Platform is simulating at the laboratory urban Air Quality and its health impacts | 19 |
| Long-Term PM_{2.5} and PM₁₀ Nitrate Trends from Filter Networks: Correction of Temperature-dependent Measurement Bias Using Multi-Year Filter–MARGA Intercomparison Data | 20 |
| Computational investigation of multiphase chemical mechanisms in atmospheric aerosols and water droplets | 21 |
| Chemistry on Urban Surfaces as a Driver of Air Pollution in the Cities | 22 |
| Rethinking Stratospheric Aerosols: Sources, Composition, and Unexpected Impacts | 23 |
| Revealing the important role of OVOCs on photochemistry in Coastal Hong Kong | 24 |

| | |
|---|-----------|
| Constraining the Unconstrained: Isotopic Evidence Debunks Modeled Pathways of Haze Sulfate Formation | 25 |
| Airborne microplastics: A review of current perspectives and environmental implications | 26 |
| Quantifying Hourly Wildfire Smoke Exposure and Acute Health Risks with Cascade Machine Learning | 27 |
| Vehicle emissions under real driving conditions: investigating the impact of semi-volatile compounds on air quality | 28 |
| The CHIMERE model as a tool to identify the best strategies to improve air quality and develop innovative AI-based techniques | 29 |
| Early-life nutritional additives, home environment, and outdoor air pollution associated with childhood food allergies: A multi-center mother-child study in China | 33 |
| Vacuum ultraviolet photoionization mass spectrometry and its applications in atmospheric environment | 34 |
| Uptake of atmospheric pollutants on road asphalt pavements: an underestimated sink in urban environments | 35 |
| Atmospheric oxidation capacity dynamics-driven meteorology and multi-precursor interactions modulate O₃ variation in Hangzhou, China | 36 |
| Microscopic Insights into Firework and Biomass Burning Derived Haze Particles During the Diwali Festival in Delhi, India | 37 |

| | |
|--|-----------|
| Machine Learning for Long-term NO₂ Photolysis Reconstruction and its Impact on Secondary Pollution | 38 |
| Specific ion chemistry at the air-water interface of nitrite/nitrate containing droplets | 39 |
| Data-Driven Methodologies for Accurate Source Apportionment of Atmospheric Pollution and Practical Applications | 40 |
| Construction of the First Fingerprint Spectrum for Biogenic Carbonyls Emitted from a Tropical Rainforest | 41 |
| Experimental Reexamination of the CH₂OO and (CH₃)₂COO Criegee Intermediate Reactions with SO₂ | 42 |
| Particle–gas transfer processes during the photolysis of cis-pinonic acid: a comparative study between bulk and single-particle approaches | 43 |
| Spontaneous Sulfur(IV) Oxidation at Droplet Interfaces | 44 |
| Oxidation of Dimethyl Sulfide at Air-Water Bubbles Surfaces | 45 |
| Ammonia (NH₃) Monitoring and Its Impact on Air Pollution and Climate Change in Agricultural and Semi-Urban Sites from Central France | 46 |
| Ozonolysis of Myrtenal on Saharan Sand: Impact of Particle Diameter, Surface Coating and Relative Humidity | 47 |
| Less NO_x emission reductions are a potential cause for low effectiveness of sulfate aerosol reductions in China | 48 |
| Urban–rural divergence of wintertime organic aerosol molecular fingerprints in PM_{2.5} revealed by FT–ICR MS | 50 |

| | |
|--|-----------|
| Real-time Detection of Black Smoke from Ships based on Improved YOLOv5 with Multi-Feature Fusion Method | 51 |
| JUNON: Environmental Digital Twins in the Centre Val de Loire | 53 |
| Street level spatiotemporal assessment of 6PPD-Q emissions and inhalation risks for humans and wild birds on Chongming Island | 54 |
| Accurate discrimination of endogenous and exogenous VOCs in exhaled breath and exposure risk assessment | 55 |
| Spontaneous Fe(III) Reduction at the Air–Water Interface Promotes Fenton OH Formation in Atmospheric Microdroplets | 56 |
| Effect of Surfactants on Spontaneous H₂O₂ Formation at Air-water Interface | 57 |
| Emission Characteristics and Environmental Risks of White Oil and Liquid Paraffin Combustion | 58 |
| Bent Quadrupole for QTOF-MS Simulated by COMSOL Multiphysics: Ion Transmission Efficiency and Its Influencing Parameters | 59 |
| Development of a Miniaturized TD–Trap Gas Chromatography System and Its Application in Atmospheric VOCs Monitoring | 60 |
| Simulation of Global Cloud Water Acidity Based on the Adaptive Damped Newton’ s Method | 61 |
| Core-Shell Three- Way Catalysts for Natural Gas Vehicle Exhaust Aftertreatment | 62 |
| Dark Freezing of Iodide-containing Aqueous Droplets as a Potential Source of Reactive Iodine in Polar Marine Regions | 64 |

| | |
|--|-----------|
| Technological advances in solvents drive substantial reductions in VOC emissions and associated impacts from industrial coating use | 65 |
| Research on the Optical Properties of Secondary Organic Aerosols Based on Laboratory Simulations: Progress and Prospects | 66 |
| Biogenic Oxygenated VOCs: Dynamics and Responses under Global Change ... | 68 |

Advances in remote sensing techniques for atmospheric trace gases in China

Wenqing Liu

Anhui Institute of Optics and Fine Mechanics, HFIPS, CAS

Institute of Environment, Hefei Comprehensive National Science Center

Environmental monitoring technology is an important support for the construction of ecological civilization. Atmospheric gases and their changes not only affect the present and future world, but also have always been the focus of international scientific research.

With the advancement of the "pollution reduction and carbon emission reduction" strategy, significant changes have occurred in the sources, emission components, and emission concentrations of pollution sources/greenhouse gases. The monitoring technology system for atmospheric trace components is developing towards high precision, dynamism, and intelligence. The development of new technologies such as satellite remote sensing and unmanned aerial vehicle (UAV) remote sensing has made it possible to obtain pollutant data from space, forming an integrated multi-pollutant monitoring system that combines space, air and ground. This system integrates satellites, unmanned aerial vehicles and ground monitoring equipment to achieve comprehensive and precise monitoring of air pollutants and greenhouse gases. Provide technical and equipment support for the construction of an ecological environment protection and monitoring system from mountain peaks to the ocean in our country.

Rapid HCl Production from Chlorine Oxidation Sustains Coastal Atmospheric Chlorine Cycling

Weihsun Sun^{1†}, Hengqing Shen^{1†}, Xiaorui Chen^{1,2}, Yifan Jiang¹, Poon Steven¹, Tao Wang^{1*}

¹Department of Civil and Environmental Engineering, The Hong Kong Polytechnic University, Hong Kong 999077, China. tao.wang@polyu.edu.hk

²Southern Marine Science and Engineering Guangdong Laboratory (Zhuhai), School of Atmospheric Sciences, Sun Yat-sen University, Zhuhai 519082, China.

[†]These authors contributed equally to this work.

Hydrogen chloride (HCl), a major tropospheric reservoir of reactive chlorine. In coastal environment, it is thought to primarily originate from acid displacement of particulate chloride (Cl^-). Here we demonstrate that chlorine radical oxidation of volatile organic compounds (VOCs) dominates HCl formation (64%) at a semi-polluted coastal site with elevated levels of molecular chlorine (Cl_2), exceeding the acid displacement of Cl^- (36%). Rapid HCl formation from chlorine radical oxidation, coupled with concurrent Cl^- activation to molecular chlorine (Cl_2), shifts the HCl- Cl^- partitioning equilibrium and drives efficient aerosol uptake of gaseous HCl. The dynamic balance between Cl^- depletion and replenishment reveal a previously overlooked self-sustaining multiphase chlorine cycling, where HCl acts not as terminal sink but as central hub sustaining chlorine cycling. This cycle (Cl -HCl- Cl - Cl) amplifies daytime OH, HO_2 , and RO_2 concentrations by 11%, 19%, and 30%, respectively, and increases net O_x production by 28%. Our study reveals a feedback loop that enhances atmospheric oxidation in this coastal site and potentially other areas.

Global air-pollution policy effectiveness for curbing major ozone precursor emissions over two decades

Ningning Yao^{1,2}, Huan Xi^{1,2}, Jie Zhang^{1,2}, Lang Chen^{1,2}, Zhe Song^{1,2,3}, Zhengnan Cen^{1,2}, Pengfei Li⁴, Alexander Baklanov⁵, Jens Hesselbjerg Christensen⁵, John H. Seinfeld⁶, and Shaocai Yu^{2,1,3*}

¹Collaborative Innovation Center for Statistical Data Engineering, Technology and Application; School of Statistics and Mathematics, Zhejiang Gongshang University, Hangzhou, 310018, China

²Zhejiang Key Laboratory of Solid Waste Pollution Control and Resource Utilization, School of Environmental Sciences and Engineering, Zhejiang Gongshang University, Hangzhou 310018, China

³Research Center for Air Pollution and Health, Key Laboratory of Environmental Remediation and Ecological Health, Ministry of Education, College of Environment and Resource Sciences, Zhejiang University, Hangzhou, 310058, China

⁴State Key Laboratory of Infrared Physics, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, Shanghai, 200031, China

⁵Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark

⁶Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125, USA *Email: shaocaiyu@zjgsu.edu.cn

Ground-level ozone (O₃), formed through photochemical reactions of NO_x, CO, and VOCs, poses significant threats to human health, agriculture, and ecosystems. Despite widespread deployment of diverse environmental policies targeting these precursors, their real-world effectiveness and optimal combinations remain unclear. Here, we employ structural-break detection with a machine-learning enhanced model to identify and attribute O₃ precursor emission reductions without predefining intervention timing or policy types. We detect 50 statistically significant breakpoints in NO_x, CO, and VOC emissions, with average reductions of 11.9%, 17.9%, and 13.6%, respectively, and larger declines observed in developed economies. We further find that integrated policy packages combining regulation, pricing, and RD&D support outperform single-instrument approaches. However, association rule analysis reveals diminishing returns and functional redundancy when layering more than two instruments, especially in developed economies where core emission pathways are well targeted. In developing countries, effective combinations often include investment-linked instruments with standards or pricing, though excessive layering similarly yields marginal gains. This data-driven approach offers a scalable tool for ex-post policy attribution and highlights the critical need for designing functionally complementary, context-specific policy portfolios to efficiently mitigate O₃ precursors globally.

The Nitrogen Oxides Chemistry in Polar Urban Environment Revealed by N and O stable isotopes

Joel Savarino¹, Sarah Albertin², Slimane Bekki³, Natalie Brett³, Meeta Cesler-Maloney⁴, James H. Flynn⁵, Fangzhou Gao⁵, Brice Barret⁶, Nicolas Caillon¹, Barbara d'Anna⁷, Elsa Dieudonné⁸, Alexis Lamothe¹, Soline Richard¹, Brice Temine-Roussel⁷, Becky Alexander⁹, Steve R. Arnold³, Stefano Decesari¹⁰, Gilberto J. Fochesatto¹¹, Jingqiu Mao⁴, William Simpson⁴, Kathy Law³

¹Institut des Geosciences de l'Environnement, UGA/CNRS, France, joel.savarino@cnrs.fr

²Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder, CO, USA and Chemical Sciences Laboratory, National Oceanic and Atmospheric Administration, Boulder, CO, USA

³Sorbonne Université, UVSQ, CNRS, LATMOS/IPSL, Paris, France,

⁴Geophysical Institute and Department of Chemistry and Biochemistry, University of Alaska Fairbanks, Fairbanks, AK, USA

⁵Earth & Atmospheric Sciences, University of Houston, Houston, TX 77204, USA,

⁶Université Toulouse III – Paul Sabatier, CNRS, LAERO, 31062 Toulouse, France,

⁷Aix Marseille Univ, CNRS, LCE, 13000 Marseille, France,

⁸Université du Littoral Côte d'Opale, Laboratoire de Physico-Chimie de l'Atmosphère, 59140 Dunkerque, France,

⁹Department of Atmospheric Sciences, University of Washington, Seattle, WA 98195, USA

¹⁰CNR-ISAC, National Research Council of Italy, Institute of Atmospheric Sciences and Climate, Bologna, IT 40129, Italy,

¹¹Department of Atmospheric Sciences, College of Natural Science and Mathematics, University of Alaska, Fairbanks, AK 99775, USA.

Nitrogen (N) and oxygen (O) stable isotopes measured in atmospheric reactive N (Nr) species can help trace emission sources of nitrogen oxides (NO_x). However, large uncertainties subsist regarding the factors controlling the variability of N and O isotopes in Nr species, preventing a precise isotope-based chemistry and emission source apportionment. This work presents a comprehensive analysis of the enrichment of the $\delta^{15}\text{N}$ and $\Delta^{17}\text{O}$ in atmospheric nitrogen dioxide (NO₂) collected during the Alaskan Layered Pollution and Chemical Analysis (ALPACA) 2022 international winter campaign in Fairbanks, Alaska.

Both isotopic parameters show a very good correlation with the NO_x regime encountered during this field campaign. After correcting our $\delta^{15}\text{N}(\text{NO}_2)$ measurements for N fractionation effects, a $\delta^{15}\text{N}$ -Based source apportionment analysis identifies vehicle and space heating oil emissions as the dominant sources of breathing-level NO_x at this urban site. Despite their large NO_x emissions, coal-fired power plants with elevated chimney stacks (> 26 m) appear to make a small contribution to surface NO_x levels in downtown Fairbanks (likely less than 18 % on average). The combined uncertainties of the $\delta^{15}\text{N}$ of NO_x from heating oil combustion and of the influence of low temperatures on the $\delta^{15}\text{N}$ of NO_x emitted by vehicle exhaust prevent a more detailed partitioning of surface NO_x sources in Fairbanks.

We found two distinctive regimes for the $\Delta^{17}\text{O}$ of NO₂. During the day, $\Delta^{17}\text{O}$ increases with the NO₂ photolysis flux ($J_{\text{NO}_2} \times [\text{NO}_2]$), reflecting the progressive establishment of the photochemical steady state as solar radiation increases throughout February. Thus, $\Delta^{17}\text{O}$ reflects the NO–NO₂ system returning to an equilibrium steady state over a timescale dependent on NO₂ photolysis. In other words, this result shows that during the day, it is not until end of February than the Leighton cycle is fully established. At night, $\Delta^{17}\text{O}(\text{NO}_2)$ scales proportionally with the NO₂/NO_x ratio and reaches values well- below the limit set by the NO + O₃ reaction, requiring a source of NO₂ that is independent from the NO + O₃.

Tire Antioxidants and their Quinone Derivatives in Aerosol, Clouds

Jianmin Chen and Runqi Zhang

Environmental Science and Engineering, Fudan University, Shanghai, China.

Email: jmchen@fudan.edu.cn

Substituted p-phenylenediamines (PPDs) are widely employed as antioxidant additives in rubber products, particularly in tire manufacturing, to delay oxidative degradation. Here, we report tire antioxidants and their quinone derivatives in aerosol, clouds. We systematically investigated the occurrence, chemical composition, transformation behaviors, and influencing factors of PPDs and PPD-Qs in fine particulate matter (PM_{2.5}) during the summer from 2018 to 2024 in urban Shanghai, which is a representative megacity in eastern China. Using ultrahigh-performance liquid chromatography coupled with higher solution mass spectrometry (UHPLC-HRMS), we identified 25 PPD-related compounds in total. 7 parent PPDs and 6 corresponding PPD-Qs were selected for quantitative analysis. The concentrations of individual PPDs and PPD-Qs ranged from 45.7 to 1580, and 83.9 to 1130 pg/m³, respectively. Both the total concentration of PPDs (ΣPPDs) and that of PPD-Qs (ΣPPD-Qs) exhibited significant interannual increases over the study period. This trend was highly associated with the increasing frequency and intensity of summer heatwave events observed in recent years. Further analysis revealed that the ambient temperature and ozone concentration play crucial roles.

In cloud water collected in at Tianmu Mountain (1151 m a.s.l.), China, from April 7 to September 26, 2024. Fig. 1 showed the identification of PPDs and PPD-Qs in cloud water the concentrations of PPD ranged from 3.02 to 43.69 ng/L, markedly exceeding those of their transformation products (PPD-Qs, 0.21 – 11.45 ng/L).

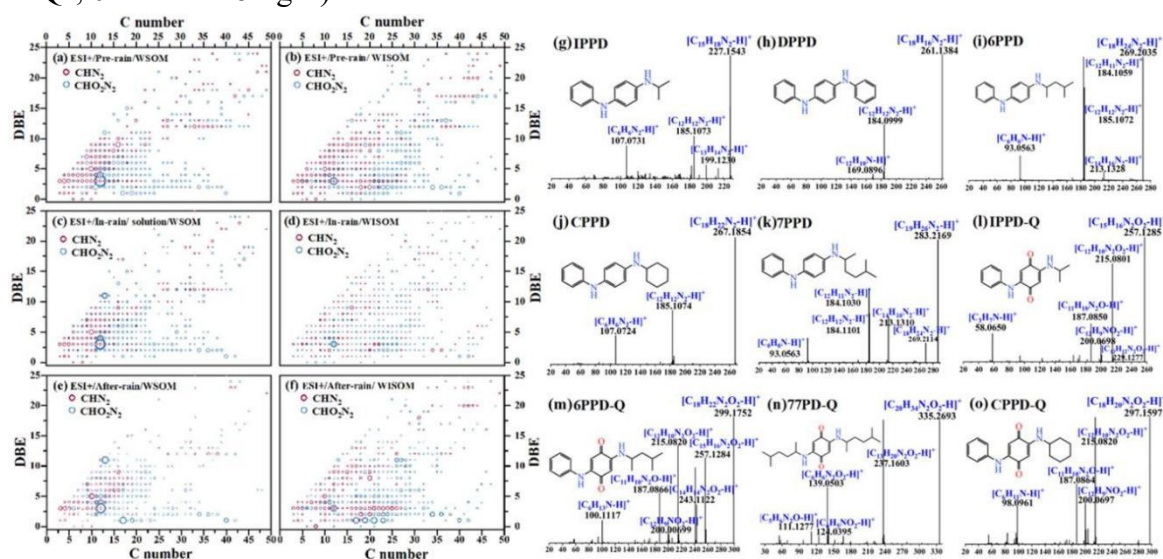


Fig. 1. Identify PPDs and PPD-Qs in cloud water. Double Bond equivalent (DBE) and C number of CHN₂ and CHO₂N₂ compounds detected in ESI+ on Pre-rain(a, b), In-rain(c, d) and After-rain(e, f) days. Representative MS/MS fragmentation spectra of PPDs (g–k) and PPD-Qs (i–o)

PPDs exhibited greater accumulation in water-insoluble organic matter (WISOM) than in water-soluble organic matter (WSOM), with enrichment factors ranging from 1.13 to 1.88, indicating a stronger tendency for particle-phase partitioning. Precipitation processes were found to influence the oxidative conversion of PPDs to PPD-Qs. This study provides the characterization of the distribution and environmental behavior of PPDs and their quinone derivatives, highlighting the previously overlooked role of clouds in determining the fate of rubber-derived pollutants. The findings provide critical insights and establish a baseline for future ecological and human health risk assessments.

KEYWORDS: Tire antioxidants, Aerosol, Cloud, PPDs, PPD-Qs, LC-Q-TOF-MS, LC-Orbitrap MS

Molecular-scale Study of Molecules of Atmospheric Interest Using Cryogenic Matrices

S. Coussan^a, J. Mascetti^b, G. Bourdon^{b,c}, E. Villenave^c, S. Sobanska^b

^a Aix-Marseille Univ., CNRS, PIIM, Marseille 133997, France

^b Institut des Sciences Moléculaires, UMR CNRS 5255, Univ. Bordeaux, Talence cedex F-33405, France

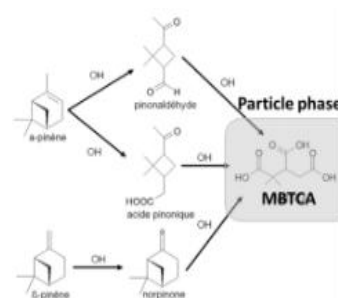
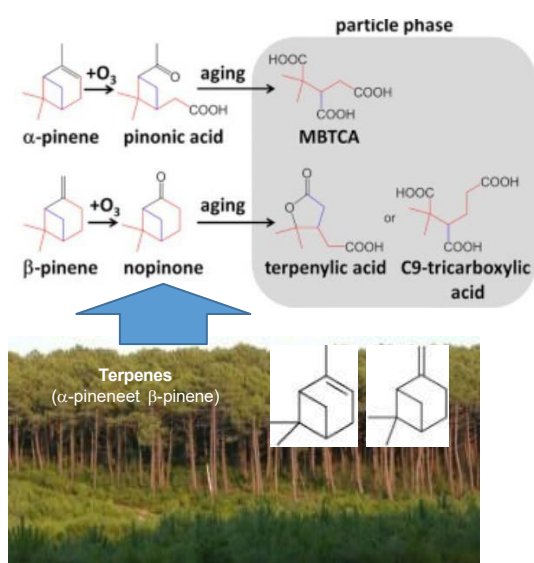
^c CNRS, EPOC, EPHE, UMR 5805 CNRS, Univ. Bordeaux, Pessac cedex F-33615, France

Complexity arises from a sequence of simple fundamental events, first atomic and then molecular. It is therefore particularly useful to study extremely complex systems, such as the Earth's atmosphere, at different scales, ranging from the molecular scale to the micrometric scale, that of aerosols in particular. If we focus specifically on the oxidation chain of terpenes, particularly α - and β -pinene to MBTCA, it is particularly important to understand the effects of hydration and UV and visible radiation at each stage. This aging process is not well characterized, yet the molecules involved can subsequently become solvated in aerosols or on their surface, thereby generating reactivity in turn. The purpose of our presentation is to highlight the advantages of a technique particularly suited to molecular studies, namely cryogenic matrices. This will be illustrated through two examples: MBTCA and cis-pinonic acid.

Hydration of atmospheric interest molecules

ANR SOAPHY, ISM Bordeaux, EPOC Bordeaux, PIIM Marseille, ICCF Clermont

–Ferrand



Coussan*, S., Aupetit, C., Mascetti, J., Villenave, E., Sobanska*, S., J. Phys. Chem. A, 2025, 129, 1280–1292

Source Apportionment of PM₁₀ in Nouméa and Health Risk Assessment: Influence of the Nickel Smelter on Air Quality at Griscelli School

Estelle Roth^{1*}, Peggy Gunkel-Grillon², Abdelkhaleq Chakir¹

^{1*}Climate Impacts on Environment, AEROLAB emr7007, Université de Reims, France, estelle.roth@univ-reims.fr

^{2*}Institut des Sciences Exactes et Appliquées, Université de la Nouvelle-Calédonie, France

New Caledonia is a remote South Pacific island where the main industrial activities are open-pit mining and nickel (Ni) metallurgy. The island's geology is characterized by lateritic soils enriched in Ni, manganese (Mn), and chromium (Cr), elements that may pose health risks, particularly when present in inhalable particulate form. In Nouméa, the capital city of New Caledonia, a ferronickel production plant operates in close proximity to residential areas, including Griscelli School. In response to public concern, especially regarding children's health, the local air quality monitoring agency, Scal'Air, conducted an intensive measurement campaign to identify pollution sources and assess associated health risks.

PM₁₀ samples were collected daily over a period exceeding two months and analyzed for 12 elements, including both metals and non-metals. In parallel, NO_x, SO_x, wind speed, and wind direction were recorded hourly. Source apportionment was performed using a combination of Principal Component Analysis (PCA) /APCS (Absolute Principal Component Scores) and Positive Matrix Factorization (PMF). Health risk assessment was conducted following methodologies recommended by the U.S. Environmental Protection Agency (US EPA).

Hourly PM₁₀ concentrations ranged from 1.5 µg/m³ to 106.9 µg/m³, with an average concentration of 12.6 µg/m³. The regulatory daily limit value of 50 µg/m³ for the protection of human health was not exceeded during the sampling period. However, while overall PM₁₀ mass concentrations remained below regulatory thresholds, nickel concentrations showed significant variability. The mean Ni concentration was 57.4 ng/m³, with a median value of 13.7 ng/m³, reflecting strong day-to-day variability (0.2 to 615 ng/m³). Notably, 30% of daily Ni concentrations exceeded the annual target value of 20 ng/m³ established for air quality protection. Health risk assessment based on the measured elemental concentrations revealed a high non-carcinogenic risk associated primarily with elevated nickel concentrations, while the carcinogenic risk was found to be within acceptable limits. PCA/APCS analysis identified five principal components and sources. To improve source apportionment PMF analysis was carried out combining metallic and non-metallic elements with gases leading to 6 sources. Coupling wind direction data with the industrial and heavy fuel oil combustion contribution factors clearly demonstrated the significant impact of the nickel smelter on local air quality.

Online molecular composition and processing of aqueous secondary organic aerosol in clouds at a mountain site in southeastern China

Yali Jin^{1,2,3,4}, Hao Luo^{1,6}, Siqi Tang¹, Shuhui Xue¹, Chengyu Nie¹, Xiaocong Peng⁷, Yan Zheng⁹, Weiqi Xu⁸, Guohua Zhang⁷, Xiaole Pan⁸, Yele Sun⁸, Qi Chen⁹, Lanzhong Liu⁸, and Defeng Zhao^{1,3,4,5*}

¹Department of Atmospheric and Oceanic Sciences & Institute of Atmospheric Sciences, Fudan University, Shanghai, 200438, China

²Shanghai Frontiers Science Center of Atmosphere-Ocean Interaction, Fudan University, Shanghai, 200438, China

³Shanghai Key Laboratory of Ocean-land-atmosphere Boundary Dynamics and Climate Change, Fudan University, Shanghai, 200438, China

⁴National Observations and Research Station for Wetland Ecosystems of the Yangtze Estuary, Fudan University, Shanghai, 200438, China

⁵Institute of Eco-Chongming (IEC), 20 Cuiniao Rd., Chongming, Shanghai, 202162, China, dfzhao@fudan.edu.cn

⁶Inner Mongolia Key Laboratory of Pollution Control and Low Carbon Resource Utilization, Inner Mongolia University, Inner Mongolia, 010021, China

⁷State Key Laboratory of Advanced Environmental Technology, Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou, 510640, China

⁸State Key Laboratory of Atmospheric Environment and Extreme Meteorology, Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing, 100029, China

⁹State Key Laboratory of Regional Environment and Sustainability, College of Environmental Sciences and Engineering, Peking University, Beijing, 100871, China

Aqueous secondary organic aerosol (aqSOA) contributes substantially to organic aerosol (OA), affecting air quality, human health, and climate. However, the molecular composition and processing of aqSOA in clouds remain unclear due to limited online field measurements. We measured molecular composition of OA online (time resolution 20 s) and tracked its processing at a mountain site in southeastern China, using an Extractive ElectroSpray Ionization inlet coupled with a Time-of-Flight Mass Spectrometer (EESI-ToF-MS). We identified 2084 molecular formulas and compared OA composition from three sample types: cloud droplet residuals (CDR), interstitial aerosol particles (INT), and cloud-free aerosol particles (CF) in representative cloud episodes. CHO class was the dominant constituent, followed by CHON class. In most cloud episodes, the fraction of CHO was lower in CDR than that in INT and CF, while the fraction of CHON was higher, which may result from the uptake of organonitrates or nitration in cloud water. Compounds in CDR had more carbon number and higher molecular weight than CF, which is attributed to accretion reactions in cloud water. We identified 39 significantly enriched compounds in CDR compared with CF, which could be potentially used as aqSOA tracers formed via cloud processing. This study also reveals rapid changes in aqSOA composition, which highlight the necessity for high time resolution measurements to capture the processing of aqSOA in clouds. Overall, this study provides clear information on processing of aqSOA in clouds and highlights the importance of accretion reactions, which have implications on the composition and physicochemical properties of SOA.

Cloud chemical composition: pesticides in water droplets

Gilles Mailhot^{1,2*}, Angelica Bianco¹, Pauline Nibert¹, Yi Wu^{1,2}, Jean-Luc Baray¹, Marcello Brigante², Laurent Deguillaume¹, Davide Vione³, and Pascale Besse-Hoggan¹

^{1*}Laboratoire de Météorologie Physique, UMR CNRS 6016, Université Clermont Auvergne, France, gilles.mailhot@uca.fr

^{2*}Institut de Chimie de Clermont-Ferrand, UMR CNRS 6296, Université Clermont Auvergne, France

³Università degli Studi di Torino, Dipartimento di Chimica, Via P. Giuria 5, Torino 10125, Italy

Since more than 20 years clouds have been sampled at the puy de Dôme observatory (France) using a collector specifically designed for high volume sampling ^[1]. The physico-chemical analysis and the backtrajectory calculation enabled the classification of cloud water samples into four classes: highly marine, marine, continental and polluted ^[2]. Target analysis were developed to quantify the concentration of short chain carboxylic acids, amino acids and, more recently, sugars ^[3, 4]. Pesticide contamination is a growing and alarming concern for both environment and human health. Widely used in agriculture to control pests and disease carriers, pesticides undergo extensive long-range atmospheric transport in the gas phase, aerosols and, as shown here, in clouds ^[5]. We measured the concentration of 32 pesticides at the puy de Dôme observatory (France) in the sub- $\mu\text{g L}^{-1}$ to $\mu\text{g L}^{-1}$ range in cloud water, largely arising from regional to long-range transport that also involves pesticides currently banned for agricultural use in France. Half of the samples showed a total concentration of pesticides over $0.5 \mu\text{g L}^{-1}$, which is the European drinking water limit. If 2,4-dinitrophenol, which can also be produced by photochemical reactions, is excluded, two samples still present a total concentration over $0.5 \mu\text{g L}^{-1}$. The frequent detection of pesticides in rainwater may thus depend on their presence in clouds, as well as atmospheric washout. Estimates of pesticides quantity in clouds over France, ranging from 6.4 ± 3.2 to 139 ± 75 tons, suggest that their amounts in the cloud aqueous phase are potentially high and that these compounds would affect areas that are not directly impacted by agricultural activities.

- [1] Väitilingom M., Bernard C., Ribeiro M., Berthod C., Bianco A., Deguillaume L., Design and evaluation of BOOGIE: a collector for the analysis of cloud composition and processes, *Atmos. Meas. Tech.*, 18, 1073–1090, 2025.
- [2] Deguillaume, L., Charbouillot, T., Joly, M., et al. , *Atmos. Chem. Phys.*, 14, 1485–1506, 2014.
- [3] Bianco, A., Vyard, G., Deguillaume, L. et al. Improving the characterization of dissolved organic carbon in cloud water: Amino acids and their impact on the oxidant capacity. *Scientific Reports* 6, 37420, 2016.
- [4] Bianco A., Pailler L., Joly M., Delort A.-M., Darfeuil S., Jaffrezo J.-L., Deguillaume L., Sugars in clouds: Measurements and modelling investigation of their aqueous photodegradation, *Atmos. Environ.*, Volume 350, 2025.
- [5] Bianco A., Nibert P., Wu Y., Baray J.-L., Brigante M., Mailhot G., Deguillaume L., Vione D., Cabanes D. J. E., Méjean M., and Besse-Hoggan P., Are Clouds a Neglected Reservoir of Pesticides? *Environ. Science & Technology* 2025 59 (40), 21579-21588

The reactions of ozone with alkenes and subsequent chemistry

Max McGillen¹

¹Institut de Combustion Aérodynamique Réactivité et Environnement (ICARE),
CNRS-Orléans, France max.mcgillen@cnrs-orleans.fr

A large quantity and variety of natural and anthropogenic alkenes are emitted into the atmosphere, for which reactions with ozone represent a major sink. These reactions have many interesting attributes that warrant further attention. This begins with the 1,3-cycloaddition mechanism, which makes ozonolysis reactions unusually sensitive to the inductive and steric factors imposed by substitutions about the olefinic bond. Following this, the reaction enters a complex potential energy landscape, where a variety of chemical fates await the nascent Criegee intermediates. For higher energy Criegee intermediates, prompt unimolecular reaction (i.e. isomerization and fragmentation) channels are dominant. Conversely, for the lower energy Criegee intermediates, bimolecular reactions (i.e. insertion and cycloaddition) channels become important. Following this, a diverse array of reaction products emerges, many of which are peroxidic, and almost none of which have been studied in detail.

In this invited talk, I will describe some of the recent progress that has been made in the study of this important class of reaction, and show some recent results from our experimental facilities at CNRS-Orléans.

Molecular Characteristics, Origins and Atmospheric Reaction Behavior of Atmospheric Amines in Four Chinese Cities

Jian Wang¹, Bin Han¹, Jing Wang¹, Xinhua Wang¹, Jia Xu¹, Liyao Guo¹, Wen Yang¹, Shala Tuohetaerhan², Christian George³, Kangwei Li¹, Jianmin Chen⁴, Tongyi Ning¹, Guiqian Tang⁵, Merched Azzi⁶, and Zhipeng Bai^{1*}

¹State Key Laboratory of Environmental Criteria and Risk Assessment, Chinese Research Academy of Environmental Sciences, Beijing, China, baizp@craes.org.cn

²Xinjiang Academy of Ecological and Environmental Sciences, Urumchi, China

³University Lyon, Université Claude Bernard Lyon 1, CNRS, IRCELYON, Lyon, France

⁴Department of Environmental science & Engineering, Fudan University, Shanghai, China ⁵State Key Laboratory of Atmospheric Environment and Extreme Meteorology, Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing, China

⁶Department of Climate Change, Energy, the Environment and Water (DCCEEW) of New South Wales, Australia

Amines in the atmosphere, as an important component of reduced nitrogen compounds, have attracted increasing attention in recent years due to their potential use in different industrial applications such as the CO₂ capture technologies, and for its potential impacts on air quality. Presently little information on the molecular composition of amines in urban atmospheres is available. In this study, we have collected 40 PM_{2.5} samples from four typical cities (Xining, Baotou, Jinan, and Shenyang) in China during the winter of 2015 to study their chemical compositions. Ultra-high-resolution mass spectrometry (UHRMS) was used for non-targeted analysis, and a dual-mode ionization approach (positive and negative) was applied to reduce uncertainty and systematically characterise the composition of amines among reduced nitrogen compounds in aerosols. The data analysis show that: (1) Amines in PM_{2.5} exhibit significant molecular diversity. In addition to the fatty amine homologous C₃H₉(CH₂)_nN₁ series, complex amine-containing molecules with amide, amino, and nitro functional groups were also detected. (2) The carbon chain length distribution of fatty amine homologues (C₃–C₈) suggests that these compounds mainly originate from sources such as biomass burning. (3) The detection of aniline-, anthracene-, and other aromatic amines indicates that aromatic amines produced by fossil fuel combustion can enter the aerosol phase through pathways associated with the reduced nitrogen cycle. (4) By estimating the reaction rate constants of primary, secondary, and tertiary amines in the four cities, the temperature and humidity dependence of reactions between amines and atmospheric oxidants (O₃) was revealed.

This study characterises the complex composition of amines in aerosols from different cities and provides important scientific insights for a deeper understanding of the sources and reaction behaviours of amines in urban atmospheres. In addition, the results can be used to assess the accuracy of existing chemical reaction mechanisms used for simulating the state of the ambient air compositions under different ambient conditions.

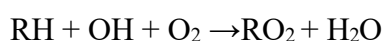
Selfreaction of peroxy radicals re-investigated by laser photolysis / cw Cavity Ring Down Spectroscopy

Christa Fittschen¹, Cuihong Zhang^{1,2}, Xiaofeng Tang², Coralie Schoemaeker¹ and Laure Pillier¹

¹PC2A, University Lille, France

^{2*}Anhui Institute of Optics and Fine Mechanics, Chinese Academy of Science, China
christa.fittschen@univ-lille.fr

Peroxy radicals, RO₂, are key species in the atmosphere. They are formed from a reaction of OH radicals with hydrocarbons:



In polluted environments, RO₂ radicals react predominantly with NO, leading to formation of NO₂, and eventually through photolysis of NO₂ to formation of O₃.

At low NO_x concentrations such as in the marine boundary layer or the background troposphere, the life-time of RO₂ radicals increases and other reaction pathways such as self- and cross reaction with other RO₂ or with HO₂ radicals become competitive. To study these reactions, UV absorption spectroscopy has been employed in the past: this technique gives good sensitivity for peroxy radicals, but poor selectivity as these radicals have broad absorption features in the UV.

We have established a technique allowing to follow peroxy radicals with a better selectivity compared to UV, but with still good sensitivity by coupling laser photolysis to cw-Cavity Ring Down Spectroscopy in the near IR.

Here, we will present some recent results on measurements of rate constants and branching ratios of the self-reaction of selected peroxy radicals [1-5]. Radicals are generated by laser photolysis, and the detection of the peroxy radicals is done by cw-Cavity Ring Down Spectroscopy in the near IR, a rather selective method compared to UV absorption spectroscopy.

Literature:

- [1] Dimeric product of peroxy radical self-reaction probed with VUV photoionization mass spectrometry and theoretical calculations: The case of C₂H₅OOC₂H₅, Yue H., C. Zhang, X. Lin, Z. Wen, W. Zhang, S. Mostafa, P. Luo, Z. Zhang, P. Hemberger, C. Fittschen, X. Tang, *International Journal of Molecular Sciences*, 2023; 24, 3731
- [2] Self-reaction of Acetonyl Peroxy Radicals and their Reaction with Cl-Atoms, Assali, M, C. Fittschen C, *The Journal of Physical Chemistry A*, 2022; 2126 (28), 4585–4597.
- [3] Rate Constants and Branching Ratios for the Self-Reaction of Acetyl Peroxy (CH₃C(O)O₂) and its Reaction with CH₃O₂, Assali, M, C. Fittschen C, *Atmosphere*, 2022, 13(2), 186
- [4] Rate Constant and Branching Ratio for the Reaction of Ethyl Peroxy Radicals with Itself and with Ethoxy Radicals, Shamas M, Assali M, Zhang C, Tang X, Zhang W, Pillier L, Schoemaeker C, Fittschen C, *Earth and Space Chemistry*, 2022; 6 (1), 181 – 188,
- [5] Absolute Absorption Cross Section of the $\tilde{A} \leftarrow \tilde{X}$ Electronic Transition of the Ethyl Peroxy Radical and Rate Constant of its Cross Reaction with HO₂, Zhang C, Shamas M, Assali M, Tang X, Zhang W, Pillier L, Schoemaeker C, Fittschen C, *Photonics*, 2021, 8, 296

Development of Green Methanol in Shipping and Methanol-SCR Denitration Technology

Liehao Wei¹ and Shitao Peng^{1*}

¹ Environmental Technology Research Center, Tianjin Research Institute for Water Transport Engineering, M.O.T., China.

weiliehao@twite.ac.cn; pengshitao@twite.ac.cn

Since the International Maritime Organization (IMO) adopted its landmark “Net-Zero” framework, the global shipping industry has intensified efforts toward green and low-carbon transformation. Among emerging decarbonization pathways, alternative fuels stand out for their scalability and demonstrable lifecycle emission reduction potential. Green methanol—produced from renewable hydrogen and biogenic or captured CO₂—has emerged as a leading marine fuel candidate, owing to its favorable attributes: near-zero well-to-wake carbon intensity, compatibility with existing dual-fuel engine architectures, ease of storage and bunkering infrastructure adaptation, and intrinsic oxygen content that supports cleaner combustion.

Concurrently, stringent NO_x Tier III emission limits—applicable in Emission Control Areas (ECAs) for newbuilds since 2021—pose a critical challenge for methanol-fueled ships. Conventional ammonia-based selective catalytic reduction (NH₃-SCR) systems face operational limitations in this context: (i) irreversible catalyst deactivation due to ammonium bisulfate (ABS) deposition under low-exhaust-temperature conditions typical of slow-speed marine engines; (ii) substantial spatial footprint and system complexity; and (iii) risk of toxic hydrogen cyanide (HCN) formation during reaction between HCHO and NH₃. In contrast, methanol-selective catalytic reduction (Methanol-SCR) leverages unreacted methanol inherently present in the exhaust stream of partially combusted methanol engines, eliminating the need for auxiliary reductant storage, dosing, and thermal management subsystems. This approach not only circumvents sulfate-related catalyst fouling entirely but also enables compact, integrated aftertreatment designs with lower capital and operational expenditures.

Therefore, this paper reviews the development trend of green methanol in the context of shipping emissions reduction, analyzes the research progress and application prospects of methanol-SCR denitration technology, and provides new insights for the shipping industry to reduce pollution and carbon emissions and achieve green and sustainable development.

Tackling Seasonal Smog: Breaking Crop Residue Burning's Grip

Weiwei Chen¹, Bowen Shi¹, Jing Fu¹, Lin Liang¹

¹State Key Laboratory of Black Soils Conservation and Utilization, Northeast Institute of Geography and Agroecology, Chinese Academy of Sciences, Changchun 130102, China, chenweiwei@iga.ac.cn

From India's subsidized straw balers to Vietnam's awareness campaigns, major developing economies are deploying a growing arsenal of localized measures to combat the seasonal smog from agricultural residue burning. These efforts, however, remain fragmented, targeting the immediate symptoms of pollution but failing to address its socioeconomic roots. A comprehensive national strategy that systematically balances clean air, public health, and farmer livelihoods remains conspicuously absent from most policy agendas. Nowhere is this governance gap more evident than in China's Northeast, where the annual "smog season" persists with striking intensity, demanding an urgent and fundamental rethink of integrated mitigation approaches.

The Northeast China Plain is ranked among the most severely affected regions in the world for extreme seasonal air pollution events driven by agricultural activity. In late November 2025, the city of Jilin experienced a historic smog crisis, with hourly PM_{2.5} concentrations exceeding 2,000 µg/m³, exceeding the World Health Organization's 24-hour guideline value by over 145-fold and marking some of the highest values ever recorded in China. This episode enveloped the metropolitan area in persistent darkness, 28 districts and counties endured cumulative exposures exceeding 500µg/m³ for more than 300 hours, and posing severe risks to public health. Such acute pollution episodes have become a recurrent phenomenon across Heilongjiang, Liaoning, and parts of Inner Mongolia during the autumn harvest. The primary cause is not only the large-scale, spatially and temporally unregulated burning of crop residues within individual provinces, but more critically, the transport of pollutants both within and across provincial boundaries and their superposition, which synergistically sustain elevated regional pollution levels for prolonged periods.

While China has adopted a targeted and nuanced approach in its straw burning policy, transitioning from a rigid nationwide ban to a system of designated no-burn and limited-burn zones to utilize favorable meteorological windows for planned burning, the execution has fallen short of its goals due to vague coordination mechanisms and insufficient technological support. The ongoing inadequacy in real-time monitoring, precise weather forecasting, and cross-jurisdictional coordination during the 2025 burning window led to widespread uncontrolled fires. As a result, excluding robust operational management from the policy's execution will inevitably trigger more severe pollution crises. This disconnects between policy adoption and managerial rigor poses an immediate and escalating threat to public health and regional environmental security.

Given the existing targeted and nuanced policy framework and the national strategic focus on coordinating agriculture and environmental protection, we urge the National Development and Reform Commission, the Ministry of Ecology and Environment, and Northeast China's provincial authorities to jointly develop a technology-empowered, cross-regional platform for planned crop residue burning control. Based on the vigorous promotion of comprehensive residue utilization, the platform will cover the entire management chain from pre-burning planning and in-process monitoring to post-burn assessment. Omitting rigorous, technology-driven execution and inter-provincial coordination from this governance model will greatly undermine these goals and perpetuate a preventable public health crisis. For all developing economies grappling with the crop residue dilemma, China's experience demonstrates that the critical path forward lies not merely in policy design, but in building the indispensable managerial and technological capacity to close the implementation gap.

Electronically Engineered Hierarchical Heterojunction Catalysts for Low-Concentration NO Photocatalytic Purification

Jun He* and Zhiyu Xiao

Department of Chemical and Environmental Engineering, Climate and Environmental Solutions Research Center, University of Nottingham Ningbo China, Ningbo, China

*jun.he@nottingham.edu.cn

The photocatalytic oxidation of low-concentration nitrogen monoxide (NO) at ppb level presents a significant challenge for air remediation, demanding materials that combine high efficiency, visible-light response, and excellent selectivity. This research project establishes and validates a coherent, hierarchical "electronic engineering" strategy to systematically overcome the intrinsic limitations of graphitic carbon nitride (g-C₃N₄), namely rapid charge recombination, inefficient interfacial charge transfer, and a scarcity of highly active sites. The work progresses through three designed stages of complexity and innovation. Initially, a ternary Z-scheme heterojunction, Co(OH)₂/CeO₂-g-C₃N₄ (CoCe-CN), was constructed via a facile one-step hydrothermal method. Here, Co(OH)₂ was strategically incorporated as an electron-mediating bridge between CeO₂ and g-C₃N₄, accelerating interfacial electron transfer and introducing supplementary ·OH radical generation pathways. The optimal 50CoCe-CN catalyst achieved a notable 53.5% conversion efficiency for 600 ppb NO under visible light, 1.82 times that of pristine g-C₃N₄, with DFT calculations and elemental mapping providing direct evidence for the novel multi-layer synergistic structure.

Building on this, the strategy evolved to engineer a stronger interfacial connection. A pyrene-based covalent organic framework (TAPPy-DMTP-COF) was grown in-situ on g-C₃N₄ nanosheets via a Schiff base reaction, forming a chemically bonded Type-II heterojunction (TAPPy-DMTP-CN). This innovation created a seamless interface with robust electron communication through -C=N- covalent linkages, significantly enhancing charge separation and yielding a NO conversion efficiency of 45.8%. The culmination of this hierarchical design is the Pt/TP-BPY-CN/g-C₃N₄ composite, which integrates atomic-level precision with the macro-scale heterojunction. Single-atom platinum (Pt) was coordinated onto the bipyridine units of the in-situ grown COF matrix. This Pt/40TPBPY-CN composite delivered a breakthrough performance, attaining 65.3% conversion of 800 ppb NO with near-100% selectivity towards nitrate (NO₃⁻).

A comprehensive mechanistic investigation, employing *in-situ* XPS and XAFS, revealed the origin of this exceptional activity. The chemically bonded heterointerface ensured efficient vectorial electron transfer, while the atomically dispersed Pt sites established a dynamic Pt²⁺/Pt⁴⁺ redox cycle. This cycle uniquely orchestrates dual reaction pathways: driving the deep oxidation of NO to nitrate while concurrently facilitating a reduction pathway to ammonium (NH₄⁺), as confirmed by extraction experiments. This work demonstrates a scalable materials design blueprint where photocatalytic efficacy is radically elevated through rational electronic structure manipulation across multiple scales—from bulk heterojunction engineering to atomic-level active site creation. The synergistic fusion of a covalent organic/inorganic interface with a bifunctional single-atom catalyst represents a novel and powerful paradigm, offering significant potential for advanced air purification and broader photocatalytic applications requiring complex, multi-step redox transformations. Future perspectives include the crucial assessment of long-term stability under realistic humid conditions and the exploration of earth-abundant single-atom analogues to enhance practical viability and sustainability.

Arctic Air Pollution: New Insights and Future Perspectives

Kathy S. Law^{1*}, Weihang Zhang¹, Natalie Brett^{1,a}, Barbara D'Anna², Brice Temime-Roussel², James Campbell³, Jingqui Mao³, William Simpson³, Joel Savarino⁴, Slimane Bekki¹, Jean-Christophe Raut¹, Brice Barret⁵, Steve Arnold⁶,

ALPACA-2022 Team

¹LATMOS-CNRS, Sorbonne Université, Paris, France, *kathy.law@latmos.ipsl.fr

^anow at: IRSTV, CNRS, Nantes, France

²LCE, CNRS, Aix-Marseille Université, Marseille, France

³Department of Chemistry and Biochemistry & Geophysical Institute, University of Alaska, Fairbanks, United States

⁴IGE, Univ. Grenoble Alpes, CNRS, INRAE, IRD, Grenoble, France

⁵Laboratoire d'Aérodynamique (LAERO), Université de Toulouse, CNRS, Toulouse, France

⁶School of Earth & Environment, University of Leeds, UK

Air pollution in the Arctic originates from mid-latitude emission regions via long-range transport and from local emissions. Black carbon, tropospheric ozone and methane act as short-lived climate forcers (SLCFs) contributing to Arctic warming. Local air pollution also contributes to poor air quality due to boreal fires in summer and anthropogenic pollution in winter. During Arctic winter in urban areas, extremely cold and stable meteorological conditions, coupled with elevated local emissions, leads to severe air pollution episodes.

Highlights are presented from the Alaskan Layered Pollution and Chemical Analysis (ALPACA) field campaign in Fairbanks, Interior Alaska that took place during winter 2022. High concentrations trace gases (CO, NO_x, VOCs, ..) and aerosols (organics, sulphate, ...) were observed, in particular during two pollution episodes, with very cold (down to -35 °C) and relatively warmer (~0 °C) conditions, respectively, contributing to air quality exceedences. Studies include investigation of pollutant sources using Lagrangian particle dispersion model simulations run with specific ALPACA-2022 surface and elevated emissions. Power plant plume simulations are improved compared to profile observations by taking into account capping by surface-based and elevated temperature inversions. Results are used to estimate the contribution of power plant emissions to breathing level air quality.

Low biases in modelled surface trace gas concentrations during pollution episodes are also examined, in particular, related to deficiencies in emissions from vehicles and space heating under harsh winter conditions. For example, low modelled surface NO_x is attributed to inefficient diesel vehicles at cold temperatures, even if diesel vehicles are only 10% of the fleet. Aromatics, one of the most abundant VOCs observed during ALPACA-2022, are also simulated. Improvements to heating emissions and gasoline vehicle emission dependencies on meteorological factors reduces model biases.

Uncertainties in modelling SLCFs are also discussed. Results are presented from studies linked to the Arctic Monitoring and Assessment Programme (AMAP), under the Arctic Council. For example, the influence of wet and dry removal on black carbon in the Arctic is investigated using the WRF-Chem model showing variations between different observation sites. The importance of local emissions over northern Alaska is also highlighted. Lastly, future perspectives emerging from the IGAC/IASC air Pollution in the Arctic: Climate, Environment and Societies (PACES) initiative are presented.

AI-based Probabilistic Air Quality Forecasting

Ao Ding¹, Aoxing Zhang^{1*}, and Tzung-May Fu^{1,2*}

¹School of Environmental Science and Engineering, Southern University of Science and Technology, China

^{2*}National Center for Applied Mathematics Shenzhen, China, fuzm@sustech.edu.cn

Current operational air quality forecasts are computationally expensive, susceptible to errors in physics and emissions, and fail to quantify weather-related uncertainty. To address these limitations, we developed an AI-based framework that synergistically integrates knowledge from chemical transport model simulations with real-world observational constraints, enabling efficient and accurate probabilistic air quality prediction. The system outperforms existing operational benchmarks, achieving lower forecast errors while also providing probabilistic diagnostics that explicitly quantify the impact of weather forecast uncertainty on air quality predictability. Moreover, our AI-based forecast system can rapidly adapt to changing emissions through fine-tuning on limited recent data. Together, these attributes establish the system as a powerful, extensible tool for next-generation probabilistic air quality forecasting, with clear potential for application to other pollutants and regions.

Characterization of secondary organic aerosol from the ozonolysis of α -pinene using laser trapping and Raman spectroscopy

Naoto Tyumyo¹, Gwendoline Bourdon^{2,3}, Eric Villenave², Sophie Sobanska³, Shoji Ishizaka¹

¹Graduate School of Advanced Science and Engineering, Hiroshima University, 1-3-1 Kagamiyama, Higashi-Hiroshima 739-8526, Japan

²Univ. Bordeaux, CNRS, EPOC, UMR 5805, F-33600 Pessac, France

³Univ. Bordeaux, CNRS, ISM, UMR 5255, F-33400 Talence, France

sophie.sobanska@u-bordeaux.fr

During their atmospheric transport, volatile organic compounds (VOCs) may undergo oxidation reactions by ozone, hydroxyl and nitrate radicals, leading to the formation of secondary organic aerosols (SOAs), which have significant impacts on human health and climate change. Among VOCs, α -pinene, emitted primarily by coniferous trees, is recognized as one of the major biogenic precursors of SOAs worldwide, because of its high emission and reactivity. To form SOA from volatile α -pinene via ozone oxidation reactions, the generation of low-vapor pressure compounds capable of acting as condensation nuclei is essential. Both laboratory and field studies have identified low volatile dimers as key components in SOA formation. Although mechanisms involving stabilized Criegee intermediates and peroxy radicals have been proposed for dimer formation in the gas phase, the detailed processes remain widely debated due to the high diversity of reaction products and the inherent complexity of their formation mechanisms. To clarify certain steps of the SOA formation mechanism from ozone-initiated oxidation of α -pinene, a laser trapping technique coupled with Raman spectroscopy was employed for in situ analysis of individual SOA particles. In this study, single micrometer-sized α -pinene SOA particles were successfully trapped in the gas phase. To our knowledge, this represents the first successful application of laser trapping of α -pinene SOA particles directly in the gas phase. Raman analysis of the levitating particle revealed a complex mixture of species likely to evolve over time, reflecting the aging of the particle. An intense Raman peak observed at about 852 cm⁻¹ was attributed to the O–O stretching vibration of peroxides. This finding provides direct evidence for the presence of peroxy functional groups in the dimers, likely formed via stabilized Criegee intermediates. These results demonstrate the capability of laser trapping combined with Raman spectroscopy for studying SOA formation and aging.

Acknowledgments

This research was supported by the JSPS KAKENHI Grant Numbers JP21H01964. The authors would like to thank the Agence Nationale de la Recherche (ANR) for supporting the SOAPHY project (ANR- 21-CE29-0031), the Région Nouvelle Aquitaine for funding the LEVIAERO project (convention n°AAPR2022-2021-17126210) and the INSU LEFE Program of the CNRS for supporting the LEVITEAU project. Gwendoline Bourdon thanks the University of Bordeaux for the international exchange grant.

Exposure Studies of Living/biological Organisms: how can smog chambers revolutionize such exposure studies? Illustration: how the PolluRisk Platform is simulating at the laboratory urban Air Quality and its health impacts

Patrice Coll¹, Ambre Delater¹, Mathieu Cazaunau², Spyros N. Pandis³, Christina Vasilakopoulou¹, Sophie Lanone⁴ and The PolluRisk Team^{1,4}

¹ Université Paris Cité and Univ Paris Est Creteil, CNRS, LISA, F-75013 Paris, France

² Univ Paris Est Creteil and Université Paris Cité, CNRS, LISA, F-94010 Créteil, France

³ Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas (FORTH/ICE-HT), 26504, Patras, Greece

⁴ Univ Paris Est Creteil, INSERM, IMRB, F-94010 Créteil, France pcoll@lisa.ipsl.fr

It has been widely accepted that there are clear relations between exposure to atmospheric pollution and Health impacts (epidemiology and toxicology studies). This explicit demonstration has been supported – as an illustration - regarding mortality and morbidity effects of long-term exposure to low-level PM_{2.5}, BC, NO₂ and O₃ (analysis of European cohorts in the Elapse project).

We have developed the PolluRisk platform, that reproduces for days the atmospheric phases (gases/aerosols) similar those of cities that are highly, mid- or low-polluted. It is mainly resulting from the coupling of an atmospheric simulation chamber (cesam.cnrs.fr) and of exposure devices able to host preclinical models (isolators from Noroit® company). The principle of such an atmospheric simulation is described on the platform website: pollurisk.eu

The experimental protocol consists in the continuous injection of primary pollutants (NO_x, COVs mix, SO₂, soot, inorganic salts and potentially mineral dust particles if needed) at low concentrations (ppb levels) in air in the chamber. With a 4 hours residence time in the chamber, the mixture is exposed to an artificial solar irradiation, allowing secondary pollutants such as O₃, NO₂, HCHO, etc. as well as complex polyfunctional organics including Secondary Organic Aerosol (SOA) to be formed, reaching a chemical steady state. Isolators are then “fed” with a constant flow of such a mixture. The “reference” isolator is filled up with filtered air only.

We will illustrate the results regarding 2 experiments (one simulating a summer mid-polluted city atmosphere and one simulating a winter mid-polluted city atmosphere, both for a duration of 7 days). We will present 1/ the SOA characterization including Organics, Nitrate or Sulfate content 2/ the functionalized particulate compounds observed 3/ some biological characterizations of the exposed mice lungs. These results clearly state the interest of Atmospheric Simulation chambers to support such exposure studies devoted to Health Impacts of Air Quality.

We will conclude sharing the perspectives relative to such innovative approach : a/ scientific AQ questions to tackle b/ investigating the accuracy of AQ survey methodologies including potential oxidants c/ direct links to Environmental Health and Public Health policies.

Long-Term PM_{2.5} and PM₁₀ Nitrate Trends from Filter Networks: Correction of Temperature-dependent Measurement Bias Using Multi-Year Filter–MARGA Intercomparison Data

Zijing Zhang¹ and Jian Zhen Yu^{1,2*}

¹Division of Environment and Sustainability, Hong Kong University of Science & Technology, Hong Kong, China

^{2*}Department of Chemistry, Hong Kong University of Science & Technology, Hong Kong, China, jian.yu@ust.hk

Nitrate is a major component of atmospheric particulate matter (PM), and its accurate quantification is critical for assessing air quality, evaluating emission control policies, and constraining atmospheric models. While offline filter-based methods are widely used due to their cost-effectiveness and operational simplicity, their reliability for nitrate is compromised by volatilization and sampling artifacts. Here, we evaluate offline filter measurements against online Monitor for Aerosols and Gases in ambient Air (MARGA) systems for PM_{2.5} and PM₁₀ nitrate at an urban and a suburban site in Hong Kong over multi-year periods. Daily filter measurements were directly compared with corresponding 24 h averages derived from hourly MARGA data. PM_{2.5} sulfate and ammonium showed excellent agreement between methods (slopes ≈ 1 , $R^2 \geq 0.87$), whereas nitrate exhibited larger scatter and a substantial intercept, indicating higher uncertainty for filter-based nitrate. Temperature emerged as the dominant driver of this bias. Using 23 °C as a threshold, we find that at > 23 °C, offline filters severely underestimate PM_{2.5} nitrate and often fail to capture its variability, yielding relationships with MARGA that are too weak and distorted for meaningful calibration. At < 23 °C, underestimation persists, but strong, approximately linear correlations allow robust empirical calibration. In comparison, PM₁₀ nitrate measured by filters agrees well with MARGA across both temperature regimes ($R^2 \approx 0.85$), reflecting its lower volatility and predominant occurrence as stable coarse-mode salts (e.g., NaNO₃, Ca(NO₃)₂, Mg(NO₃)₂). However, the regression slopes and intercepts for PM₁₀ nitrate differ systematically between high- and low-temperature conditions, implying a need for temperature-specific calibrations.

Overall, our results demonstrate that offline filter-based nitrate data must be used with caution, particularly for PM_{2.5} under warm conditions. We recommend (i) treating PM_{2.5} nitrate filter data at higher ambient temperatures (e.g., > 23 °C) as unreliable and generally non-calibratable, and (ii) applying temperature-stratified calibrations against online instruments such as MARGA for both PM_{2.5} at lower ambient temperature (e.g., < 23 °C) and PM₁₀ nitrate to enhance the reliability of long-term nitrate datasets and derived coarse-mode estimates.

Acknowledgements: We thank the Research Grants Council of Hong Kong (R6011-18 and SRFS2526- 6S05) for funding and the Hong Kong Environmental Protection Department for provision of the real- time PM_{2.5} and MARGA datasets.

Computational investigation of multiphase chemical mechanisms in atmospheric aerosols and water droplets

Rawan Abouhaidar^b, Denis Duflot^a, Céline Toubin^a

^aUniv. Lille, CNRS, UMR 8523 – PhLAM – Physique des Lasers Atomes et Molécules, F-59000 Lille, France. celine.toubin@univ-lille.fr

^bUniversité Paris-Saclay, Univ Evry, CY Cergy Paris Universit., CNRS, LAMBE UMR 8587, 91025 Evry- Courcouronnes, France.

Gas–liquid and air–liquid interfaces play a central role in atmospheric chemistry by controlling reaction kinetics, phase partitioning, and chemical transformations. Gaining molecular-level insight into these interfacial processes is essential for predicting atmospheric behavior and its implications for climate and the environment. Molecular dynamics (MD) and quantum mechanical (QM) approaches provide complementary perspectives on the multiphase chemistry and mechanisms of freezing.

This talk highlights applications of these molecular-level methods. MD simulations elucidate interfacial organization and partitioning between surface and bulk phases, which strongly influence uptake processes, surface properties, and ice nucleation. In particular, graph theory analysis has revealed how short-chain alcohols modify the hydrogen-bonding network of interfacial water, offering new perspectives on the early stages of freezing relevant to climate science. In parallel, QM and hybrid QM/QM' methods captured heterogeneous reactivity, including explicit solvent effects, and predict heterogeneous rate constants that may differ by several orders of magnitude from gas-phase reactions.

References

- [1] Abouhaidar, R. ; D. Duflot, C. Toubin, Theoretical characterization of the kinetics of the multiphase ozonolysis of an aqueous maleic acid droplet, *Aerosol Science and Technology*, 58(4), 337–355. <https://doi.org/10.1080/02786826.2023.2286341>
- [2] AbouHaidar, R., Bougueroua, S., Duflot, D., Gaigeot, M.P., Wyslouzil, B., Toubin C., Unraveling Aqueous Alcohol Freezing: new theoretical tools from graph theory to extract molecular processes in MD simulations, *Faraday Discussions* 2025. <https://doi.org/10.1039/D4FD00165F>

¹ E-mail: celine.toubin@univ-lille.fr

Chemistry on Urban Surfaces as a Driver of Air Pollution in the Cities

Sasho Gligorovski

Environmental Science and Engineering

Guangdong Technion - Israel Institute of Technology, Shantou, China sasho.g@gtiit.edu.cn

In the cities, urban surfaces, such as paved roads and parking lots, rooftops, buildings areas, cover 60% of the total urban area, and increase up to 80-100% in the central business district.

For example, considering the city of Paris, asphalt pavements provide 130 times higher surface area than aerosols emitted in a polluted day (considering $40 \mu\text{g m}^{-3}$, specific surface area of $30 \text{ m}^2 \text{ g}^{-1}$ of the aerosols and homogeneous concentration of particles in a boundary layer of 100 meters, i.e. an extreme upper limit). Considering the building glass surface in Guangzhou, we estimated a total building surface area of 0.52 billion m^2 . (Deng et al., 2022) As a comparison, the boundary-layer aerosol surface area is roughly 0.22 billion m^2 for the same study region, if we assume a $25 \mu\text{g m}^{-3}$ aerosol concentration (roughly annual mean concentration for Guangzhou), $1 \mu\text{m}$ aerosol diameter, and 800 m boundary layer height. (Deng et al., 2022)

Although urban surfaces particularly asphalt pavements covering 40% of urban areas provide surface area exceeding atmospheric aerosols by two orders of magnitude (130 times in Paris), yet their role in air quality remains practically unknown.

Myriads of pollutants which are emitted into the air by automobiles, factories and a host of other sources present in the cities where we live, can settle on the building surfaces in form of a grime. Hence, urban grime adsorbed on glass surfaces is a mixture of organic compounds and inorganic ions coated on the building surfaces. Sunlight acting on urban grime very rapidly releases gas phase nitrogen oxides (NO) and nitrous acid (HONO) back into the atmosphere, by the light-induced heterogeneous reactions of nitrogen dioxide (NO_2) with organic compounds such as polycyclic aromatic hydrocarbons (PAHs) trapped in the grime. HONO is very important player in urban atmospheric chemistry as represents the main primary source of hydroxyl radicals (OH) in urban air. Preliminary data demonstrate explosive nitrous acid (HONO) formation from light-induced NO_2 reactions on fresh asphalt at atmospherically relevant concentrations (10 ppb) a mechanism involving photosensitized chemistry of polycyclic aromatic hydrocarbons with ammonia promotion, previously discovered on urban grime (Liu et al., 2023).

Some of the released N-containing organic compounds by this chemistry make a part of the still poorly characterized light-absorbing organic compounds known as “brown carbon” indicating the importance of heterogeneous NO_2 conversion processing on urban surfaces.

Organic sulfur (OS) compounds have been globally identified in ambient secondary organic aerosols (SOA), but their contribution to organic mass remains inadequately quantified, and the current models considerably underestimate ambient SOA formation. OS compounds are surface active and may also play a role in cloud formation. To illuminate this intricate system, we investigated the reactive uptake of SO_2 on urban grime in the dark and under simulated sunlight irradiation at different RHs and applied a kinetic multilayer model of aerosol surface and bulk chemistry. The heterogeneous reaction of SO_2 with authentic urban grime under near-ultraviolet sunlight irradiation leads to a large suite of various organic compounds including OS released in the gas phase. Model estimations indicate that at the core area of Guangzhou, building surface uptake of SO_2 is 15 times larger than uptake of SO_2 on aerosol surfaces, yielding $\sim 20 \text{ ng m}^{-3}$ of OS that represents an important fraction of the observed OS compounds (60 to 200 ng m^{-3}) in ambient aerosols of Chinese megacities. Hence, the chemistry on urban surfaces initiates the formation of HONO, nitrogen and sulfur containing organic compounds, “brown carbon” and secondary organic aerosols (SOA) in the cities where majority of people live.

1. Liu, et al., J. Am. Chem. Soc., 2023, 145, 21, 11488–11493.
2. Deng, et al., Sci. Adv., 2022, 8, eabq6830.

Rethinking Stratospheric Aerosols: Sources, Composition, and Unexpected Impacts

Slimane Bekki¹, Sergey Khaykin¹, Gwenael Berthet², Maylis Gaulin¹, Eric d'Almeida¹

¹LATMOS-IPSL, CNRS, UVSQ, Sorbonne Uni., France ²LPC2E, CNRS, Orleans Univ.

slimane.bekki@latmos.ipsl.fr

The stratosphere, extending roughly from 12 to 50 km above Earth's surface, contains aerosols-microscopic particles suspended in the air that vary widely in size, shape, and chemical composition. These particles influence the atmospheric radiative balance by scattering and absorbing incoming solar radiation, thereby affecting climate. They also play a role in stratospheric chemistry, particularly in the balance of ozone, by providing surfaces for heterogeneous chemical reactions and by acting as condensation nuclei for polar stratospheric clouds.

For decades, stratospheric aerosols were assumed to consist primarily of sulfuric acid, largely because variability in the global stratospheric aerosol layer appeared to be driven by sulfur injections from major volcanic eruptions. However, recent observations have challenged this view and highlighted a broader range of aerosol sources and processes. Two events have been especially transformative: the extreme Australian wildfires of 2019–2020 (the “Australian New Year’s” event) and the January 2022 eruption of the Hunga Tonga–Hunga Ha’apai volcano. Both events injected substantial material into the stratosphere and produced impacts that were unexpected and, in some cases, unprecedented in the historical observational record.

In parallel, recent in-situ measurements have revealed that the composition of stratospheric aerosols is much more diverse than previously recognized. They commonly contain meteoritic material and may also include carbonaceous elements. Interestingly, ~10% of stratospheric aerosols contain a small contribution from human space activities, such as rocket launches and the re-entry of space debris.

This talk will review recent observational advances that have improved our understanding of the chemical and physical processes governing stratospheric aerosols, their properties, distributions, and atmospheric impacts. It will also discuss emerging questions regarding the potential implications of rapidly increasing spaceflight activities for the ozone layer and Earth's climate.

Revealing the important role of OVOCs on photochemistry in Coastal Hong Kong

Zhe WANG*, Lirong HUI, Xin Feng, Yang XU, Yi CHEN, Yao CHEN

¹ Division of Environment and Sustainability, The Hong Kong University of Science and Technology
z.wang@ust.hk

Oxygenated organic compounds are key reactive pollutants that significantly impact air quality and human health. They play critical roles in tropospheric photochemistry and oxidation capacity, profoundly influencing radical cycling and O₃ formation. Despite their importance, the precise quantification of these compounds remains a significant challenge. Here we present a comprehensive field study of volatile organic compounds (VOCs) and oxygenated VOCs in the coastal atmosphere of Hong Kong, employing a combination of real-time online mass spectrometry and offline sampling methods. The measurements revealed the substantial abundance of OVOCs and their significant contributions (~50%) to photochemical reactivity and O₃ formation potential.

Further observation-based modeling analysis demonstrated that the OVOCs related reactions can contribute to 30-65% of peroxy radical formation and recycling, thereby enhancing daytime O₃ formation. In addition, a GC-PTR coupled method was employed to resolve the isobaric interferences and fragmentation in real time mass spectrometry, and revealed substantial underestimation of long-chain aldehydes but overestimation of isoprene, benzene, styrene, and phenol. These biases propagated into photochemical modelling and would lead to large uncertainties in estimating photochemical radical and ozone chemistry. These findings underscore the critical role of OVOCs in coastal atmospheric chemistry and highlight the importance of isomer-resolved, interference-aware measurements for improving air-quality assessments and pollution control strategies.

Constraining the Unconstrained: Isotopic Evidence Debunks Modeled Pathways of Haze Sulfate Formation

Lei Geng^{1*}, Xueyin Ruan^{1*}, Guangming Su²

^{1*}School of Earth and Space Sciences, University of Science and Technology of China, Hefei, Anhui, China, genglei@ustc.edu.cn

²Institut de physique du Globe de Paris, Paris, France

Sulfate is a key aerosol component, being critical to the outbreak of haze pollution in China. Numerous studies have been conducted to discern the source and formation pathways of sulfate in China Haze, yet no consensus has reached. Atmospheric chemical transport model is one of the most popular tools that the community uses to probe how sulfate is formed. However, in order to reproduce the observed high sulfate content in Haze, such models are often tuned with unrealistic kinetic parameters. Another challenging but less been tackled issue is that how to justify the relative contributions of different formation pathways to atmospheric sulfate burden. Currently, most models rely on the modeled production rate of sulfate from each pathway, assuming the rate represents the contribution as long as the model can reproduce the observed sulfate concentration. This is not only a methodological failure, but also with no means to constrain the modeled production rates.

The oxygen-17 isotope anomaly (i.e., $\Delta^{17}\text{O}$) is a mass independent isotope fractionation signal originating from the photochemical formation of O_3 , and this $\Delta^{17}\text{O}$ signal can be transferred during oxidation chemistry, providing a unique means to probe the flux of individual chemical reaction. Here we develop a $\Delta^{17}\text{O}$ traced chemical transport model based on WRF-Chem, where the $\Delta^{17}\text{O}$ tracer serves to track the fate of sulfate produced in each formation pathway, i.e., from its chemical formation to transport, phase changes (i.e., gas-aerosol, aerosol-cloud), deposition and etc. By doing this, the real contribution of each formation pathway to atmospheric sulfate burden can be constrained. The model was then used to simulate a haze episode in Eastern China, with observed sulfate concentrations and its $\Delta^{17}\text{O}$ as observational constraints. The results show that although the model can successfully reproduce the observed high sulfate concentrations with tuned parameters, it fails to reproduce the observed $\Delta^{17}\text{O}$. The latter indicates the modeled formation pathways are wrong but its combination happens to agree with the observed mass concentrations. Our results highlight the general idea we want to convey that all models are probably wrong on the source apportionments of atmospheric sulfate despite that some of them can get the concentration right, and call for the widespread adoption of isotope-enabled measurements as a routine benchmark to evaluate chemical transport models for source apportionment.

Airborne microplastics: A review of current perspectives and environmental implications

Longyi Shao ^{a*}, Yaxin Cao ^a, Yaowei Li ^{b*}, Pengju Liu ^a, Susu Fan ^a

^a College of Geoscience and Surveying Engineering, China University of Mining and Technology (Beijing), Beijing 100083, China

^b Hebei North University, Zhangjiakou 075000, China

^c School of Environment, Tsinghua University, Beijing, 100084, China

* ShaoL@cumtb.edu.cn

Microplastics (MPs), as an entirely anthropogenic type of pollution, are considered to be stratigraphic markers of the Anthropocene Epoch, and have become of increasing public concern over the past decade. Recent studies have revealed that the atmosphere is an efficient medium to disseminate MPs from their sources to remote mountains and marine areas. However, current research on atmospheric MPs (i.e. airborne MPs) is generally less highlighted than MP water and soil pollution studies due to the lack of standard methods for the identification and quantification of atmospheric MPs. This paper reviews the published literature on airborne MPs, gives an overview of the advantages and disadvantages of current airborne MPs collection techniques, extraction methods and identification (i.e., ‘passive’ and ‘active’ sampling, density separation and visual identification), and lays a foundation for future studies. The physical and chemical characteristics, classification, spatial and temporal scale distributions, sources, transport, and environmental impacts of airborne MPs are summarized. There are substantial research gaps in the quantification of airborne MPs and the exploration of toxicity mechanisms of inhalable MPs. The establishment of accredited methods is an urgent challenge for a better understanding on airborne MPs and their environmental and health effects. As one of the constituents in many aerosols, airborne MPs should be treated as a recognized pollutant for long-term monitoring, and the factors that specifically affect airborne MPs could be better addressed by means of the characterization of individual MPs. In the future, the effects and interaction of MPs in the atmosphere, lithosphere and hydrosphere are also of critical importance.

Keywords: Airborne microplastics, analytical methods, Anthropocene, human health, physicochemical characteristics, source and transport.

Quantifying Hourly Wildfire Smoke Exposure and Acute Health Risks with Cascade Machine Learning

Shupeng Zhu^{1*} and Xiyao Chen¹, Luyao Wang¹, Anqi Jiao², Jun Wu²

^{1*} School of Earth Sciences, Zhejiang University, China

² Department of Environmental and Occupational Health, University of California, Irvine, USA, shupengz@zju.edu.cn

The rising frequency and severity of wildfires have intensified concerns regarding their adverse impacts on public health. However, accurately quantifying acute wildfire smoke exposure and its associated health impacts remains challenging due to limitations in existing high-resolution exposure data. Here, we develop a novel Cascade-Machine-Learning framework to generate unprecedented hourly wildfire-specific PM_{2.5} concentrations at a 1 km × 1 km resolution across California, achieving substantial accuracy improvements over traditional chemical transport models and satellite-derived datasets. Leveraging this high-resolution dataset with health records from the University of California, we identify critical relationships between short-term wildfire smoke exposure and acute pneumonia-related health risks. Notably, we introduce a new exposure metric, Pmax, capturing the intensity of hourly peak exposures relative to daily accumulated exposure, and reveal that short-lived, pulse-type wildfire smoke events are associated with nearly tenfold higher pneumonia-related medical risks compared to sustained exposure at equivalent daily average concentrations. Our results further highlight heightened vulnerability among individuals younger than 18 years and the African American populations. This work underscores the urgent need for temporally detailed exposure assessment in wildfire health studies and provides a robust scientific foundation for targeted public health interventions and emergency preparedness in an era of intensifying wildfire risks.

Vehicle emissions under real driving conditions: investigating the impact of semi-volatile compounds on air quality

Amira Jabbari-Hichri¹, Yassine Azizi^{2*}, Bernard Guiot^{2*}, Antoinette Boreave¹, Christian George¹

¹IRCELYON, University of Lyon, CNRS, Lyon, 69626 Villeurbanne Cedex, France

^{2*} CRMT, 69570 Dardilly, France, antoinette.boreave@ircelyon.univ-lyon1.fr

Vehicle emissions significantly affect air quality, particularly through the release of particulate matter (PM), which pose severe health risks such as respiratory and cardiovascular diseases¹. The world health organization (WHO) has updated guidelines to restrict exposure to these pollutants². Traditional emission models often overlook semi-volatile organic compounds (SVOCs) and intermediate-volatility organic compounds (IVOCs), which play crucial roles in forming secondary organic aerosols (SOAs)³. These compounds contribute to the formation of fine particulate matter (PM) and can have significant health implications due to their ability to penetrate deep into the respiratory system⁴.

This study investigates the impact of the emissions coming from various automotive vehicles on air quality, with a specific focus on semi-volatile organic compounds (SVOCs) measured across different real driving conditions, including urban, rural, and highway. A number of advanced on-line analytical instruments were used to gain a detailed understanding on the emitted compounds. The particle concentration and its distribution size, using a TSI EEPS 3090 and the Horiba OBS ONE SPN23 and SPN10, meanwhile the gas phase analysis was carried out using a Horiba FTX. In addition to real-time measurements, a novel collection system was developed to capture tailpipe emissions as a function of vehicle speed. Those various speed conditions dependent emissions, condensed in liquid phase through a cooling process, were subsequently analyzed offline using an UPLC-Orbitrap-MS. The compounds identified were then classified according to their volatility using the Volatility Basis Set (VBS)⁵.

The relationship between the molecular mass of the emitted compounds and their volatility, based on the engine speed during various test drives was established, providing deeper insights into car emissions of SVOCs and IVOCs. These findings are important for enhancing the accuracy of air quality models and developing targeted strategies to reduce pollution.

References

- [1] Hussain M, Madl P, Khan A (2011), Part-I. *Health* 2(2):51–59.
- [2] World Health Organization (2021), Geneva, World Health Organization.
- [3] Robinson AL, Donahue NM, Shrivastava MK, Weitkamp EA, Sage AM, Grieshop AP, Lane TE, Pierce JR, Pandis SN (2007), *Science* 315(5816):1259–1262.
- [4] Sun J, Shen ZX, Zhang T, Kong SF, Zhang HA, Zhang Q, Niu XY, Huang SS, Xu HM, Ho KF, Cao JJ (2022), *Environmental, International* 165:107344.
- [5] Li Y, Pöschl U, Shiraiwa M (2016), *Atmospheric Chemistry and Physics* 16(6):3327-3344.

The CHIMERE model as a tool to identify the best strategies to improve air quality and develop innovative AI-based techniques

Bertrand Bessagnet¹, Arineh Cholakian¹, Sylvain Mailler¹, Laurent Menut¹, Romain Pennel¹, Guillaume Siour², Myrto Valari¹, Enrico Pisoni³, Anthony Rey Pommier³, Philippe Thunis⁴, Maxime Beauchamp⁵, Alexander de Meij⁶,

¹Laboratoire de Météorologie Dynamique (LMD)/IPSL, Ecole Polytechnique, Institut Polytechnique de Paris, ENS, Université PSL, Sorbonne Université, CNRS, France

²Univ Paris Est Creteil and Université Paris Cité, CNRS, LISA, France

³European Commission, Joint Research Centre, Italy

⁴Ex European Commission, Joint Research Centre, Italy

⁵Danish Meteorological Institute, NCKF, Denmark

⁶METCLIM, Italy

Introduction

Air pollution, and particularly particulate pollution, is considered a major health risk. The WHO has lowered its guideline values in 2021, notably setting the annual limit for PM_{2.5} (particles smaller than 2.5 µm) concentrations at 5 µg m⁻³ in 2021 (World Health Organization, 2021). Despite clear improvements of air quality in China since 2013, Asia is still the continent the most impacted by poor air quality with countries like India, Bangladesh Nepal and Pakistan now the most affected by particulate pollution (State of Global Air, 2023). Furthermore, the Intergovernmental Panel on Climate Change (IPCC, 2023) clearly identified air quality as a key lever for action in the fight against climate change. Various international protocols, recommendations, and guideline values have led to national regulations worldwide on air quality. The new air quality directive proposes an increase use of modelling tools which requires a framework (EU, 2024). Modeling is a suitable approach for studying air quality and complement the monitoring strategy, but these numerical tools constantly need improvement and evaluation before they can be used operationally by public authorities responsible for national air quality policy.

Discussion

Within the French national framework, the CHIMERE tool, a chemistry transport model developed by the CNRS, LMD and LISA of IPSL (Menut et al., 2024) is the French national model used for research (Bessagnet et al., 2025; Cholakian et al., 2023; Lapere et al., 2023; Mailler et al., 2017; Maison et al., 2024) and operational contexts (Bessagnet et al., 2014; Rouil et al., 2009). The model is widely used throughout the world for research, forecasting by international organization and institutions (Figure 1). CHIMERE can simulate the atmospheric composition from urban scales at 1 km resolution up to 100 km resolution at the hemispheric level as shown in Figure 2 (Bessagnet et al., 2017; Mailler et al., 2017).

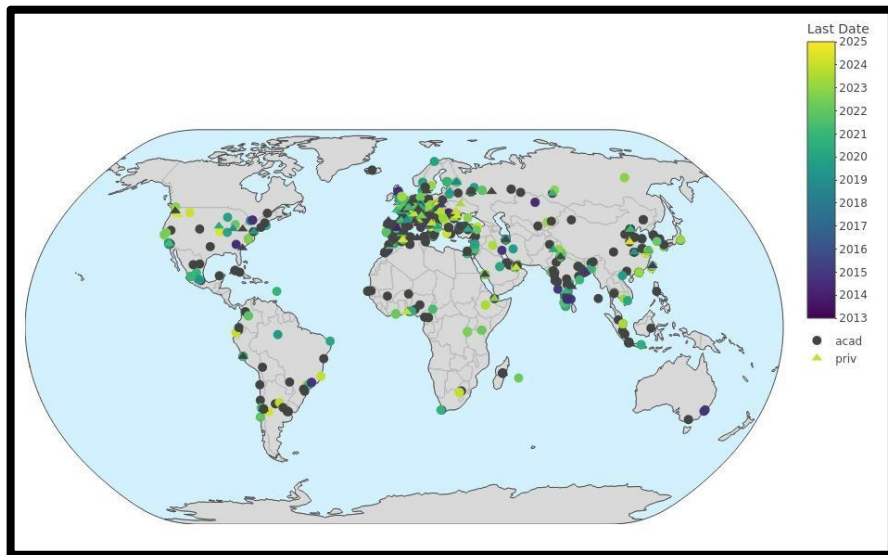


Figure 1: Map of CHIMERE users throughout the world

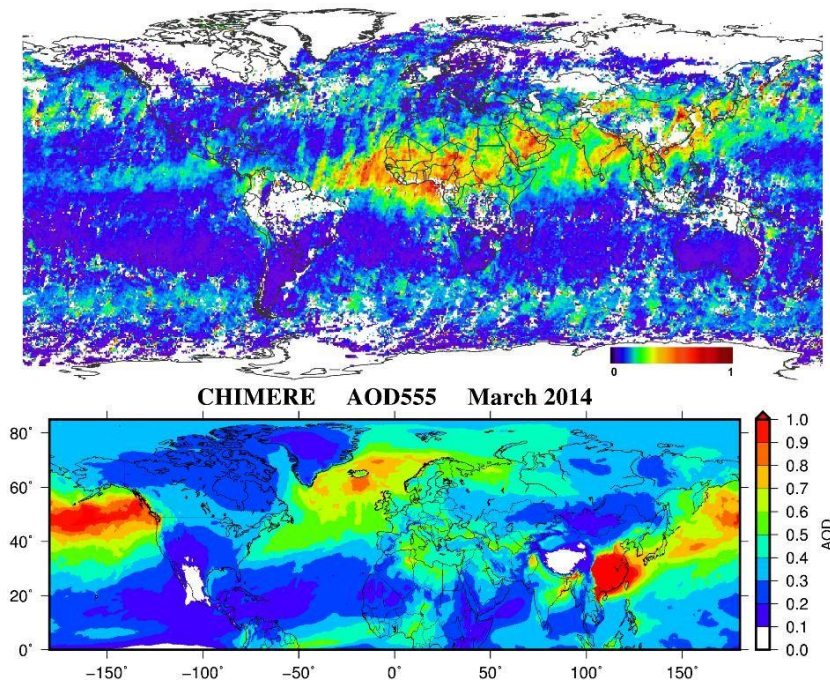
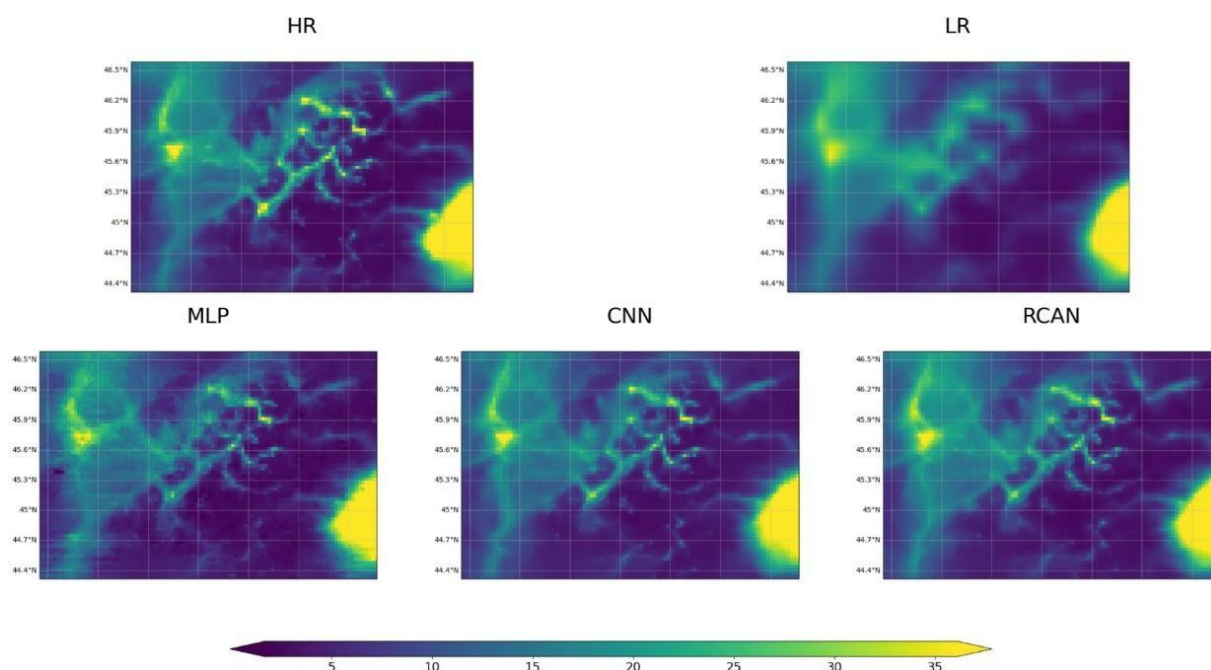


Figure 2: (Top) MISR (on board TERRA satellite instrument) monthly mean Aerosol Optical Depth 555 nm for March 2014 with cloud screening; and (Bottom) mean AOD 555 nm simulated by CHIMERE without cloud screening.

New approaches have emerged over the past decade, and the community is embracing machine learning techniques to develop new approaches that primarily use measurements, but also embed model results. Since 2020, CHIMERE is also used to develop techniques based on Artificial Intelligence techniques (Bessagnet et al., 2021). In (Bessagnet et al., 2021), the best Neural Network (NN) architecture (RCAN) displays very good performances in terms of prediction of pollutant

concentrations observed at stations with respect to the raw super-resolution CHIMERE simulation. The ability of the NN to mimic the high resolution (HR) was demonstrated with a correlation



exceeding 0.95 as well (Figure 3), doing much better than the low resolution (LR). Moreover, CHIMERE has been used to develop metamodels like the SHERPA model (Pisoni et al., 2024; Thunis et al., 2016) which is a screening model to identify the source of air pollution and quickly test options to improve air quality.

Figure 3: PM_{2.5} mean concentrations over a validation period for CHIMERE high-resolution (HR) and coarse resolution (LR) (top line) and three Neural Network-based super resolution architectures (bottom line): from left to right, pixel-based independent multi-layer perceptron (MLP), Convolutional neural network (CNN) and Residual channel attention network (RCAN)

Conclusions

In this presentation, we present the recent model developments and how this kind of model can be used to design new techniques to address the challenge of the high resolution over large domains. Some applications in Asia and Europe will be presented. We will highlight the necessity to develop both (i) the physical/chemical processes in the chemistry transport models like CHIMERE, (ii) in parallel machine learning techniques to generate simplified models able to produce outputs in a few seconds *i.e.* several orders faster than usual chemistry transport models.

References:

- [1] Bessagnet, B., Beauchamp, M., Guerreiro, C., de Leeuw, F., Tsyro, S., Colette, A., Meleux, F., Rouil, L., Ruysenaars, P., Sauter, F., Velders, G. J. M., Foltescu, V. L., and van Aardenne, J.: Can further mitigation of ammonia emissions reduce exceedances of particulate matter air quality standards?, *Environmental Science & Policy*, 44, 149–163,

<https://doi.org/10.1016/j.envsci.2014.07.011>, 2014.

- [2] Bessagnet, B., Menut, L., Colette, A., Couvidat, F., Dan, M., Mailler, S., Létinois, L., Pont, V., and Rouil, L.: An evaluation of the CHIMERE chemistry transport model to simulate dust outbreaks across the Northern Hemisphere in March 2014, *Atmosphere*, 8, 2017.
- [3] Bessagnet, B., Beauchamp, M., Menut, L., Fablet, R., Pisoni, E., and Thunis, P.: Deep learning techniques applied to super-resolution chemistry transport modeling for operational uses, *Environ. Res. Commun.*, 3, 085001, <https://doi.org/10.1088/2515-7620/ac17f7>, 2021.
- [4] Bessagnet, B., Thapa, N., Bajgai, D. P., Sahu, R., Saikia, A., Cholakian, A., Menut, L., Siour, G., Wangchuk, T., Crippa, M., and Gurung, K.: High resolution air quality simulation in the Himalayan valleys, a case study in Bhutan, *Atmospheric Chemistry and Physics*, 25, 18675–18696, <https://doi.org/10.5194/acp-25-18675-2025>, 2025.
- [5] Cholakian, A., Beekmann, M., Siour, G., Coll, I., Cirtog, M., Ormeño, E., Flaud, P.-M., Perraudin, E., and Villenave, E.: Simulation of organic aerosol, its precursors, and related oxidants in the Landes pine forest in southwestern France: accounting for domain-specific land use and physical conditions, *Atmos. Chem. Phys.*, 23, 3679–3706, <https://doi.org/10.5194/acp-23-3679-2023>, 2023.
- [6] EU: Directive (EU) 2024/2881 of the European Parliament and of the Council of 23 October 2024 on ambient air quality and cleaner air for Europe (recast), 2024.
- [7] State of Global Air: <https://www.stateofglobalair.org/health/ozone#ozone-toll>, last access: 20 December 2023.
- [8] IPCC: AR6 Synthesis Report: Climate Change 2023, IPCC, Interlaken, Switzerland, 2023.
- [9] Lapere, R., Huneeus, N., Mailler, S., Menut, L., and Couvidat, F.: Meteorological export and deposition fluxes of black carbon on glaciers of the central Chilean Andes, *Atmos. Chem. Phys.*, 23, 1749–1768, <https://doi.org/10.5194/acp-23-1749-2023>, 2023.
- [10] Mailler, S., Menut, L., Khvorostyanov, D., Valari, M., Couvidat, F., Siour, G., Turquety, S., Briant, R., Tuccella, P., Bessagnet, B., Colette, A., Létinois, L., Markakis, K., and Meleux, F.: CHIMERE-2017: from urban to hemispheric chemistry-transport modeling, *Geoscientific Model Development*, 10, 2397–2423, <https://doi.org/10.5194/gmd-10-2397-2017>, 2017.
- [11] Maison, A., Lugon, L., Park, S.-J., Baudic, A., Cantrell, C., Couvidat, F., D’Anna, B., Di Biagio, C., Gratien, A., Gros, V., Kalalian, C., Kammer, J., Michoud, V., Petit, J.-E., Shahin, M., Simon, L., Valari, M., Vigneron, J., Tuzet, A., and Sartelet, K.: Significant impact of urban tree biogenic emissions on air quality estimated by a bottom-up inventory and chemistry transport modeling, *Atmospheric Chemistry and Physics*, 24, 6011–6046, <https://doi.org/10.5194/acp-24-6011-2024>, 2024.
- [12] Menut, L., Cholakian, A., Pennel, R., Siour, G., Mailler, S., Valari, M., Lugon, L., and Meurdesoif, Y.: The CHIMERE chemistry-transport model v2023r1, *Geoscientific Model Development*, 17, 5431–5457, <https://doi.org/10.5194/gmd-17-5431-2024>, 2024.
- [13] Pisoni, E., De Marchi, D., di Taranto, A., Bessagnet, B., Sajani, S. Z., De Meij, A., and Thunis, P.: SHERPA-Cloud: An open-source online model to simulate air quality management policies in Europe, *Environmental Modelling & Software*, 106031, <https://doi.org/10.1016/j.envsoft.2024.106031>, 2024.
- [14] Rouil, L., Honore, C., Vautard, R., Beekmann, M., Bessagnet, B., Malherbe, L., Meleux, F., Dufour, A., Elichegaray, C., Flaud, J.-M., Menut, L., Martin, D., Peuch, A., Peuch, V.-H., and Poisson, N.: PREV’AIR An Operational Forecasting and Mapping System for Air Quality in Europe, *Bulletin of the American Meteorological Society*, 90, 73–83, 2009.
- [15] Thunis, P., Degraeuwe, B., Pisoni, E., Ferrari, F., and Clappier, A.: On the design and assessment of regional air quality plans: The SHERPA approach, *Journal of Environmental Management*, 183, 952–958, <https://doi.org/10.1016/j.jenvman.2016.09.049>, 2016.
- [16] World Health Organization: WHO global air quality guidelines: particulate matter (PM_{2.5} and PM₁₀), ozone, nitrogen dioxide, sulfur dioxide and carbon monoxide, WHO, Geneva, 2021.

Early-life nutritional additives, home environment, and outdoor air pollution associated with childhood food allergies: A multi-center mother-child study in China

Chan Lu^{1*}, Yufang Shan¹, Yuqing Chen¹, Ying Jiang¹, Wen Deng¹, Fèlix Faming Wang²

¹XiangYa School of Public Health, Central South University, China, chanlu@csu.edu.cn

²School of Environmental Science and Engineering, Tianjin University, China

Background: Nutritional additives and environments have been linked with food allergy (FA), but little research has explored their early-life interactions on childhood FA.

Objectives: To explore the effects of early-life nutritional additives (NAs), home environmental factors (HEFs), and outdoor air pollutant (OAP) exposures, and their interactions on childhood FAs.

Methods: Between 2022 and 2023, a large family-based retrospective cohort study was conducted across five cities in China. We collected 20,730 surveyed questionnaires, covering data on health outcomes, NAs, HEFs, lifestyle habits, and demographic characteristics of mother-child pairs and family members. Parents or guardians were required to return the completed forms within one week. Given the higher prevalence of FAs in younger children and the limited number of older children, we restricted our analysis to families with at least one child aged 0–6 years from 6,859 families. A double-sampling check of 10% of completed questionnaires confirmed >98% completeness and minimal logic errors, indicating high data reliability. Multilevel logistic regression models were conducted to investigate the independent and joint effects of early-life NAs, HEFs, OAP exposures on childhood FAs.

Results: Among 6,859 mother-child pairs, 703 children (10.2%) were diagnosed with FA. Prevalence of childhood FA varies significantly across cities, highest in Xiangxi (11.47%) and lowest in Liangshan (6.30%), with significant differences for all FA types except fruit/vegetable allergy. Maternal intake of NAs including iron, vitamins A, B, C, D, E, cod-liver oil, docosahexaenoic acid (DHA), protein powder, and prebiotic/probiotics/synbiotics during pregnancy was all related to a lower risk of childhood FA, with ORs (95% CIs) ranging from 0.63 (0.52-0.77) to 0.80 (0.68-0.95). Whereas, maternal intake of folic acid, calcium, and pregnant formula milk powder was not related to childhood FA. Childhood intake of NAs including iron, selenium, vitamin A, B, C, E, and cod-liver oil after birth reduced FA risk, with ORs (95% CIs) ranging from 0.61 (0.51-0.73) to 0.83 (0.71-0.98). Inversely, childhood intake of vitamin D and probiotics/probiotic/synbiotics was related to an increased risk of FA. However, childhood intake of calcium and zinc were not related to FA. Using ceramic tile/stone/cement floor, silicone rubber baby bottle, and fresh air filter reduced FA risk, with ORs (95% CIs) of 0.81 (0.67-0.98), 0.73 (0.57-0.93), and 0.74 (0.56-0.97). Comparatively, using glass baby bottle, plastic toy, air conditioning in summer, natural/coal gas, and mosquitos increased FA risk, ORs (95% CIs) ranging from 1.20 (1.02-1.42) to 2.05 (1.47-2.86). NO₂ exposure during the first trimester was consistently associated with FA (ORs: 1.24–1.32 per IQR). In multi-pollutant models, postnatal PM₁₀ and O₃ exposures remained significant (ORs: 1.24 and 1.12 per IQR). Gestational week-specific risks included PM_{2.5-10} (weeks 6, 18), NO₂ (weeks 3, 6, 18, 33), CO (week 9), and O₃ (weeks 27, 33). Effects were stronger for seafood and other FAs and in girls, older children, non-breastfed infants, and families with lower parental education and parental FA. Children without parental FA were more sensitive to NO₂ exposure during early pregnancy, whereas those with parental FA were more affected by CO and O₃. Nutritional supplements taken by mothers in utero and children after birth mitigated adverse effects of HEFs and OAP exposure on childhood FA, while amplified the protective effects.

Conclusions: Early-life NAs, HEFs, and OAP exposures independently and jointly impact childhood FA. Our study supports the hypothesis of “Fetal origin of childhood FA” and indicates a “nutrition-environment interaction” through gut-immunity axis.

Vacuum ultraviolet photoionization mass spectrometry and its applications in atmospheric environment

Xiaofeng Tang*, Zuoying Wen, Xuejun Gu, Xiaoxiao Lin, Weijun Zhng Hefei Institutes of Physical Science, Chinese Academy of Sciences, China Email: tangxf@aiofm.ac.cn

The origins of atmospheric pollution are complicated and often comprise a series of chemical reactions involving abundant volatile organic compounds (VOCs), free radicals and aerosol particles. How to analyze these species operando is a hot, significant and challenging topic in atmospheric environment. In this presentation, I will introduce the principle of vacuum ultraviolet (VUV) photoionization mass spectrometry, and present our home-made VUV photoionization time-of-flight mass spectrometers (VUV-PIMS) as well as photoelectron photoion coincidence (PEPICO) mass spectrometers. Several kinds of light sources, i.e. VUV discharge lamps and synchrotron radiations at Hefei and SOLEIL, have been connected with VUV-PIMS, directly providing mass information of molecular ions benefiting from its “soft” ionization at the threshold ionization energy of molecules. Some novel strategies have been developed to enhance the detection sensitivity of VUV-PIMS. In combination with synchrotron radiation light sources, mass-selected photoionization spectra or mass-selected threshold photoelectron spectra corresponding to each mass can be obtained by scanning synchrotron photon energy, very powerful to probe the elusive molecular structures and to identify complex isomers. In addition, the applications of VUV-PIMS to analyze atmospheric VOCs, free radicals and their reactions, and the chemical compositions of aerosol particles will be presented.

Uptake of atmospheric pollutants on road asphalt pavements: an underestimated sink in urban environments

M. J. Rossi^{1,2}, Adrien Gandolfo³, A. Lostier², A. Roose², C. George³, T. Salameh², F. Thevenet², H. Chen^{2,4,5} & M. N. Romanias²

¹École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

²IMT Nord Europe, Lille, France

³IRCELYON, CNRS, France

⁴School of Environmental and Chemical Engineering, Shanghai University, Shanghai, China

⁵State Environmental Protection Key Laboratory of Formation and Prevention of Urban Air Pollution Complex, Shanghai Academy of Environment Sciences, Shanghai, PR China

adrien.gandolfo@ircelyon.univ-lyon1.fr

Impervious macroscopic urban surfaces, such as paved roads, parking lots, rooftops, and building facades, cover about 60% of the total urban area, increasing to 80-100% in central business districts. Interestingly, the high coverage of these surfaces makes urban environments especially susceptible to climate change because of the urban heat island (UHI) effect. Although macroscopic urban surfaces are very common, their role as sites for heterogeneous reactions with atmospheric gases relevant to air quality has mostly been overlooked.

The uptake or transformation of atmospheric pollutants on asphalt pavements is barely documented, although it could be a significant atmospheric process due to the large surface area of asphalt pavements. Ignoring the role of heterogeneous processes in urban environments (areas with a high surface-to-volume ratio) might limit our understanding of the fate of key atmospheric pollutants.

In this study, we investigate the uptake of key atmospheric pollutants: nitrogen dioxide (NO₂), ozone (O₃), and two model organic molecules, methanol (CH₃OH) and formaldehyde (HCHO), on real-world asphalt pavements. The uptake experiments were conducted at room temperature (293 K) and under dry conditions within a Knudsen flow reactor coupled with a modulated molecular beam mass spectrometer. The environmental implications of our laboratory results are discussed through a series of box-model simulations that include NO₂, O₃, and HCHO loss on macroscopic surfaces.

Our experiments demonstrate a significant uptake of NO₂ on all weathered road pavements, while, within experimental accuracy, no uptake of NO₂ was observed on non-weathered asphalt pavement. The uptake of O₃ was observed on both non-weathered and aged asphalt pavements, with values on non-weathered samples being notably smaller than on aged surfaces. The simulations revealed that heterogeneous loss of pollutants influenced the levels of OH and NO₃ radicals, thereby affecting the oxidative capacity of urban atmospheres.

Atmospheric oxidation capacity dynamics-driven meteorology and multi-precursor interactions modulate O₃ variation in Hangzhou, China

Deming Han* and Wenjing Li

Zhejiang Key Laboratory of Environment and Health of New Pollutants, School of Environment, Hangzhou Institute for Advanced Study, University of Chinese Academy of Sciences, Hangzhou 310024, China; handeem@ucas.ac.cn

Ground-level ozone (O₃) pollution remains persistently high in China, despite the implementation of rigorous emission reduction measures targeting primary pollutants. The atmospheric oxidation capacity (AOC) serves as an essential driving force for O₃ formation; yet, its underlying mechanism is still not fully elucidated. Herein, we conducted a one-year observation campaign in Hangzhou, China, to characterize the temporal variations in O₃, and to clarify the drivers and reaction mechanisms of AOC, RO_x· radicals, and O₃ formation. We found the maximum O₃ concentrations occurred in summer, during which the average AOC value ($2.01 \pm 2.85 \times 10^7$ molecule cm⁻³ s⁻¹) was 2.4–6 times higher than in other seasons. Daytime AOC was driven by the hydroxyl radical (OH·, 83.00%–95.20%), which was itself generated mainly through O₃ photolysis in all seasons except winter. Furthermore, nitrogen oxide (NO_x) and relative humidity (RH) were identified as the principle individual factors controlling O₃ formation under low and moderate AOC scenarios, whereas the temperature-NO_x interaction and temperature-oxygenated volatile organic compounds (OVOCs) interaction emerged as the most critical factors under moderate and high AOC conditions, respectively. Our findings highlight the importance of devising O₃ mitigation strategies that account for AOC dynamics and multi-pollutant interactions, thereby supporting the development of tailored, region-specific control measures.

Microscopic Insights into Firework and Biomass Burning Derived Haze Particles During the Diwali Festival in Delhi, India

Lei Liu¹, Weijun Li^{2,*}, and Zongbo Shi³

¹Hangzhou International Innovation Institute, Beihang University, Hangzhou 311115, China
liulei5233@buaa.edu.cn

²Department of Atmospheric Sciences, School of Earth Sciences, Zhejiang University, Hangzhou 310058, China

³School of Geography, Earth and Environmental Sciences, University of Birmingham, Birmingham B15 2TT, UK

Delhi, one of the world's most densely populated megacities, experiences extreme haze episodes, especially during the Diwali Festival—a nationwide event characterized by intense fireworks coinciding with post-monsoon biomass burning. While bulk measurements show sharp pollution spikes with hourly PM_{2.5} exceeding 800 $\mu\text{g m}^{-3}$ during Diwali, direct microscopic evidence linking specific aerosol types to these concurrent sources remains limited. Here, we combined transmission electron microscopy (TEM) with real-time bulk chemical analyses to characterize fine particles and track their physicochemical evolution throughout the Diwali Festival. Before Diwali, high number fractions of potassium (K)-rich particles (25.2%), carbonaceous particles (primary organic aerosol (POA) and soot, 28.9%), and their internal mixtures (K-POA/soot, 37.1%), associated with spherical POA (i.e., tar balls), indicate significant biomass burning influences. During Diwali, we observed a large number of Al₂O₃ monomers (30–300 nm) and their agglomerates, either as bare (36.4–40.6%) or uniformly coated by K₂SO₄ shells (Al₂O₃-K, 46.6–47.5%), presumably from pyrotechnic combustion of fireworks. After Diwali, ultrafine Al₂O₃ particles (<100 nm) persisted, undergoing coagulation with aged biomass-burning particles, forming unique complex Al₂O₃-K-POA/soot particles. These findings suggest Al₂O₃ as a robust microscopic tracer of fireworks and provide direct microscopic evidence on particle evolution reflecting the combined impacts of fireworks and biomass burning on severe hazes in Delhi.

Keywords: megacity Delhi, Diwali Festival, Firework emission, Transmission electron microscopy (TEM), Individual particle analysis, Particle morphology, Ultrafine particles

Machine Learning for Long-term NO₂ Photolysis Reconstruction and its Impact on Secondary Pollution

Tong Li¹, Li Zhou^{2*} and Fumo Yang²

¹ College of Architecture and Environment, Sichuan University, China

^{2*}Country College of Carbon Neutrality Future Technology, Sichuan University, China,

lizhou@scu.edu.cn

The nitrogen dioxide (NO₂) photolysis rate coefficient J_{NO_2} is a critical parameter for assessing the intensity of atmospheric photochemical reactions and ozone (O₃) formation. Continuous, long-term direct measurements of J_{NO_2} are heavily limited by practical constraints in environmental settings. Reconstructing historical J_{NO_2} data allows researchers to accurately evaluate regional photochemical processes, atmospheric oxidation capacity, and the underlying drivers of secondary pollution. The Sichuan Basin, specifically the megacity of Chengdu, experiences complex meteorological conditions and severe compound air pollution involving PM_{2.5} and O₃, which complicates traditional atmospheric modeling.

In this study, we developed a machine learning-based method to reconstruct hourly J_{NO_2} values, applying it to a megacity in the Sichuan Basin from 2015 to 2023. The predictive accuracy and temporal transferability of the models were rigorously tested using ten-fold cross-validation and time-split selection. The model exhibited strong performance with cross-validation $R^2 = 0.854$ and $\text{RMSE} = 8.15 \times 10^{-4} \text{ s}^{-1}$. The Shapley Additive Explanations (SHAP) method was applied to interpret the model, quantifying the specific contribution and influence of each independent variable on the J_{NO_2} predictions. Utilizing SHAP method, we identified solar activity and pollutant levels both as significant predictors for J_{NO_2} . Our long-term J_{NO_2} reconstructions indicate a strong correlation between J_{NO_2} and ozone concentration, highlighting its important role in secondary pollution. This study illustrates the effectiveness of machine learning in reconstructing hourly J_{NO_2} values, providing valuable enhancement to traditional models. The findings are crucial for understanding regional photochemical processes and for analyzing trends and causes of ozone and aerosol pollution.

Specific ion chemistry at the air-water interface of nitrite/nitrate containing droplets

Yoan Carreira Mendes Da Silva¹, Maria Angelaki¹, Adrien Gondolfo¹, D. James Donaldson^{2,3} and Christian George¹

¹Universite Claude Bernard Lyon 1, CNRS, IRCELYON, UMR 5256, Villeurbanne F-69100, France, yoan.carreira-mendes@ircelyon.univ-lyon1.fr

²Department of Chemistry, University of Toronto, 80 George Street, Toronto, Ontario, Canada M5S 3H6,

An increasing number of studies report that OH radicals and hydrogen peroxide (H₂O₂) can be spontaneously formed at the air-water interface of water droplets^{1–3}. This interfacial chemistry can be an important source of oxidants in the atmosphere. In salt droplets (NaCl, NaBr, NaI, NaSCN, ...), H₂O₂ production has been reported to be linked to the Hofmeister series⁴, suggesting that this spontaneous chemistry is related to interfacial solvation properties. However, in these studies, droplets containing nitrate (NO₃⁻) or nitrite (NO₂⁻) anions were not investigated. These two ions, particularly NO₃⁻ play a key role in atmospheric chemistry. Therefore, the present experimental study investigates the spontaneous production of H₂O₂ in water droplets containing these anions under dark conditions. In a double-wall reactor covered by black fabric, a nebulizer is used to generate NO₃⁻/NO₂⁻ droplets in a range of 0.1–10 μm, from NaNO₃ or NaNO₂ solutions. During the experiment NO_x and HONO are monitored using gas-phase analyzers. After 30 minutes of experiments, the liquid droplets gathered in an impactor is collected to measure H₂O₂ production with an H₂O₂ analyzer.

Compared to ions that we have already studied using the same experimental approach (i.e., Cl⁻, Br⁻)^{4,5}, H₂O₂ production in droplets containing NO₂⁻ or NO₃⁻ is either enhanced or inhibited, depending on the NO₂⁻ or NO₃⁻ concentrations. Below a critical concentration, both NO₂⁻ and NO₃⁻ enhance the H₂O₂ production, we believe as a consequence of their ability to disrupt the water structure at the interface. At larger concentrations, a specific interfacial NO₂⁻ or NO₃⁻ chemistry starts to be important, producing gas phase species such as HONO and NO₂. Measuring the dependence of the gas phase production of H₂O₂, NO_x and HONO on solution parameters allows us to propose a mechanism to explain this specific interfacial chemistry of NO₂⁻ and NO₃⁻. This study provides new insight into the “spontaneous” interfacial chemistry of droplets, highlighting that NO₂⁻/NO₃⁻-containing droplets could be a significant nighttime source of nitrogen species before daytime photolysis.

- [1] Heindel, J. P.; Hao, H.; LaCour, R. A.; Head-Gordon, T. Spontaneous Formation of Hydrogen Peroxide in Water Microdroplets. *J. Phys. Chem. Lett.* 2022,13 (43), 10035–10041. <https://doi.org/10.1021/acs.jpcllett.2c01721>.
- [2] Lee, J. K.; Walker, K. L.; Han, H. S.; Kang, J.; Prinz, F. B.; Waymouth, R. M.; Nam, H. G.; Zare, R. N. Spontaneous Generation of Hydrogen Peroxide from Aqueous Microdroplets. *Proceedings of the National Academy of Sciences* 2019, 116 (39), 19294–19298. <https://doi.org/10.1073/pnas.1911883116>.
- [3] Mehrgardi, M. A.; Mofidfar, M.; Zare, R. N. Sprayed Water Microdroplets Are Able to Generate Hydrogen Peroxide Spontaneously. *J. Am. Chem. Soc.* 2022, 144 (17), 7606–7609. <https://doi.org/10.1021/jacs.2c02890>.
- [4] Carreira Mendes Da Silva, Y.; Angelaki, M.; Donaldson, D. J.; George, C. Specific Ion Properties Induce Spontaneous H₂O₂ Production at the Air–Water Interface. *J. Am. Chem. Soc.* 2025, 147 (31), 27768–27776. <https://doi.org/10.1021/jacs.5c06512>.
- [5] Angelaki, M.; Carreira Mendes Da Silva, Y.; Perrier, S.; George, C. Quantification and Mechanistic Investigation of the Spontaneous H₂O₂ Generation at the Interfaces of Salt-Containing Aqueous Droplets. *Journal of the American Chemical Society* 0 (0), null. <https://doi.org/10.1021/jacs.3c14040>.

Data-Driven Methodologies for Accurate Source Apportionment of Atmospheric Pollution and Practical Applications

Tianjiao Dai¹, Qili Dai², Yinchang Feng², Junfeng Chen¹, Rongcheng Chen, and Zheng Wang^{1*}

^{1*}China Waterborne Transport Research Institute, China, wangzh@wti.ac.cn

²Key Laboratory of Urban Air Particulate Pollution Prevention and Control of Ministry of Ecology and Environment, College of Environmental Science and Engineering, Nankai University, China

Against the backdrop of increasingly pressing demands for air pollution control and refined emission inventory management, precise source apportionment of atmospheric pollution has become a critical scientific issue requiring urgent breakthrough. This study develops a source apportionment framework that integrates multidimensional information including meteorological conditions, pollution monitoring, and emission inventories based on multi-source observations and data-driven approaches. We propose a spatially-refined integrated source apportionment method combining Positive Matrix Factorization (PMF) and Bayesian receptor modeling. The methodology is validated using coarse particulate matter (PM) mass concentrations with pronounced spatial heterogeneity. By coupling information on the spatial distribution and activity levels of local emission sources, we quantify the probability distribution of source contributions at different monitoring locations, enabling high-precision identification and quantitative apportionment of major pollution sources. Future work will further investigate precise source apportionment of atmospheric pollution in typical port multi-pollutant scenarios, providing technical support for synergistic control of pollution reduction and carbon neutrality and enhancement of port environmental quality.

Construction of the First Fingerprint Spectrum for Biogenic Carbonyls Emitted from a Tropical Rainforest

Qinqin Li^{1,2*}, Zijian Chen¹, Daocheng Gong^{1,2}, Xi Chen¹, Jiangyong Li^{1,2}, Qinghua Chang¹, Sijun Chen¹, Ruiyun Xu¹, Yiqing Li¹, Zimo Zeng¹, Boguang Wang^{1,2*}

¹College of Environment and Climate, Institute for Environmental and Climate Research, Jinan University, China

²Guangdong Provincial Observation and Research Station for Atmospheric Environment and Carbon Neutrality in Nanling Forests, China

*liqinqin@jnu.edu.cn, tbongue@jnu.edu.cn

Carbonyls is critical to biosphere-atmosphere interactions, profoundly influencing atmospheric chemical recycling and ecological function, yet fully scripts for their biogenic emissions remains challenging. Here, we conducted in situ measurements of biogenic carbonyls emitted from 50 typical rainforest species in South China. The emission patterns of biogenic carbonyls varied dramatically between different species. Straight-chained ketones and aromatic aldehydes are key biogenic carbonyl compounds emitted from the tropic plants. The emission rates were also calculated using both G93 and T80 models, which presenting a relatively strong emission potential of biogenic carbonyls from the tropic rainforest. The emission of biogenic carbonyls estimating using MAGEN model are extremely underestimated. The newly constructed biogenic carbonyls emission inventory provides an improved dataset for re-examining the roles of biogenic emissions on the air quality and climate feedback.

Experimental Reexamination of the CH₂OO and (CH₃)₂COO Criegee Intermediate Reactions with SO₂

Chenyang Xue¹, Pengcheng Wang¹, Rabi Chhantyal-Pun², Véronique Daële¹, Abdelwahid Mellouki^{1,3}, Max R. McGillen^{1*}

¹ CNRS, Institut de Combustion Aérothermique Réactivité et Environnement (ICARE), Orléans, 45071, France

² School of Chemistry, University of Nottingham, Nottingham, NG7 2RD, U.K.

³ Mohammed VI Polytechnic University, Ben Guerir 43150, Morocco

chenyang.xue@cnrs-orleans.fr

The reactions of SO₂ with Criegee intermediates are considered to be a significant source of sulfate in the atmosphere, with implications for aerosol formation in various environments. Despite this, discrepancies remain in the rate coefficients of these reactions, especially regarding the acetone oxide Criegee intermediate, and by extension, other substituted Criegee intermediates. In this study, we utilize a recently developed relative rate technique for determining the rate coefficients of CH₂OO + SO₂ and (CH₃)₂COO + SO₂ at room temperature and atmospheric pressure, yielding values of 3.18×10^{-11} and 4.26×10^{-10} cm³ molecule⁻¹ s⁻¹ respectively. For CH₂OO, we find excellent consistency with the various absolute measurements available in the literature. However, for (CH₃)₂COO, our determination is more than a factor of 3 higher, suggesting that current data evaluations may require revision, affording a better constraint on the effects of these reactions on atmospheric chemistry.

Particle–gas transfer processes during the photolysis of cis-pinonic acid: a comparative study between bulk and single-particle approaches

Gwendoline Bourdon^{1*,2}, Pierre-Marie Flaud², Emilie Perraudin², Eric Villenave², Sophie Sobanska¹

^{1*} ISM UMR 5255 CNRS, Univ. Bordeaux, Talence, France, gwendoline.bourdon@u-bordeaux.fr

² EPOC UMR 5805 CNRS, Univ. Bordeaux, Pessac, France

Summary: At the global scale, biogenic volatile organic compounds (BVOCs) are predominantly emitted by vegetation (e.g., monoterpenes such as α - and β -pinene) and contribute to the formation of biogenic secondary organic aerosols (BSOAs), which are estimated to account for 30–50% of the global organic aerosol budget¹. Once formed, BSOAs can undergo further transformations through multiphase aging processes. These reactions modify both the chemical composition and physico-chemical properties of aerosols, such as hygroscopicity, viscosity, and gas–particle partitioning, thereby influencing their atmospheric fate, air quality, and climate impacts. Cis-pinonic acid (CPA) is a key compound in the formation processes of biogenic secondary organic aerosols originating from the photo-oxidation of α -pinene^{2,3}. Owing to its low vapor pressure ($\sim 7 \times 10^{-5}$ Pa) and high Henry's law constant (2×10^7 M atm⁻¹), CPA can partition between the gas phase and particulate matter in the atmosphere. Despite the well-established role of CPA in SOA formation and aging, significant knowledge gaps remain regarding the underlying photo-oxidative mechanisms. The few mechanisms proposed so far in the literature are mainly based on studies conducted in bulk aqueous solutions or flow reactors^{4,5}. Investigations at the single-particle scale are still lacking, although it is known that reactivity in bulk systems can differ from that at the gas–particle interface, due to effects related to particle curvature and surface-to-volume ratio. At the single-particle level, levitation techniques offer unique advantages for investigating aerosol physico-chemical properties and processes, notably by eliminating substrate-induced artifacts while allowing precise control of environmental parameters (e.g. temperature and relative humidity)⁶. In this context, the present study aims to elucidate the photo-oxidative aging mechanisms of CPA particles, used as a model for BSOAs generated from α -pinene photo-oxidation, in order to improve our understanding of the atmospheric fate and impact of BSOAs.

To achieve these objectives, an original experimental setup coupling acoustic levitation with high-resolution proton-transfer-reaction time-of-flight mass spectrometry (PTR-TOF-MS) was developed. This approach enables real-time monitoring of volatile compound exchanges between a single particle and the surrounding gas phase during physico-chemical processes. Comparison of bulk and single-particle experiments reveals the emission of methyl vinyl ketone from the particle, produced via a Norrish type II pathway during CPA photolysis. This innovative methodology opens new perspectives for investigating dynamic gas–particle exchanges at the single-particle scale and provides a more comprehensive understanding of atmospheric aerosol aging mechanisms.

References

- [1] Jimenez J. L., et al. *Science* 2009, 326, 1525–1529.
- [2] Kavouras I. G., et al. *Nature* 1998, 395, 683–686.
- [3] Daumit K. E. et al., *J. Phys. Chem. A* 2016, 120, 1386–1394.
- [4] Lignell H. et al., *J. Phys. Chem. A* 2013, 117, 12930–12945.
- [5] Enami S. and Sakamoto Y. *J. Phys. Chem. A* 2016, 120, 3578–3587.
- [6] Tuckerman et al., *Anal. Bioanal. Chem.*, 2002, 372, 122–127.

Acknowledgments

The authors wish to thank the ANR for financial support of the SOAPHY project (ANR-21-CE29-0031) and the Région Nouvelle Aquitaine for its support of the LEVIAERO project (convention n°AAPR2022-2021-17126210).

Spontaneous Sulfur(IV) Oxidation at Droplet Interfaces

Yuting Lyu¹ and Christian George^{1*}

¹Universite Claude Bernard Lyon 1, CNRS, IRCELYON, UMR 5256, Villeurbanne, F-69100, France, yuting.lyu@ircelyon.univ-lyon1.fr

Objective The oxidation of sulfur dioxide (SO₂) to sulfate is a key pathway in atmospheric aerosol formation and acid deposition. Conventional mechanisms attribute this process to aqueous oxidants such as ozone, hydrogen peroxide, or transition-metal-catalyzed reactions in bulk solution. However, these pathways cannot fully explain the rapid sulfate formation observed during severe haze episodes. This work investigates alternative oxidation mechanisms occurring at the air–liquid interface of atmospheric microdroplets, with a focus on the role of electron scavengers and interfacial redox chemistry.

Method Bisulfite-containing microdroplets were generated by nebulizing aqueous sodium bisulfite solutions into a humidified flow-tube reactor, allowing controlled variation of pH and gas composition (N₂ or N₂/O₂ mixtures). The droplets had diameters of approximately 0.2–4 μm and a residence time of around 36 s in the reactor. Gas-phase SO₂ emission was monitored using a fluorescence SO₂ analyzer, while sulfate formation in collected droplets was quantified by ion chromatography. Hydroxyl radical (OH·) formation was detected using terephthalic acid (TA) as a fluorescent probe.

Result Sulfate formation was observed even under oxygen-free conditions, particularly at pH 4.6 where bisulfite (HSO₃⁻) dominates. Decreased emission of SO₂ and formation of sulfate were observed under N₂ atmosphere, indicating that S(IV) oxidation can proceed without molecular oxygen. The presence of O₂ enhanced sulfate formation but was not required for the reaction to occur. Fluorescence measurements confirmed the formation of OH· in bisulfite droplets under N₂, suggesting that sulfur(IV) species can act as electron scavengers at the droplet interface. These findings support a mechanism involving interfacial electron transfer, sulfur-centered radicals (SO₃⁻ and SO₄⁻), and reactive oxygen species.

Conclusion Our results reveal a previously unrecognized oxidation pathway for S(IV) at the air–liquid interface that operates independently of molecular oxygen. Interfacial electron transfer involving electron scavengers and radical intermediates can drive sulfate formation in atmospheric droplets. This mechanism highlights the importance of interfacial chemistry in atmospheric sulfur cycling and may help explain the rapid sulfate production observed during severe haze events.

Oxidation of Dimethyl Sulfide at Air-Water Bubbles Surfaces

Laurentiu-Gabriel Movila^{1*}, Yoan Carreira Mendes Da Silva¹, Zhongyu Guo¹, D. James Donaldson² and Christian George¹

^{1*}Université Claude Bernard Lyon 1, CNRS, IRCELYON, UMR 5256, Villeurbanne F-69100, France, laurentiu.movila@ircelyon.univ-lyon1.fr

²Department of Chemistry, University of Toronto, Toronto, Ontario, Canada M5S 3H6; Department of Physical and Environmental Sciences, University of Toronto Scarborough, Toronto, ON, Canada M1C 1A4

Dimethyl Sulfide (DMS) is a significant volatile organic sulfur compound in marine and atmospheric environments where it can affect aerosol and cloud formation, being produced in large amounts by algal blooms¹. This study explores the oxidation of DMS in a simple bubbled aqueous system, simulating bubbles formed from wave breaking in ocean and sea, without external oxidants or catalysts. Similar to OH radical formation at the interface of aqueous droplets², the air-water interface of air bubbles in water might show the same phenomenon and thus lead to the OH initiated oxidation of DMS. The study aims to also highlight the role of O₂ as electron scavenger to promote in OH radical formation. The OH-initiated oxidation of DMS is expected to lead to the formation of products such as dimethyl sulfoxide (DMSO), dimethyl sulfone (DMSO₂), methanesulfonic acid (MSA) and sulfate (SO₄²⁻)^{3,4}.

Solutions of DMS in deionized water were bubbled with either air or nitrogen (N₂) through frits of different pore size, to vary bubble S/V ratios. The gas expelled from bubbles' bursting at the aqueous surface was sampled with a Proton Transfer Reaction Mass Spectrometry (PTR-MS) to monitor the real-time formation for volatile oxidation products, specifically DMSO and DMSO₂. Orbitrap Mass Spectrometry (Orbitrap-MS) was employed for offline detection of MSA in the liquid phase, while Ion Chromatography (IC) is planned for future analysis of SO₄²⁻. Experiments were conducted under controlled conditions at room temperature, showing good reproducibility.

Results showed significant DMSO₂ formation during air bubbling, indicating its role as an oxidation product, while DMSO formation seemed to be minimal, suggesting a minor role as an intermediate or rapid conversion of DMS to DMSO₂ via a different pathway. Orbitrap-MS confirmed the presence in the detection limit of MSA, a stable end product of DMS oxidation. Oxygen-free conditions (N₂) suppressed oxidation of DMS, proving the essential role of O₂ in OH radicals formation and DMS oxidation.

This study highlights a new, environmentally relevant oxidation pathway for DMS, driven by OH radicals formed at the interfaces of air bubbles in water, without the presence of oxidants or catalysts, highlighting the importance of air-water interfacial processes, which may represent an underappreciated pathway for sulfur species oxidation in marine environments.

- [1] Alcolombri U, Ben-Dor S, Feldmesser E, Levin Y, Tawfik DS, Vardi A. Identification of the algal dimethyl sulfide-releasing enzyme: A missing link in the marine sulfur cycle. *Science*. 2015;348(6242):1466-1469. doi:10.1126/science.aab1586
- [2] Lee JK, Walker KL, Han HS, et al. Spontaneous generation of hydrogen peroxide from aqueous microdroplets. *Proc Natl Acad Sci USA*. 2019;116(39):19294-19298. doi:10.1073/pnas.1911883116
- [3] Chen G, Davis DD, Kasibhatla P, et al. A Study of DMS Oxidation in the Tropics: Comparison of Christmas Island Field Observations of DMS, SO₂, and DMSO with Model Simulations.
- [4] Mardyukov A, Schreiner PR. Atmospherically Relevant Radicals Derived from the Oxidation of Dimethyl Sulfide. *Acc Chem Res*. 2018;51(2):475-483. doi:10.1021/acs.accounts.7b00536

Ammonia (NH₃) Monitoring and Its Impact on Air Pollution and Climate Change in Agricultural and Semi-Urban Sites from Central France

Abdellatif Rafik¹, Pengcheng Wang¹, B. Grosselin¹, Corinne Robin², Amélie De Fillipis², Abderrazak Yahyaoui², Max McGillen¹, Véronique Daële¹

¹Institut de Combustion Aérothermique Réactivité Environnement (ICARE-UPR 3021) / CNRS, Orléans - FRANCE

^{2*} Association de surveillance de la qualité de l'air en Région Centre-Val de Loire LIG'AIR, St-Cyr-en-Val - FRANCE

veronique.daele@cnr-orleans.fr

Ammonia (NH₃) is a major precursor of secondary inorganic aerosols and plays a central role in atmospheric chemistry, contributing indirectly to ecosystem acidification, and eutrophication. Despite its predominantly agricultural origin, its regional-scale atmospheric dynamics remain insufficiently documented. This study investigates the temporal variability, meteorological controls, and chemical interactions of NH₃ in the Centre-Val de Loire region (France), where agriculture accounts for 96–99% of emissions (~30,375 t yr⁻¹) slightly higher than the national average (94%). Continuous active high-resolution NH₃ measurements were conducted at a rural crop-dominated site (Oysonville) and at a semi-urban site (Supersite Voltaire CNRS-Orléans) over the 2022–2026 period. These observations were complemented by passive sampling using Radiello tubes at eight sites during late winter and early spring, corresponding to the main fertilizer spreading period. Spatial and temporal variability of NH₃ was investigated across sites with contrasting land-use characteristics, with particular focus on agricultural periods such as fertilizer application. The annual mean NH₃ concentration at the agricultural site was 3.4 μg m⁻³, with hourly maxima reaching 31.5 μg m⁻³. Pronounced increases were observed during fertilizer application periods, with monthly means peaking in March and weekly values exceeding 20 μg m⁻³ during intensive spreading. Concentrations decreased markedly following rainfall events, in some cases dropping below 4 μg m⁻³. Passive and active measurements showed strong agreement (R² > 0.9), although passive samplers underestimated concentrations by 2.7 μg m⁻³ (–28%). In addition, the influence of other meteorological parameters (wind speed, relative humidity) and NO_x, O₃ was examined to identify the main processes governing NH₃ variability, including emission intensity, atmospheric dispersion, wet scavenging, and gas–particle partitioning. These findings provide an integrated regional characterization of NH₃ dynamics and support improved emission management and air-quality modeling in temperate agricultural systems.

Ozonolysis of Myrtenal on Saharan Sand: Impact of Particle Diameter, Surface Coating and Relative Humidity

Mohamad Ghaleb Alossaily¹, Abdelkhaleq Chakir¹, Estelle Roth^{1*}

^{1*}Climate Impacts on Environment, AEROLAB EMR7007, Université de Reims, France, estelle.roth@univ-reims.fr

Heterogeneous reactions of biogenic volatile organic compounds (BVOCs) on mineral dust surfaces represent an important yet still uncertain sink in the atmosphere. In this work, we investigate the heterogeneous ozonolysis of myrtenal, a monoterpene aldehyde emitted by vegetation, on Saharan sand as a proxy for mineral dust.

Experiments were conducted in a photochemical reactor under controlled conditions to quantify the reactivity of myrtenal deposited on sand particles with ozone. The influence of key physicochemical parameters was explored, including surface coating, sand particle diameter, and relative humidity (RH). Myrtenal decay was monitored using GC-FID, and apparent pseudo-first-order rate constants were derived to assess the impact of surface properties and environmental conditions on the reaction kinetics.

Results show that the rate of ozonolysis reaction taking place on Saharan sand is significantly slower compared to the gas-phase reaction. The reactivity was strongly dependent on the particle size, with smaller sand particles exhibiting enhanced reactivity due to their higher surface area. Higher surface coatings altered the accessibility and reactivity of active sites, therefore showed lower reactivity. In addition, relative humidity played a key role, affecting both surface chemistry and ozone–VOC interactions, with notable changes in reaction rates observed across the investigated RH range.

These findings demonstrate that mineral dust properties and ambient humidity critically control the heterogeneous ozonolysis of myrtenal. This study highlights the importance of accounting for dust–VOC–ozone interactions in atmospheric models, particularly in regions influenced by Saharan dust transport, where such processes may significantly impact VOC lifetimes and secondary oxidation chemistry.

Less NO_x emission reductions are a potential cause for low effectiveness of sulfate aerosol reductions in China

Zhe Song^{1,2,3}, Huan Xi^{1,2}, Ningning Yao^{1,2}, Lang Chen^{1,2}, Zhengnan Cen^{1,2}, Pengfei Li⁴, Daniel Rosenfeld⁵ and Shaocai Yu^{2,3,6}

¹Laboratory for Statistical Monitoring and Intelligent Governance of Common Prosperity, Collaborative Innovation Center of Statistical Data Engineering Technology & Application, School of Statistics and Data Science, Zhejiang Gongshang University, Hangzhou 310018, China;

²Zhejiang Key Laboratory of Solid Waste Pollution Control and Resource Utilization, School of Environmental Sciences and Engineering, Zhejiang Gongshang University, Hangzhou 310018, China;

³Research Center for Air Pollution and Health; Key Laboratory of Environmental Remediation and Ecological Health, Ministry of Education, College of Environment and Resource Sciences, Zhejiang University, Hangzhou, Zhejiang 310058, China;

⁴State Key Laboratory of Infrared Physics, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, Shanghai 200031, China;

⁵Institute of Earth Sciences, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel;

⁶School of Statistics and Data Science, Zhejiang Gongshang University, Hangzhou 310018, China.

Despite the substantial progress China has made in controlling sulfur dioxide (SO₂) emissions in recent years, observations indicate that the decline in sulfate aerosol (SO₄²⁻) concentrations has not been proportional to the reduction in SO₂ emissions, suggesting that the formation of SO₄²⁻ is influenced by more complex chemical processes. In this study, a comprehensive emission inventory and the WRF–CMAQ regional air quality modeling system were used, together with emission and meteorological data for Western Europe (WE), Eastern North America (ENA), and East Asia (EA) for the years 2007 and 2020, to investigate the impacts of changes in SO₂ and nitrogen oxides (NO_x) emissions on atmospheric acidity and sulfate formation. The results show that in WE and ENA, both SO₂ and NO_x emissions declined significantly between 2007 and 2020, leading to reduced atmospheric acidity, reflected by an increase in the adjusted gas ratio (adjGR) and a substantial decrease in SO₄²⁻ concentrations. In contrast, although SO₂ emissions in EA—particularly in China—were markedly reduced, the relatively smaller reduction in NO_x emissions resulted in limited changes in adjGR and only modest decreases in SO₄²⁻ concentrations. Mechanistic analysis indicates that the persistently high NO_x emissions in EA limited the reduction in atmospheric acidity and enhanced the contribution of the ozone oxidation pathway, thereby promoting the formation of SO₄²⁻. These

findings highlight that controlling SO₂ emissions alone is insufficient to effectively reduce sulfate aerosol concentrations. Coordinated reductions of NO_x and ammonia (NH₃) are also required to achieve more effective improvements in regional air quality and climate impacts.

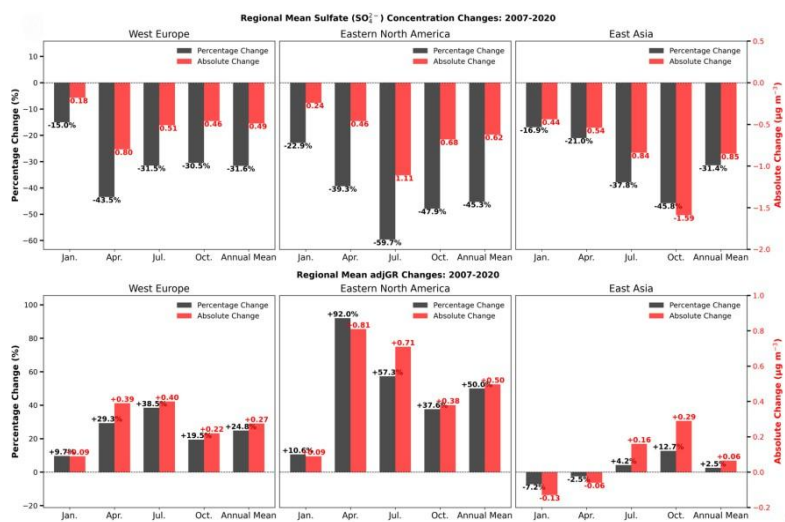


Figure 1: Seasonal changes of mean sulfate (SO₄²⁻) concentrations (top row) and adjusted gas ratio (adjGR, bottom row) over West Europe, Eastern North America, and East Asia in January, April, July, and October of 2007 and 2020, simulated by the WRF-CMAQ model. Left axes show percentage changes (black bars), right axes show absolute changes (red bars)

Urban–rural divergence of wintertime organic aerosol molecular fingerprints in PM_{2.5} revealed by FT–ICR MS

Shanshan Tang

Hangzhou International Innovation Institute, Beihang University, Hangzhou 311115, China
tangshanshan@buaa.edu.cn

Winter haze over the North China Plain (NCP) remains a major air quality challenge. Molecular level constraints on water soluble organic carbon (WSOC) are needed to clarify how contrasting urban versus rural emission mixtures, together with subsequent atmospheric processing, shape organic aerosol composition and inform mitigation. Here we investigated wintertime PM_{2.5} collected at an urban site and a rural site using Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS), together with measurements of bulk aerosol components (PM_{2.5}, OC, WSOC, and major inorganic ions). In the full molecular pool, the urban WSOC showed an enhanced contribution of nitrogen-containing formulas, with CHON accounting for 29.1% compared with 21.3% at the rural site, whereas the rural WSOC exhibited a slightly higher CHOS contribution (27.1%). A site-unique formula framework amplified these divergences. Urban-unique formulas were dominated by CHON (47.6%), while rural-unique formulas were strongly enriched in sulfur-containing species, with CHOS+CHONS reaching 67.9%. Atom-number fingerprints revealed that urban-unique CHON was characterized by a stronger N₂ subpopulation and higher oxygen-number bins, whereas rural-unique CHON was dominated by N₁ formulas, consistent with distinct nitrogen functionalities and processing environments. This work provides robust molecular evidence for pronounced urban–rural divergence in wintertime organic aerosol composition in the NCP, offering a basis for source and process informed strategies to reduce haze pollution.

Keywords: PM_{2.5}, FT–ICR MS, Urban–rural divergence, Molecular fingerprints

Real-time Detection of Black Smoke from Ships based on Improved YOLOv5 with Multi-Feature Fusion Method

Ling Xiao¹, Jianbo Hu^{1*}, Lin Jiang², Lei Wang², Guanghui Yang³

^{1*}Tianjin Research Institute for Water Transport Engineering. M. O. T, Tianjin 300456, China
Country, xiaoling20260309@163.com

²Shanghai Maritime Safety Administration of the People's republic of China, Shanghai 200086, China

³Dongguan Maritime Safety Administration of the People's republic of China, Guangdong 523990, China

Ship black smoke, a visible manifestation of airborne pollutant emissions from vessels, poses a significant threat to air quality in port cities and their surrounding areas. manual inspection methods. Traditional approaches, are limited applicability under varying environmental conditions, and substantial human resource requirements, rendering them inadequate for comprehensive surveillance of dense maritime traffic. To address these limitations, this study aims to develop an automatic ship black smoke recognition algorithm based on an improved YOLOv5 architecture with multi-feature fusion, enabling real-time warning and intelligent supervision of smoking vessels using video stream data from surveillance cameras installed near critical waterways.

To support modeling and rigorous validation, this study constructed a specialized dataset of ship black smock through systematic field data collection, and subsequently annotated and preprocessed the dataset. Six high-definition surveillance cameras were strategically deployed at locations with unobstructed views along the Yangtze River Estuary and the Huangpu River, including Baoshan Maritime Safety Administration area, Huangpu Maritime Administration area (upstream of Nanpu Bridge), Fisherman's Wharf in Baoshan District, and Nandu Ferry. Video data were collected from June 2023 to May 2024, capturing diverse meteorological conditions, illumination scenarios, background environments, vessel types, and smoke opacities. Using ScreenToGif software, video frames were extracted at 15-frame intervals, yielding 15,618 images containing ship black smoke plumes, supplemented by 48 online images for enhanced diversity. All images were meticulously annotated using the labeling tool following YOLO format, with bounding boxes carefully delineating smoke plume regions while excluding vessel stacks. The dataset was partitioned into training (80%), validation (10%), and test (10%) sets. To enhance model generalization under low-light conditions, adaptive Gamma transformation was applied during preprocessing to improve contrast and reveal smoke edge features otherwise obscured by poor illumination.

Building upon the YOLOv5x architecture, we conducted model improvement and training. We developed an enhanced detection framework incorporating cross-scale feature fusion structures and an improved loss function. The methodological innovations include: (1) Integration of Convolutional Block Attention Mechanism (CBAM) into the backbone network to enhance spatial localization of smoke plumes and suppress background interference. (2) Replacement of the traditional Path Aggregation Network (PANet) with a lightweight bidirectional feature pyramid network (BiFPN) for efficient multi-scale feature fusion, enabling robust detection of smoke plumes exhibiting significant scale variations. (3) Adoption of EIoU_Loss as the localization loss function, replacing CIoU_Loss to overcome ambiguous aspect ratio representation and enable faster convergence with more precise

bounding box regression. Additionally, systematic integration of negative samples—including wire ropes, cloud shadows, and background clutter—was implemented through negative sample mining, effectively suppressing false detections while maintaining high recall rates. Seven attention mechanisms (ECA, C3-ECA, SE, CBAM, GAM, CA, NAM) were systematically evaluated to identify optimal configuration. Models were trained with initial learning rate 0.01, batch size 8, image size 640×640 pixels, and 1000 epochs with early stopping patience of 100. Extensive comparative experiments demonstrated that the CBAM achieved superior performance among all evaluated variants. The CBAM-enhanced YOLOv5x model attained a mean average precision at IoU threshold 0.5 (mAP50) of 0.985 and mAP50-95 of 0.635, representing improvements of 5.2% and 1.6%, respectively, over the baseline YOLOv5x model (mAP50 0.933, mAP50-95 0.625). Precision reached 96.9% , while recall achieved 97.3%. The CBAM mechanism's ability to capture both channel relationships and spatial information proved particularly advantageous for smoke plume localization amid complex backgrounds. The BiFPN integration enabled effective multi-scale feature fusion, while EIoU_Loss improved bounding box regression accuracy and convergence speed. Negative sample mining substantially reduced false positives, successfully eliminating misclassifications of wire ropes, cloud shadows, and background clutter. To validate practical applicability, a 20-day field validation campaign at the Yangtze River Estuary monitored 5,224 cruising vessels during daytime hours (07:00-17:00 daily). The proposed algorithm successfully identified 155 black smoke emission events, corresponding to 2.96% of monitored vessels, demonstrating high consistency with concurrent manual monitoring.

This study presents an improved YOLOv5 model integrating spatial attention and a bidirectional feature pyramid network for the automatic identification of ship black smock in complex waterway environments. By embedding the attention mechanism into the feature network to enhance spatial semantic representation and leveraging a bidirectional feature pyramid to optimize multi-scale feature fusion, the method effectively improves the detection accuracy of semi-transparent, non-rigid black smock with blurred boundaries. Experimental results on a self-constructed multi-scenario ship black smock dataset demonstrate that the algorithm achieves good detection performance and generalization capability under diverse lighting, weather, and background conditions. Furthermore, the systematic negative sample mining strategy employed in this study proves effective in reducing the false positive rate during practical deployment. Nevertheless, the current method exhibits limitations when processing low-visibility scenes under extreme weather conditions and nighttime scenarios. Subsequent research will focus on model lightweighting and compression techniques, multi-modal sensor fusion strategies, and adaptive learning mechanisms tailored for emerging ship types and emission patterns, aiming to enhance the all-weather environmental adaptability of the detection system. This study provides a technical pathway for deploying unattended visual monitoring systems for ships in port emission control areas, contributing to the advancement of sustainable shipping and port air quality management.

Keywords: Ship; Black Smoke; YOLOv5; Attention Mechanism; Multi-Feature Fusion; Recognition

JUNON: Environmental Digital Twins in the Centre Val de Loire

Sébastien DUPRAZ, Véronique DAELE and Anouk FRONZES

Our society is currently undergoing radical change in a number of ways, affecting its environment (global warming, emerging pollutants), its practices (ecological and energy transition), and its perceptions and modes of communication (digital transition). In this context, transdisciplinarity takes on its full meaning and manages to consider, from different angles, common problems in order to provide more complete and integrated answers. It is with this in mind that the ARD JUNON program was conceived, with the aim of responding to the major regional challenges that lie ahead. At a time of digital and environmental transition, the Region and its partners have set their sights on creating a unique, innovative digital hub dedicated to the environment and the management of natural resources. The key element of this approach is the development of Digital Twins for Water, Soil and Air, using the latest developments in Artificial Intelligence. The Digital Twins enable real structures and processes to be reproduced throughout their evolution using Machine Learning approaches. The JUNON program also involves some twenty research teams and a total budget of over 12 million euro distributed across ten collaborative projects working together to create and exploit new digital twins, as well as establishing new public and commercial services to manage our natural resources more sustainably.

Street level spatiotemporal assessment of 6PPD-Q emissions and inhalation risks for humans and wild birds on Chongming Island

Anass Malah^{1*}, Xinke Wang¹, and Jianmin Chen^{1*}

¹Shanghai Key Laboratory of Atmospheric Particle Pollution and Prevention, Department of Environmental Science and Engineering, Institute of Atmospheric Sciences, Fudan University, Shanghai, China

anass_malah@fudan.edu.cn

Summary

Problem statement. In recent years, 6PPD-quinone (6PPD-Q) has gained global attention after being identified as the cause of massive die-offs in adult Coho salmon. Since then, several studies have reported the presence of 6PPD-Q in rivers, stormwater, and sediments and have highlighted its neurotoxic and cardiotoxic risks to humans. Yet, most research still focuses on aquatic pathways and runoff, while the air and soil pathways remain less explored. Moreover, existing assessments are mainly conducted at regional or national scales, even though near-road areas are where people walk, cycle, and where birds forage and rest. Consequently, there is a need for fine scale spatiotemporal assessments that link traffic activity, emission pressure, and exposure risks.

Context. Chongming Island represents a relevant case study to address this gap. Located at the mouth of the Yangtze River, the island combines expanding residential areas with nationally important wetlands. Also, its eastern part hosts an important bird nature reserve of more than 111 species of migratory water birds along the East Asian- Australasian Flyway, including several globally threatened species. Meanwhile, road infrastructure and population have progressively increased across the island, while industrial activity remains relatively limited compared with other districts of Shanghai, indicating that road traffic may represent the dominant local emission source.

Research objective. This study aims to develop a street-level spatiotemporal assessment of 6PPD-Q on Chongming Island and to evaluate inhalation risks for residents and wild birds.

Methodology. Traffic data from four representative months in 2024 were combined with tire-wear emission factors and estimates of 6PPD content and its transformation to 6PPD-Q. Moreover, three environmental pathways (air, water, and soil) were estimated using transfer coefficients from multimedia fate studies. Then, air pathway emissions were used in a Gaussian line-source model to estimate street-level concentrations and calculate inhalation doses for children, adults, and selected bird groups (shorebirds and ducks).

Results. Emissions show moderate seasonal variation, with passenger cars contributing about 68–70% of the total 6PPD-Q pressure, followed by heavy trucks (19–20%) and buses (about 11%). Approximately 59% of emissions are estimated to be emitted to soil, 27% to surface water, and 14% to the atmosphere. Also, results showed that spatial patterns align with major road corridors, where highway and major roads emerge as hotspots. Inhalation risks follow similar spatial patterns, with higher intake values for children than adults, while inhalation doses were smaller for shorebirds compared with ducks.

Conclusion. Although the analysis relies on only four representative months, which does not fully capture annual variability, it provides a first street-level perspective on 6PPD-Q emission pressure and inhalation exposure on Chongming Island. Besides, by linking traffic activity, road network structure, and exposure patterns, this study highlights how near-road environments shape local pollution risks for both humans and wildlife.

Accurate discrimination of endogenous and exogenous VOCs in exhaled breath and exposure risk assessment

Zhengen Cen¹, Xiang Li² and Shaocai Yu^{3*}

¹ School of Statistics and Data Science, Zhejiang Gongshang University, China

² Department of Environmental Science and Engineering, Fudan University, China

^{3*} School of Environmental Science and Engineering, Zhejiang Gongshang University, China, shaocaiyu@zju.edu.cn

Objective Exhaled breath contains a large number of trace volatile organic compounds (VOCs), which reflect both metabolic activity and environmental exposure. Exhaled VOCs mainly originate from two sources, including exogenous compounds inhaled from the environment and endogenous compounds released by host metabolism and microbial activity. After entering the body, exogenous VOCs can be distributed and accumulated in blood and tissues and can later be exhaled again. Accurate discrimination between endogenous and exogenous VOCs in breath is therefore essential for non-invasive exposure assessment and health monitoring.

Methods Breath samples from 271 volunteers and 101 ambient air samples were collected and analyzed qualitatively and quantitatively using TD-GC×GC-TOF MS/FID, from which 50 common exhaled VOCs were identified. A quantitative structure-property relationship (QSPR) model based on a genetic algorithm and artificial neural network (GA-ANN) was developed to predict the nonlinear relationship between chemical structure and the blood-air partition coefficient ($\lambda_{b:a}$) of VOCs. This model was further integrated with a physiologically based compartmental kinetic model to estimate the production rate, clearance rate, alveolar concentration, and tissue distribution of VOCs in the body. On this basis, a framework was established to distinguish endogenous from exogenous VOCs in exhaled breath, followed by health risk assessment of both internal and external exposure.

Results The results showed that the traditional alveolar gradient method and the breath tracker method had clear limitations in determining the origin of VOCs. After model correction, 32 of the 50 VOCs were classified as endogenous, 13 as exogenous, and 5 as mixed-source compounds. The overall non-carcinogenic risk of external exposure was low, but the risk increased with age and longer exposure duration. The overall risk associated with internal exposure was higher than that associated with external exposure and was closely related to metabolic status and physiological function. The limited dilution of aromatic hydrocarbons in adipose tissue suggests a more persistent health risk. Prolonged external exposure could also drive the transition of some VOCs from a sink to a source within the body, turning humans into secondary emitters of pollutants. The $\lambda_{b:a}$ was identified as an important factor governing this process.

Conclusion This study established a systematic approach for source discrimination and kinetic analysis of exhaled VOCs. The findings show that directly measured exhaled concentrations are easily affected by environmental background, whereas corrected alveolar concentrations better represent true endogenous signals. This approach improves the accuracy and interpretability of exposure assessment and provides reliable methodological support for the application of breathomics in pollution control, precision medicine, and environmental health.

Spontaneous Fe(III) Reduction at the Air–Water Interface Promotes Fenton OH Formation in Atmospheric Microdroplets

Peng CHENG¹, Christian George^{1*}

¹Universite Claude Bernard Lyon 1, CNRS, IRCELYON, UMR 5256, Villeurbanne, F-69100, France, peng.cheng@ircelyon.univ-lyon1.fr

Objective

In cloud water and aerosol droplets, the Fenton reaction and Fenton-like reactions are considered important sources of •OH, with efficiency highly dependent on the continuous supply of Fe(II) and the closed-loop Fe(III)/Fe(II) cycle. Notably, field observations often show that Fe(II) accounts for about 30–50% of the total soluble iron in the atmospheric liquid phase, suggesting the existence of an efficient Fe(II) regeneration pathway in oxidizing environments. However, traditional views are mostly based on bulk homogeneous systems, and it remains unclear whether there exists an "additional reduction channel" at the air-water interface of atmospheric microdroplets that can sustain Fe(II) under dark conditions, thereby amplifying the •OH yield of Fenton reactions. This study aims to clarify whether interface-induced spontaneous reduction of Fe(III) provides a key driving force for the generation of •OH in microdroplets, and to quantitatively assess its contribution to the

•OH budget.

Method

an aqueous microdroplet system containing Fe(III) was set up by spraying Fe(III) solution, and controlled residence time and environmental conditions to conduct online/offline measurements under dark conditions. By systematically modulating inorganic chemical parameters (salinity, anionic composition, pH/alkalinity, dissolved oxygen, etc.), the response of the Fe(III) reduction to Fe(II) conversion in the environment was investigated. Fe(II) was quantified using a selective complexation colorimetric method, while H₂O₂ was tracked using fluorescence-based method. Simultaneously, the effective formation of •OH was assessed using a •OH probe. Control experiments were combined to distinguish the contributions of the bulk phase and the interface. Reaction kinetic modeling was used to simulate the experimental data.

Results

The results showed that Fe(III) in the microdroplets underwent a significant spontaneous interfacial reduction reaction to generate Fe(II) under dark conditions, indicating that the air-water interface provides a unique reduction driving force and microenvironment compared to the bulk phase. Importantly, Fe(II) formation was strongly dependent on the atmospheric O₂ concentration: changes in O₂ concentration led to significant changes in Fe(II) yield and formation kinetics, highlighting the role of O₂ as a key regulator of the interfacial redox cycle. Fe(II) formation further affected the formation of H₂O₂/•OH. The main reason for this is likely that the spontaneous interfacial reduction continuously replenishes Fe(II) and reacts with H₂O₂ via a Fenton reaction (Eq.1).



Conclusion

This study proposes and verifies that interface-induced spontaneous reduction of Fe(III) is a crucial "a key driver" for the (Fenton-like) reaction in atmospheric microdroplets, sustaining the Fe(II) cycle under dark conditions and significantly influencing the formation and budget of •OH. This mechanism emphasizes that the microdroplet interface effect and its promoting effect on iron cycle closure must be explicitly considered when assessing the atmospheric liquid phase oxidation capacity, providing a new molecular mechanism basis for improving the parameterization of cloud water/aerosol liquid phase •OH source.

Effect of Surfactants on Spontaneous H₂O₂ Formation at Air-water Interface

Zhongyu GUO¹, Christian George^{1*}

¹Universite Claude Bernard Lyon 1, CNRS, IRCELYON, UMR 5256, Villeurbanne, F-69100, France, zhongyu.guo@ircelyon.univ-lyon1.fr

Objective

Hydrogen peroxide (H₂O₂) has been proved to form spontaneously at the air–water interface of atmospheric droplets, which can contribute to interfacial oxidative chemistry. Atmospheric droplets commonly contain both organic surfactants and inorganic salts, yet how these components jointly regulate interfacial H₂O₂ formation remains poorly constrained. This study aims to quantify the effects of surfactant concentration, salt concentration, and surfactant headgroup chemistry on spontaneous H₂O₂ production at the air–water interface.

Method

Aqueous microdroplets containing nonanoic acid (NA), a ubiquitous fatty-acid surfactant in atmospheric aerosols, were generated with systematically varied surfactant and salt concentrations. Interfacial H₂O₂ formation was quantified using a fluorescence-based H₂O₂ analyzer. To probe headgroup-dependent effects on H₂O₂ formation, NA was replaced with ionic surfactants featuring distinct headgroup chemistries. Ab initio molecular dynamics simulations were conducted to resolve surfactant organization at the molecular level and elucidate underlying mechanisms.

Results

Increasing NA concentration modestly suppresses H₂O₂ formation, consistent with hydroxyl radical scavenging at low surfactant concentrations. In contrast, salt addition to NA-containing droplets induces a pronounced nonmonotonic (“V-shaped”) dependence of H₂O₂ formation on salt concentration. Simulations show that the H₂O₂ minimum coincides with enhanced anchoring of NA headgroups, which densifies hydrophobic tails and reduces possible H₂O₂ precursors, namely interfacial free water, OH⁻, and O₂ accessibility. Ionic surfactants exhibit similar concentration-driven suppression, but salt responses diverge: a V-shaped dependence is observed only for headgroups capable of forming hydrogen bonds with interfacial water.

Conclusion

These results demonstrate that interfacial H₂O₂ formation is modulated by organic–inorganic combinations commonly found in atmospheric aerosols, exhibiting behaviors distinct from those observed in surfactant-only or salt-only systems. Surfactant headgroup chemistry, particularly hydrogen-bonding ability, controls salt-induced interfacial reorganization and associated oxidative outcomes. This work provides a mechanistic framework for understanding how organic–inorganic coupling, ubiquitous in atmospheric aerosols, regulates interfacial oxidative capacity in atmospheric droplets.

Emission Characteristics and Environmental Risks of White Oil and Liquid Paraffin Combustion

Wenjun Fang¹, Zhentao Wu¹, Shengsheng Lu¹, Lv Tian¹, Junyu Hu¹, Xiaobing Pang^{1*}

^{1*}College of Environment, Zhejiang University of Technology, China, pangxb@zjut.edu.cn

Despite China's progress in air pollution control, the illegal use of industrial by-products such as white oil (WO) and liquid paraffin (LP) as fuels in the catering and heating sectors has emerged as a poorly regulated emission source in China. Field surveys revealed that over 14000 tons of these fuels were sold in Shaoxing City alone within five months. This study investigates the combustion emission characteristics of WO and LP in comparison with liquefied petroleum gas (LPG), based on controlled combustion experiments.

Fuel samples were collected from over 10 restaurants in Zhejiang Province, and a controlled combustion system was designed to measure real-time emissions of CO, SO₂, CO₂, and PM_{2.5}. Results show that WO and LP combustion emits significantly higher pollutants than LPG. On a per-mass basis, CO emissions from LP (2.22 mg/g) and WO (1.82 mg/g) were approximately 110 and 90 times higher than those from LPG (0.02 mg/g), respectively. SO₂ emissions from LP (9.74 µg/g) and WO (8.72 µg/g) were approximately 30 and 25 times higher than those from LPG (0.34 µg/g). Real-time CO concentrations from LP and WO combustion ranged from 35–165 ppm and 30–145 ppm, frequently exceeding the WHO safety threshold, while the CO concentrations from LPG combustion remained below 2.6 ppm. In addition, significant oil residue accumulation was observed on burners after WO and LP combustion, providing indirect evidence of incomplete combustion and substantial volatile organic compound (VOCs) emissions, which may contribute to secondary PM_{2.5} and O₃ formation—warranting further investigation into their VOCs emission profiles. These findings highlight the substantial environmental and health risks posed by WO and LP combustion and provide scientific evidence supporting the need for regulatory updates to close current loopholes in fuel quality and air pollution control policies.

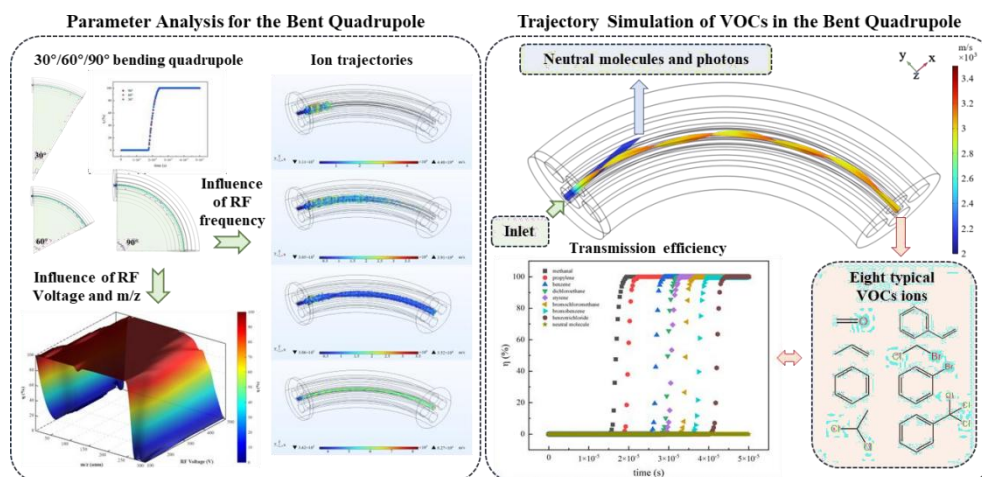
Bent Quadrupole for QTOF-MS Simulated by COMSOL Multiphysics: Ion Transmission Efficiency and Its Influencing Parameters

Junyu Hu¹, Xiaobing Pang^{1,*}, Wenjun Fang¹, Bin Jia², Gaosheng Zhao²

¹ College of Environment, Zhejiang University of Technology, China, 202005090307@zjut.edu.com

² School of Environmental and Chemical Engineering, Shanghai University, China

Abstract: The Quadrupole Time-of-Flight Mass Spectrometer (QTOF-MS) is a vital analytical tool for complex trace analysis, offering high resolution and sensitivity. However, its conventional straight ion path is severely limited by neutral noise interference and space charge effects, significantly compromising the signal-to-noise ratio and detection sensitivity. To address those limitations, this study introduces and systematically evaluates a bent quadrupole structure. Using COMSOL Multiphysics software, models with bending angles of 30°, 60°, and 90° were constructed to analyze their higher-order electric field distributions and ion confinement properties. The simulation results clearly demonstrate that the bent geometry completely eliminates interference from neutral molecules and photons, thereby thoroughly resolving the neutral noise issue. For charged ions, the transmission efficiency is negligibly affected by the bend angle but depends primarily on the applied radio frequency (RF) voltage, frequency, and the ion's mass-to-charge ratio (m/z). Simulations across parameter ranges of m/z 10-300, RF voltage 100-500 V, and RF frequency 1.0-4.0 MHz reveal that ions with lower m/z require higher RF frequencies and appropriate voltages for effective transmission, while heavier ions demand higher voltages at the same RF frequency. Further simulations of eight typical volatile organic compounds (VOCs) show that under optimized conditions, the transmission efficiencies for all VOCs approach nearly 100%. This research validates the effectiveness of the bent quadrupole in eliminating neutral noise while maintaining high ion transmission efficiency, providing an important theoretical foundation for optimizing QTOF-MS ion optics systems and enhancing trace analysis sensitivity in complex matrices.



Development of a Miniaturized TD–Trap Gas Chromatography System and Its Application in Atmospheric VOCs Monitoring

Haonan Xu¹, Xiaobing Pang^{1*}, Qiliang Su¹

¹College of Environment, Zhejiang University of Technology, China, pangxb@zjut.edu.cn

To meet the demand for highly sensitive and portable detection of volatile organic compounds (VOCs) in rapid on-site monitoring and emergency response scenarios, a miniaturized thermal desorption–cryogenic trapping (TD–Trap) gas chromatography system was developed in this study and applied to the online monitoring of atmospheric VOCs. The instrument integrates cryogenic trapping, thermal desorption, chromatographic separation, and a photoionization detector (PID) into a single platform, enabling automated enrichment, desorption, and detection of trace VOCs within an integrated system and achieving rapid analysis of trace-level compounds.

In terms of instrument design, the system simplifies the gas pathway by optimizing the gas flow and heat transfer configuration. A pump-driven direct sampling approach was adopted to replace the conventional split injector, effectively reducing system complexity. Additionally, a metal-wrapped chromatographic column was employed to enhance heat transfer efficiency, replacing the traditional air-heated column oven and significantly reducing the overall instrument size. The integrated TD–Trap cryogenic enrichment module operates over a temperature range of $-30\text{ }^{\circ}\text{C}$ to $360\text{ }^{\circ}\text{C}$, enabling efficient trapping and desorption of low-concentration VOCs and substantially improving detection sensitivity. The total weight of the instrument is only 10.5 kg, providing excellent portability and operational stability.

Performance evaluation demonstrated that the system can complete a full analytical cycle within ≤ 15 min and simultaneously separate and detect more than 20 typical VOC species. The limits of detection reach the ppt level, with detection limits for aromatic hydrocarbons as low as 500 ppt. The relative standard deviation (RSD) for repeated injections is $\leq 5\%$, indicating good repeatability, and excellent linearity was obtained with correlation coefficients (R^2) ≥ 0.99 . The optimized operating conditions were determined as follows: sampling time of 80 s, column temperature of $50\text{ }^{\circ}\text{C}$, and carrier gas flow rate of $60\text{ mL}\cdot\text{min}^{-1}$.

Field deployment in an industrial park demonstrated the capability of the instrument for continuous online monitoring of 17–20 VOC species. The system successfully captured the diurnal variation patterns and concentration trends of target compounds, indicating strong field applicability and environmental responsiveness. Overall, the developed miniaturized TD–Trap gas chromatography system combines high sensitivity, rapid analysis, and portability, providing an efficient and reliable technical approach for atmospheric VOC pollution monitoring and emergency detection.

Simulation of Global Cloud Water Acidity Based on the Adaptive Damped Newton's Method

Haoqi Wang¹, Weihao Li², Ruiqing Huo¹, Juncheng Wu¹, Yu Liu¹, Yinchang Feng¹, Xuan Wang³, Shaojie Song^{1*}

¹Key Laboratory of Urban Air Particulate Pollution Prevention and Control of Ministry of Ecology and Environment, College of Environmental Science and Engineering, Nankai University, Tianjin, 300350, China

²Department of Mathematical Sciences, Tsinghua University, Beijing, 100084, China ³School of Energy and Environment, City University of Hong Kong, Hong Kong SAR, 999077, China

Corresponding author: Shaojie Song (songs@nankai.edu.cn)

Cloud water pH is a critical parameter in atmospheric chemistry, regulating the phase partitioning of semivolatile species, the dissolution of trace metals, and the kinetic processes of aqueous-phase reactions, thereby influencing secondary aerosol formation and aerosol-cloud-radiation interactions. Current approaches for calculating cloud water acidity in widely-used atmospheric chemistry numerical models range from the early fixed-value assumption and analytical solutions (e.g., Cardano's Formula for cubic equations) to iterative techniques such as the bisection and standard Newton's methods. However, these existing approaches often struggle to maintain a balance between computational efficiency, numerical stability, and the ability to generalize across diverse and highly nonlinear chemical regimes. In this study, we developed an adaptive damped Newton's method by introducing a dynamic step-size damping factor. This method retains the rapid convergence feature of the standard Newton's method while ensuring robust global numerical stability. Our results demonstrate that the adaptive damped Newton's method effectively eliminates unphysical cloud pH overestimations and the subsequent overrating of sulfate production rates in regions enriched with alkaline dust and sea salt. This work offers a robust and scalable numerical framework that enhances the fidelity of cloud pH calculations across varying spatial scales—from mechanistic box models to global chemical transport models—thereby refining our understanding of pH-dependent atmospheric processes and the non-linear evolution of secondary aerosols.

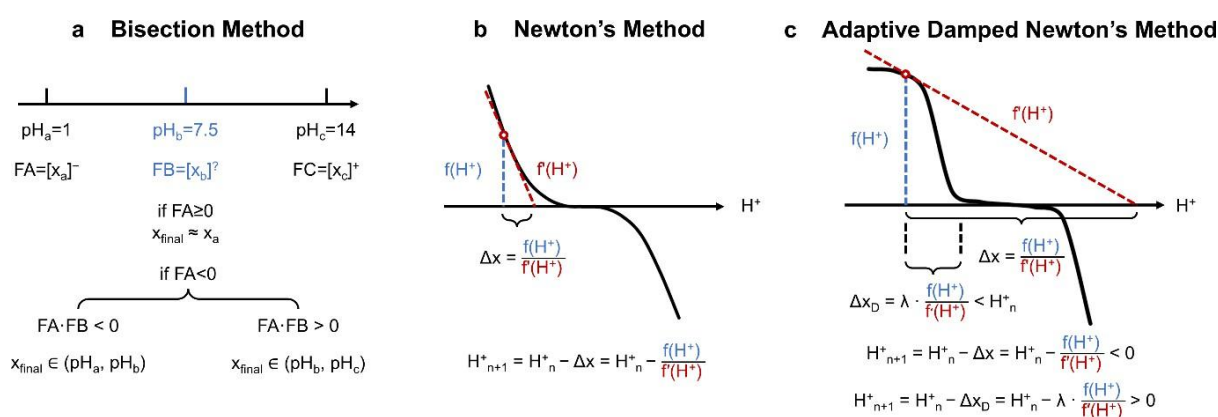


Figure. Schematic illustration of numerical root-finding algorithms: (a) bisection, (b) Newton's, and (c) adaptive damped Newton's methods.

Core-Shell Three- Way Catalysts for Natural Gas Vehicle Exhaust Aftertreatment

Run Pan^{1,3*}, AbdulAzeez Isa¹, Nicholas Musyoka¹, John L. Zhou¹, George Zheng Chen², Jun He^{1,3}

¹Department of Chemical and Environmental Engineering, University of Nottingham Ningbo China, Ningbo, China

²Department of Chemical and Environmental Engineering, University of Nottingham, UK
³Nottingham Ningbo China Beacons of Excellence Research and Innovation Institute, China, run.pan@nottingham.edu.cn

Effective exhaust aftertreatment for stoichiometric natural gas vehicles (NGVs) remains challenging because methane is difficult to activate under three-way catalytic conditions, while long-term performance is limited by hydrothermal aging and sulfur poisoning. In this work, Al₂O₃-supported core-shell catalysts were investigated for NGV three-way catalysis, with emphasis on the roles of Pd-CeO₂ interfacial structure and Pd/Pt composition in controlling catalytic activity, hydrothermal stability, and sulfur tolerance under representative exhaust conditions. A Pd@CeO₂/Al₂O₃ catalyst and a series of Pd-Pt@CeO₂/Al₂O₃ analogues were studied to establish structure-performance relationships relevant to NGV exhaust aftertreatment. Compared with the non-core-shell counterpart, Pd@CeO₂/Al₂O₃ showed markedly improved performance, with T₅₀ values of 336 °C for CH₄ and 397 °C for NO, and reductions of 113 and 177 °C in the corresponding T₉₀ values. After severe hydrothermal aging, the catalyst maintained high CH₄ and NO conversions during prolonged 100 h operation. Structural characterization and theoretical analysis indicate that the improved performance is associated with stronger Pd-CeO₂ interaction, enhanced redox properties, increased oxygen-vacancy concentration, and the formation of effective interfacial active sites.

To address sulfur-induced deactivation, Pd-only, Pt-only, and Pd-Pt bimetallic core-shell catalysts with different Pd/Pt ratios were further evaluated. Although Pd-rich catalysts showed higher intrinsic CH₄ oxidation activity in sulfur-free conditions, they deactivated severely upon SO₂ exposure. In contrast, Pt-rich catalysts maintained high CH₄ and NO conversions during both short-term poisoning tests and 100 h time-on-stream operation, with activity losses below 5%. Among them, Pd_{0.2}Pt_{0.8}@Ce/Al gave the best overall performance, combining high sulfur tolerance with improved hydrothermal stability relative to the Pt-only catalyst. Spectroscopic analyses indicate electron transfer from Pd to Pt, leading to changes in surface electronic structure and sulfur adsorption behavior. Whereas Pd-rich catalysts tended to form persistent sulfate species associated with irreversible deactivation, Pt-rich catalysts predominantly generated weaker and more reversible surface sulfur species. Limited Pd incorporation also suppressed particle growth in the Pt-rich catalyst after hydrothermal aging. These results show that combining a stable core-shell structure with appropriate Pd/Pt modulation is an effective strategy for improving the activity and durability of NGV three-way catalysts under practical operating conditions.

Effects of EWNS-Based Plasma Air Purifier on Passenger Health in Vehicle Cabins

Tingjie Daun¹, Mengdie Zheng¹, Xiaobing Pang^{1*}

¹Zhejiang University of Technology, China

211124270046@zjut.edu.cn

Abstract: Vehicle cabin air pollution poses potential health risks due to the accumulation of volatile organic compounds (VOCs), aldehydes, and particulate matter in enclosed environments. Engineered Water Nanostructures (EWNS)-based plasma air purifiers have been widely applied for in-vehicle air purification; however, their physiological health effects remain insufficiently understood.

This study investigated the health impacts of an EWNS-based plasma air purifier on passengers in a controlled in-vehicle environment. A total of 50 healthy university students were recruited and subjected to a randomized controlled experimental design. Participants remained in a sealed stationary vehicle for 180 minutes under simulated driving conditions. Serum malondialdehyde (MDA), an indicator of oxidative stress, and heart rate (HR), a marker of autonomic nervous system activity, were continuously monitored.

Results showed that in the control group (purifier off), 87.5% (14/16) of subjects exhibited an increase in serum MDA levels, indicating enhanced oxidative stress. In contrast, in the experimental group (purifier on), 88% (44/50) of subjects demonstrated a decrease in MDA, with a maximum reduction of 25.2%. Heart rate analysis revealed that the average HR during the intervention phase (76.8 bpm) was significantly lower than both pre-intervention (80.1 bpm) and post-intervention (78.1 bpm) levels.

These findings suggest that EWNS-based plasma air purifiers can effectively reduce oxidative stress and regulate autonomic responses in passengers exposed to in-cabin air pollution. The potential mechanisms may involve both pollutant removal (e.g., VOC oxidation and particle aggregation) and biological modulation via low-level reactive oxygen species (ROS), possibly inducing adaptive antioxidant responses.

Overall, this study provides experimental evidence supporting the beneficial physiological effects of EWNS technology in vehicle cabins and offers new insights into the health-oriented evaluation of in-vehicle air purification systems.

Dark Freezing of Iodide-containing Aqueous Droplets as a Potential Source of Reactive Iodine in Polar Marine Regions

Junwei Song^{1,4,*}, Linyu Gao¹, Matthieu Riva¹, D. James Donaldson^{2,3}, and Christian George^{1,*}

¹ Université Claude Bernard Lyon 1, CNRS, IRCELYON, UMR 5256, Villeurbanne, F-69100

² Department of Chemistry, University of Toronto, 80 George Street, Toronto, Ontario, Canada M5S 3H6

³ Department of Physical and Environmental Sciences, University of Toronto, Scarborough, 1265 Military Trail, Toronto, ON Canada M1C 1A4

⁴ Present address: School of Marine Sciences, Sun Yat-sen University, Zhuhai 519082, China, songjw27@mail.sysu.edu.cn

Reactive iodine species including molecular iodine (I_2) significantly influences atmospheric oxidation capacity, driving new particle formation and contributing to ozone depletion in polar marine regions. However, its formation mechanisms in these cold environments, particularly at night, remain poorly understood. Here, we present experimental evidence that the dark freezing of iodide-containing bulk solutions and droplets activates iodide (I^-) without any added catalysts or oxidants. This I^- activation is markedly enhanced during the freezing of iodide-containing droplets, leading to substantial I_2 production in both the gas and aqueous phases. The production follows a Langmuir-Hinshelwood formalism, indicating that a surface-mediated process at the frozen air–water interface. A detailed mechanistic investigation reveals that the production of I_2 is driven by the hydroxyl radicals ($OH\cdot$) and hydrogen peroxide (H_2O_2) formed at the frozen interface, which subsequently oxidize I^- . We attribute the formation of $OH\cdot$ and H_2O_2 to the high electric field possibly induced by the Workman–Reynolds freezing potential. This work identifies a previously unrecognized nighttime formation mechanism of I_2 in atmospheric snow and ice, having implications for atmospheric multiphase chemistry in polar marine environments.

Technological advances in solvents drive substantial reductions in VOC emissions and associated impacts from industrial coating use

Zhihao Zhang^{1,2}, Miaofei Wang², Di Wang^{2*}, Jingnan Hu^{2*}

¹ College of Environmental Science and Engineering, Tongji University, Shanghai, 200092, China

² Chinese Research Academy of Environmental Sciences, Beijing, 100012, China,

email: hujn@craes.org.cn; wangdi@craes.org.cn

Industrial solvent use is an important source of volatile organic compound (VOC) emissions and associated environmental and health risks. However, the source-specific drivers of VOC reduction remain poorly understood, limiting the development of more targeted control strategies. This study investigated VOC emission profiles from solvent-based and water-based paints used in industrial coating processes, with particular attention to the key drivers of emission changes and associated environmental and health implications.

Field experiments revealed a substantial decline in VOC concentrations from solvent-based paints in recent years. Compared with previous studies, fugitive emission concentrations (FC) and breathing zone concentrations (BZC) decreased by 99.0% and 99.8%, respectively. Water-based paints consistently exhibited relatively low VOC levels, with only limited further reductions observed. Enhanced ventilation further reduced VOC concentrations, especially for solvent-based paints, with a 57.9% decrease under high wind speed conditions. Reactivity analysis showed a marked decline in highly reactive VOC species from solvent-based paints, which was largely associated with advances in solvent formulation.

Overall, the results indicate that technological advances in solvents have played a critical role in reducing VOC emissions and their associated impacts from industrial solvent use. These findings provide source-specific, data-driven evidence for more targeted prevention and control of reactive and toxic VOC emissions in industrial coating sources.

Research on the Optical Properties of Secondary Organic Aerosols Based on Laboratory Simulations: Progress and Prospects

Shudan Wei^{1,2}, Junling Li^{2,*}, Yufei Song², Yushi Gong², Maofa Ge³, Hong Li², Wei Wei^{1,*}

¹Department of Environmental Science and Engineering, Beijing University of Technology, Beijing 100124, China

²State Key Laboratory of Environmental Criteria and Risk Assessment, Chinese Research Academy of Environmental Sciences, Beijing 100012, China

³State Key Laboratory for Structural Chemistry of Unstable and Stable Species, Beijing National Laboratory for Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100190, China

Correspondence: Wei Wei (weiwei@bjut.edu.cn), Junling Li (lijl@craes.org.cn)

Secondary organic aerosol (SOA) constitutes a critical component of atmospheric fine particulate matter (PM_{2.5}), primarily formed via atmospheric photochemical oxidation of volatile organic compounds (VOCs). Its optical properties and formation yields are pivotal parameters for quantifying aerosol radiative forcing and climate effects. Driven by advancements in experimental techniques and analytical methodologies, substantial progress has been made in characterizing the optical properties of SOA derived from diverse VOCs precursors. This paper systematically reviews the differences in optical characteristics between biogenic and anthropogenic SOA and their governing factors. We focus on how organic precursors and their mixtures, oxidant types and concentrations, multiphase reactions, inorganic pollutants, environmental parameters, and aging processes influence the dynamic evolution of SOA optical properties by altering their chemical composition, physical characteristics, and structure. Overall, SOA derived from biogenic VOCs (BVOCs) is predominantly scattering-dominant with weak absorption. Variations arise mainly from structural features (e.g., monoterpenes vs. sesquiterpenes) and divergent oxidation pathways involving OH radicals, ozone (O₃), and nitrate radicals (NO₃). In contrast, SOA from anthropogenic VOCs (AVOCs) — particularly aromatics and nitrogen-containing heterocycles — exhibits stronger ultraviolet and visible absorption due to their conjugated skeletons and sensitivity to nitration. Under NO_x-rich conditions, these precursors readily form brown carbon (BrC) chromophores, such as nitro-aromatic compounds. The final optical activity and radiative effects are jointly determined by oligomers, organic acids, and nitrogen- or sulfur-containing species formed during multi-generation oxidation. SOA optical properties are not dictated by a single factor but are coupled and regulated by environmental conditions including NO_x levels, relative humidity (RH), temperature, inorganic

pollutants, and seed particles. NO_x modulates RO₂ radical reaction pathways, switching between the formation of "strongly absorbing nitro-products" and "weakly absorbing highly oxygenated molecules (HOMs)/peroxides." Humidity and particle acidity influence multiphase condensation and oligomerization, thereby altering chromophore formation and photobleaching rates. Furthermore, temperature and other environmental factors modulate BVOC emissions and aging processes. Meanwhile, mixed systems of biogenic and anthropogenic precursors exhibit significant non-linear effects, characterized by three co-existing mechanisms: dilution, synergy, and pollution enhancement. Coupled with gas-phase and aqueous-phase aging and phase state evolution, these factors render SOA optical parameters highly heterogeneous across spatial and temporal scales, subsequently impacting visibility, radiative forcing, cloud condensation nuclei (CCN) activity, and potential health effects. By integrating data from laboratory studies, this review aims to elucidate the intrinsic linkages between SOA optical properties and their chemical composition. These insights provide a scientific basis for the precise assessment of aerosol radiative forcing in climate models and for the development of targeted regional air quality control strategies.

Financial support: National Natural Science Foundation of China (42405104) and the National Key Research and Development Program of China (2023YFC3706102, 2024YFC3712902).

Biogenic Oxygenated VOCs: Dynamics and Responses under Global Change

Xiaoshuai Gao^{1,2}, Junling Li², Qi Jiang², Haijie Zhang², Rui Gao², Jinjuan Li^{1*}, Hong Li^{2*}

^{1*}College of Resources and Environmental Engineering, Guizhou University, China, summy_lee@163.com

^{2*}State Key Laboratory of Environmental Criteria and Risk Assessment, Chinese Research Academy of Environmental Sciences, China, lihong@craes.org.cn

Biogenic volatile organic compounds (BVOCs) are crucial to ecosystems and atmospheric environments. Although significant progress has been made in studying major components of BVOCs such as isoprene and terpenes, reviews focusing primarily on another major component, oxygenated volatile organic compounds (OVOCs), which are recognized for their significant atmospheric chemical reactivity, remain lacking. This paper reviews the direct atmospheric emission sources, emission characteristics, and influencing factors of biogenic-oxygenated volatile organic compounds (bOVOCs), with a focus on exploring the tropospheric chemical processes of bOVOCs, including their secondary formation and impacts on ozone (O₃) and secondary organic aerosols (SOA). Findings summarize that bOVOCs mainly originate from plant-covered areas such as forests, farmlands, and urban regions, as well as marine microorganisms. These emissions exhibit multi-scale heterogeneity, influenced by environmental factors and plant species. Forested areas emit a greater quantity and diversity of species, with some species showing distinct vertical distribution characteristics due to their chemical reactivity. Farmlands and marine environments primarily emit methanol, while urban areas exhibit varied emissions depending on different ornamental tree species. Increased light intensity, temperature, and leaf number are generally considered reasons for higher concentrations of bOVOCs during summer and daytime. Drought stress increases green leaf volatiles (GLVs) but affects other bOVOCs differently depending on plant species. Herbivory induces emissions of C₅ and C₆ unsaturated alcohols and aldehydes, floral oxygenated compounds, and GLVs. Mature plants typically emit the most abundant bOVOCs, with some plants exhibiting senescence-induced effects. O₃ differentially affects marine bOVOC species by influencing the metabolism of total marine plants or bacteria, increasing methanol emissions while reducing acetaldehyde flux; however, in terrestrial systems, atmospheric chemical reactions are usually predominant. The ozonolysis of unsaturated bOVOCs and other unsaturated BVOCs forms ozonide Criegee intermediates (CIs) and bOVOCs. CIs further decompose or isomerize to serve as direct sources of other bOVOCs, which then react with NH₃ to influence the formation of

nitrogen-containing organic compounds in cloud processes. Atmospheric BVOCs (e.g., isoprene, α -pinene, β -pinene, Δ -3-carene, β -caryophyllene, monoterpenes) undergo oxidation by OH and NO₃ radicals to produce highly oxidized molecules (HOMs). These HOMs decompose via intramolecular hydrogen transfer (H-shift), photolysis, or further oxidation to form alcohol, acid, and carbonyl bOVOCs. Due to their high gas-particle partitioning coefficients, HOMs and bOVOCs significantly impact SOA. This review emphasizes the complexity of biogenic OVOC sources and their significant atmospheric chemical impacts under extreme events, providing a more comprehensive perspective for understanding BVOC sources and their roles in atmospheric environmental chemistry.

Financial support: Jing-Jin-Ji Regional Integrated Environmental Improvement National Science Technology Major Project (Grant No.2025ZD1201705)