VIRTUAL WORKSHOP

# INNOVATION IN ATMOSPHERIC MEASUREMENT TECHNIQUES

## 27 JUNE, 2024

## BOOK OF ABSTRACTS

EU Green Week
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#InnovAtmo24

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CARE-C
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ICOS Integrated Carbon Observation System

IAGOS
IN-SERVICE AIRCRAFT FOR A GLOBAL OBSERVING SYSTEM

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# Welcome to the 4th Annual Innovation in Atmospheric Measurement Techniques Workshop

Dear Colleagues,
Dear Friends,

It is with great pleasure that we welcome you for a fourth consecutive year to the Innovation in Atmospheric Measurement Techniques Workshop.

Firstly, we would like to thank all of you for your participation at the workshop. In this book of abstracts, we are delighted to share with you an exciting program, reporting the main innovations in the field of atmospheric sciences, with the participation of 20 presentations discussing recent relevant advances in the field.

All this has been possible thanks to your contribution.

We do hope that you enjoy your attendance at the Workshop!

*The Hosts & Organizers*

# SCIENTIFIC PROGRAMME COMMITTEE

Sciare Jean, CARE-C, The Cyprus Institute, Cyprus

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# AGENDA

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|---|---|
| **13:00 - Opening Session** | |
| **Welcome & Introduction to the Workshop** | |
| Workshop introduction and opening | **J. Sciare**<br>The Cyprus Institute |
| **13:10 – VOCs** (Chair: Prof Stéphane Sauvage) | |
| Temporal Variability of High-Resolution VOCs Measurements in Athens, Greece | Faidra-Aikaterini Kozonaki<br>Univ. of Crete |
| MION2 Chemical Ionization and Orbitrap-Based MS Synergy: Expanding the Horizon of Trace Species Detection with Fast Polarity Switching | Anna Franck<br>Karsa |
| Newly Designed Ion Mobility Mass Spectrometer Coupled with Chemical Ionization for Real-Time Monitoring of Isomer Populations | Matthieu Riva<br>CNRS/TOFWERK |
| A Compact GC-PTR-TOF for Monitoring Volatile Organic Compounds | Megan Claflin<br>Aerodyne Research |
| Ambient Air Quality Monitoring via Mobile Platforms and PFAs Detection | Spiro Jorga<br>Tofwerk |
| **14: 00 Greenhouse Gases Emissions & Sinks** (Dr Leonard Rivier) | |
| A Novel Unmanned Aerial System - Greenhouse Gas Tracker for Accurate Leak Detection and Emission Quantification of Methane | R.Papaconstantinou<br>The Cyprus Institute |
| Mobile Monitoring Platforms for Methane Source Identification | Veronika Pospisilova<br>Tofwerk |
| A New All-In-One Instrument for Air-Quality and Greenhouse-Gas Monitoring | Jonas Bruckhuisen<br>Miro Analytical |
| Application of Deep Learning Methods for the Creation of the First National Tree Airborne Inventory of Cyprus and the Estimation of Carbon Stock | Anna Zenonos<br>The Cyprus Institute |
| **14:40 - Aerosols And Clouds** (Chair:Prof Nikos Mihalopoulos) | |
| Condensation Particle Counter for Extended Unsupervised Use | Joonas Purén<br>Airmodus Oy |
| Twst Cloud Properties Sensor | Zachary Payne<br>Aerodyne Research Inc |
| Deducing the Composition of Aerosol and Cloud Particles with the Autofluorescence Nephelometer (AFN) | Darrel Baumgardner<br>DMT |
| The Portable Ice Nucleation Experiment Pine: A New Online Instrument for Automated Long-Term Field Observations and Laboratory Studies of Ice-Nucleating Particles | Benjamin Murray<br>University of Leeds |
| Traceable Calibration for In-Situ Aerosol Absorption Instrumentation | Griša Močnik<br>Haze Instruments d.o.o. |
| **15:30** | **Coffee Break** |
| **15: 50 - Aerosol Optical Properties** (Chair: Dr Ulrich Bundke) | |
| 3d Plume Mapping with UAVs And Lidar Technology | Maria Kezoudi<br>The Cyprus Institute |
| Aerosol Retrievals and Pm2.5 Concentration Estimations from Nephelometers Using Grasp Algorithm and Machine Learning Method | Chong Li<br>GRASP SAS |
| **16:10 - Air Quality Parameters** (Chair: Prof Jean Sciare) | |

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|---|---|
| Cavity Attenuated Phase Shift (CAPS) Instrument For Simultaneous Measurement Of $NO_x$ And $NO_2$ | Zachary Payne<br>Aerodyne Research Inc |
| Particulate Matter Concentration Evaluation of Vaisala's AQT560 Against Multiple Equivalence Reference Methods | Kimmo Neitola<br>Vaisala |
| Improving Low-Cost Optical Sensors Accuracy Using Machine Learning | Marianna Chaves<br>Federal University of Paraná |
| Sensor-Based Air Quality Systems for Accurate Emissions Monitoring | Irene Lara<br>Kunak Technologies |
| **17:00 -** | **End of Workshop** |

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**Temporal Variability of High-Resolution VOCs Measurements in Athens, Greece**

**Faidra-Aikaterini Kozonaki**
University of Crete

Volatile Organic Compounds (VOCs), emitted from both natural and anthropogenic sources, play an important role in atmospheric chemistry. Continuous monitoring in urban and rural areas is essential for a thorough understanding of their levels and source apportionment. This study presents VOCs measurements conducted from July 2023 to January 2024 at the Thissio Air Monitoring Station of the National Observatory in Athens, Greece, by means of a PTR-Q-MS 500 system. Emphasis was given to BTEX, isoprene, monoterpenes, and acetonitrile due to their importance in atmospheric processes and their role as tracers of specific emission processes. Distinct day-to-day variability was observed linked with the impact of the air masses reaching the area. During August (background period with limited local traffic impact due to summer holidays) mean levels of 0.27±0.18, 0.35±0.05, 0.50±0.21, 0.25±0.13 ppb were observed for benzene, acetonitrile, isoprene and monoterpenes respectively. A notable increase of almost 100%, in acetonitrile, and 50% in isoprene and benzene levels was observed during the impact of a fire plume, that occurred in August 2023 in the Parnitha mountain W-NW of Athens. Enhancement was also observed during the Christmas and New Year period, which is characterized by domestic wood-burning processes.

The mean period levels of benzene reached almost 1 ppb, whereas duplication of monoterpenes levels compared to the summer-time fire period was observed, suggesting thus different emission profiles between the two combustion processes. For example, acetonitrile depicted a maximum concentration of higher than 1 ppb and approximately 3 ppb on an hourly basis, during the winter holidays period compared with the forest fire period respectively, whereas benzene and isoprene followed the opposite trend. In both cases strong correlation was observed between acetonitrile and the wood-burning fraction of Black Carbon ($R2 > 0.8$ for the winter wb), serving as an indicator of the dominant emission sources.

**Authors**

Kozonaki, F.A., Liakakou, E., Kalkavouras, P., Desservetaz, M., Kaltsonoudis, C., Pandis, S. N., Mihalopoulos, N.

# MION2 Chemical Ionization and Orbitrap-Based MS Synergy: Expanding the Horizon of Trace Species Detection with Fast Polarity Switching

**Anna Franck**
Karsa

Chemical Ionization Mass Spectrometry is a powerful, soft and highly selective technique for the rapid and sensitive detection of reactive trace gases relevant to atmospheric chemistry, secondary organic aerosol formation, and air quality. The comprehensive detection and quantification of different species with different volatilities, degree of oxygenation, and functional groups requires using more than one ion scheme. To facilitate multiple ion schemes with only one mass spectrometer, the Multi-Scheme Chemical Ionization Inlet (MION2) has been developed (Rissanen et al.,2019, He et al.,2023).

An Orbitrap Fourier transform mass spectrometer offers high-resolution, accurate-mass performance and polarity switching. The MION2 and the Orbitrap set up provides a unique advantage of polarity switching within seconds. This novel feature extends the possibilities of chemical ionization and also opens new ways for studying the temporal evolution of reactive organic species, as demonstrated in the example of alpha-pinene ozonolysis (Cai et al., 2024).

A recent modelling study by Finkenzeller et al. (2024) using computational fluid dynamics 3D physico-chemical models presented the reagent ion and gas trajectories in the MION2, evaluated its efficiency in ion production and delivery to the mass spectrometer, and showed the difference with the Eisele-type inlet. The highlighted results from the study will also be presented at the workshop.

In conclusion, the MION2's unique ability to rapidly switch between reagent ion chemistries and polarities, combined with its excellent detection limits, significantly expands the analytical capabilities of CIMS instruments. This advancement allows for the comprehensive analysis of a broader range of compounds, making it a crucial tool in atmospheric chemistry, secondary organic aerosol formation studies, and air quality monitoring.

**Authors**

Franck, A.[1], Cai, R.[2,3], Finkenzeller, H. [1,3], Jost, HJ[1], Mikkilä Jyri[1], Shcherbinin, A[1].

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2. Shanghai Key Laboratory of Atmospheric Particle Pollution and Prevention (LAP3), Department of Environmental Science & Engineering, Fudan University, China
3. Institute for Atmospheric and Earth System Research (INAR), University of Helsinki, Finland

**Newly Designed Ion Mobility Mass Spectrometer Coupled with Chemical Ionization for Real-Time Monitoring of Isomer Populations**

**Matthieu Riva**
CNRS/TOFWERK

Ion mobility spectrometry (IMS) using Structures for Lossless Ion Manipulations (SLIM) is an emerging powerful tool for rapid isomer separations. This technology offers high mobility resolution due to prolonged ion mobility path lengths achieved on a small form factor separation device. We interfaced SLIM IMS separation with a chemical ionization (CI) source, which allows one to sample from the gas- and particle-phase directly. As such, one can monitor dynamic isomer populations in ambient air in real time without prior sample preparation. This technology opens the door to new possibilities in atmospheric chemistry where isomer distribution is expected to play a key role in gas phase processes and in the formation of organic aerosols.

The CI-IMS-TOF instrument built by TOFWERK produces ions via a two-step chemical ionization process, which involves 1) producing reagent ions and 2) ionizing neutral analyte molecules via the reagent ions through either charge transfer or adduct formation. Once generated, these secondary ions travel into the SLIM IMS region, where a series of DC- and AC-electrodes on printed circuit boards create a traveling wave driving force. As the ions travel through the helium buffer gas, they separate based on their rotationally averaged collision cross-sections.

In the present work, various experiments were performed using an aerosol flow tube reactor and an atmospheric simulation chamber to recreate atmospheric conditions. Gas-phase oxidation of isoprene was used to explore the capabilities of the CI-IMS-TOF under atmospheric relevant conditions. Firstly, the most important oxidation products produced from the OH-oxidation of isoprene were analyzed, including methacrolein, methyl vinyl ketone, isoprene epoxy diols (IEPOX), isoprene hydroxy hydroperoxide (1,2 and 4,3-ISOPOOH), and other C5H10O3 reactive uptake products as a single component or as a mixture to evaluate the capabilities of the CI-IMS-TOF at resolving the different isomers. Secondly, the reactive uptake of IEPOX onto acidic particles and OH-initiated oxidation (low and high NO regimes) of isoprene were studied to characterize the dynamic of the isomers generated within the simulation chamber under various environmental conditions. Results will be presented to demonstrate the capabilities of the newly developed CI-IMS-TOF at resolving isomers in real-time.

**Authors**

M.Riva, S. Gerber, S. Graf, V. Yatsyna, M.Z. Kamrath, F. Lopez-Hilfiker

# A Compact GC-PTR-TOF for Monitoring Volatile Organic Compounds

**Megan Claflin**
Aerodyne Research

Long-term, routine monitoring of volatile organic compounds (VOCs) is needed to provide insight into emission sources and patterns, oxidation processes including photochemistry and radical cycling, and the formation of tropospheric ozone and secondary organic aerosol. However, instrumentation that is able to provide high quality data both in terms of fast (e.g. 1 s) temporal resolution and molecular speciation has historically been cost-prohibitive and requires advanced users for field deployment, operation, and data analysis.

Here, we present a new instrument package for the online, long-term detection of VOCs which is an in situ gas chromatograph (GC) system equipped with an integrated thermal desorption system coupled to a compact, low-cost proton-transfer reaction time-of-flight mass spectrometer (PTR TOF-MS). The entire instrument is contained in a 72 x 80 x 65 cm footprint, weighs < 100 kg, and consumes < 600 W for typical operation. Coupling the GC system with the PTR-TOF allows the automated acquisition of both direct, high-time resolution data and molecular speciation data for isomer separation and improved quantification of both the GC-PTR and direct-PTR data.

We will present a description of the instrument, the automated acquisition and analysis software, and show ambient data that demonstrates the value of continuous VOC detection with regular molecular speciation. The automated acquisition and data analysis software developed for this instrument make the operation and data analysis both robust and efficient, requiring less labor to produce accurate concentration data for a wide suite of VOCs. This compact, low cost, easy to operate system makes it feasible to deploy this technology in many locations for greater spatial resolution to acquire coinciding datasets to elucidate local, regional, and global VOC trends.

**Authors**

Megan Claflin, Brian Lerner, Harald Stark, Donna Sueper, Gabriel Isaacman-VanWertz, Felipe Lopez-Hilfiker, Manjula Canagaratna, Douglas Worsnop, John Jayne

**Ambient Air Quality Monitoring via Mobile Platforms and PFAs Detection**

**Spiro Jorga**
Tofwerk

Volatile organic and inorganic compounds (VOCs and VICs) significantly impact air quality, with high levels posing risks to health and the environment. Accurate, real-time measurement of these compounds' concentration and chemical composition is crucial for effective air quality management. TOFWERK's Vocus chemical ionization time-of-flight mass spectrometers (CI-TOF-MS) are designed for the rapid analysis of VOCs and VICs with unparalleled sensitivity, detecting levels as low as sub-parts-per-trillion, making them indispensable for air quality monitoring. In this presentation, we will discuss the application of TOFWERK's Vocus CI-TOF instruments for (1) mobile air quality and fenceline monitoring and (2) the detection of per- and polyfluoroalkyl substances (PFAS).

First, we illustrate the use of two Vocus CI-TOF instruments in a mobile laboratory to assess emissions and monitor air quality near three landfills. Mobile laboratories allow for the direct analysis of chemical emissions and their spatial distribution using rapid, sensitive instrumentation. The rapid and sensitive capabilities of the Vocus instruments, specifically the Vocus Eiger and Vocus B, were utilized in this study. The Vocus Eiger employs a proton transfer reaction (PTR) reactor, while the Vocus B uses an atmospheric pressure interface (AIM) reactor allowing the identification of numerous landfill-emitted compounds. These include various hydrocarbons, oxygenated molecules, sulfonated compounds, ammonia, acetic acid, lactic acid, and chlorofluorocarbons. Our custom-developed software platform integrated data from the mass spectrometers with readings from a Picarro H2S and CH4 analyzer and a weather station, enabling precise source attribution.

Second, we demonstrate the use of chemical ionization mass spectrometry to detect and quantify PFAS at extremely low concentrations in gas-phase samples. PFAS, a group of man-made chemicals extensively used in consumer products and manufacturing processes, are persistent in the environment and have been associated with various health risks. These compounds, often referred to as "forever chemicals," accumulate in the environment and remain a significant concern for both public health and ecological systems. One of the major challenges in PFAS research is the lack of efficient detection methods for direct, real-time measurement in the air. TOFWERK's Vocus CI-TOF-MS technology addresses this challenge by enabling the detection of PFAS at ultra-trace levels, down to parts-per-quadrillion (ppq). Our CI-TOF-MS methodology detects PFAS at parts-per-quadrillion levels, supported by calibration data and examples of PFAS detection in various sample headspaces. This real-time PFAS detection enables accurate emission tracking and improved environmental protection measures.

**Authors**

Jorga, Spiro, Pospisilova, Veronika, Abou-Ghanem, Maya

# A Novel Unmanned Aerial System - Greenhouse Gas Tracker for Accurate Leak Detection and Emission Quantification of Methane

**Roubina Papaconstantinou**
The Cyprus Institute

Emission Quantification of Methane

The rise in atmospheric abundance of greenhouse gas (GHG) emissions, specifically carbon dioxide (CO2) and methane (CH4) is of particular concern in the Mediterranean. As the second most significant anthropogenic GHG after CO2, CH4 holds a global warming potential 28 times greater than CO2 over 100 years, emphasising the urgency to address its emissions. Although policies on reducing the GHG emissions heavily rely on accurate emission estimation through atmospheric measurements, current estimates are mainly based on inventory studies. CH4 measuring methods have significantly advanced over the past two decades, ranging from ground-based, to mobile approaches and remote-sensing methods using aircraft, unmanned aerial systems (UAS) and satellites. Owing to their ease of mobility, UAS enable the quantification of point and facility-scale sources, where conventional methods may fall short (Liu et al., AMT 2024).

The Unmanned Systems Research Laboratory (USRL) of the Cyprus Institute has developed a new UAS-GHG system exploiting an ABB LGR GLA131 and 3D wind measurements on-board a “heavy-lifter” octocopter platform with advanced autopilot capabilities. The comprehensive system of state-of-the-art sensors has been tested and validated on its ability to detect a CH4 source during controlled-release experiments. The on-board gas analyser successfully detected the tracer gas at low release rates (0.15 kg/h) below a 5-meter height above the emission point.

Our investigation extended to quantifying CH4 emissions from a cattle farm in Orounda, Cyprus, utilizing the same UAS-GHG system. Data collected mapped in detail the CH4 plume dispersion downwind the farm with concentration variations during multiple flight sessions. These findings significantly contribute to understanding the dispersion of CH4 emissions, improving quantification methodologies. This work will ultimately contribute to inform strategies to reduce site-level methane emissions and mitigate climate change.

**Authors**
Roubina Papaconstantinou, Jean-Daniel Paris, Maria Kezoudi, Pierre-Yves Quehe, Christos Keleshis, Jean Sciare

**Mobile Monitoring Platforms for Methane Source Identification**

**Veronika Pospisilova**
Tofwerk

Methane emissions represent a significant environmental concern, necessitating advanced methodologies for precise identification and mitigation. Our study introduces a novel approach applying chemical ionization and source apportionment techniques within mobile monitoring platforms to enhance methane source identification accuracy.

Through collaborative efforts with the Institute of Arctic and Alpine Research (INSTAAR) at CU Boulder and the University of Maryland, funded by the Colorado Department of Public Health and Environment, we deployed Vocus Elf, compact and portable mass spectrometer for airborne measurements as part of a project that aims to identify oil and gas emissions in the Colorado Front Range using a small aircraft research platform.

Our methodology integrates methane measurements from a Picarro analyzer with TOFWERK's Vocus Elf which is capable of real-time analysis of volatile organic compounds (VOCs) with ultra-low limits of detection. Airborne data obtained from Vocus Elf PTR-MS revealed correlations between enhancements in methane concentration and VOC levels, enabling precise identification of methane emission sources.

Furthermore, we showcase the deployment of TOFWERK's Vocus Eiger and Vocus B chemical ionization mass spectrometers on a mobile laboratory van, equipped for investigating landfill emissions. This mobile platform, developed in collaboration with the Colorado Department of Public Health and Environment, enables real-time analysis of VOCs and volatile inorganic compounds (VICs), facilitating the attribution of methane emissions to specific sources.

Our findings demonstrate the effectiveness of mobile VOC and VIC measurements in identifying methane sources across diverse industries, including oil and gas operations, landfills, and agricultural practices. This adaptive methodology holds promise for addressing a wide range of environmental challenges beyond methane, including odor detection, urban pollution characterization, and emission source differentiation.

Our approach to methane source identification offers a valuable tool for environmental protection efforts, enabling informed decision-making and responsive strategies for regulation and mitigation.

**Authors**

Maya Abou-Ghanem, Abigail Koss, Omar El Hajj, and Veronika Pospisilova

**A New All-In-One Instrument for Air-Quality and Greenhouse-Gas Monitoring**

**Jonas Bruckhuisen**
Miro Analytical

Air pollution and greenhouse gas emissions are two closely linked problems. They can be attributed to a variety of sources, such as transportation and buildings, waste management and agricultural production, natural events such as forest fires and many others. Monitoring air pollutants and GHG simultaneously with high selectivity and sensitivity enables to detect and evaluate their sources and sinks and to discover the links between them.

Until recently, however, the monitoring of complex gas mixtures was usually either limited to a picture of only few gases or required the combination of several devices based on different techniques making these measurements complex and expensive. MIRO Analytical developed a novel multicompound gas analyzer (MGA) that can monitor simultaneously with high precision up to 10 greenhouse gases ($CO_2$, $N_2O$, $H_2O$ and $CH_4$), air pollutants (CO, NO, $NO_2$, $O_3$, $SO_2$ and $NH_3$) and other atmospheric trace gases (OCS, HONO, $CH_2O$) at sub ppb levels.

We provide robust, reliable and compact laser absorption spectrometer combining several mid-IR lasers (QCLs). With a time-resolution of up to 10Hz, an outstanding precision, selectivity and accuracy and an automatic water-vapor correction, it is therefore well-suited for eddy covariance investigations of both reactive species and GHG, air quality monitoring and mobile measurements.

In our contribution, we will introduce the measurement technique and will demonstrate application examples of this all-in-one atmospheric gas monitor. The system will be compared to alternative devices in parallel measurements and results of long-term observations at atmospheric measurement stations and shorter campaigns will be presented.

**Authors**

Morten Hundt, Jonas Bruckhuisen, Marco Brunner & Oleg Aseev

# Application of Deep Learning Methods for the Creation of the First National Tree Airborne Inventory of Cyprus and the Estimation of Carbon Stock

**Anna Zenonos**
The Cyprus Institute

A neural network model that has been developed by researchers in Denmark has been applied to create the first national airborne tree inventory of Cyprus. This model employs state-of-the-art methods and advanced techniques for image processing. Specifically, high-resolution orthophotos are analyzed to delineate tree crown areas and count the number of trees within each reference area. The model achieves high accuracy and produces tree crown maps that offer valuable information for the amount of tree covered area in the country and other parameters that will be further discussed during the presentation. Moreover, the tree crown area, the location and the tree height that will be estimated by using another form of data, will be eventually used for the estimation of carbon emissions and carbon stock. Trees are one of our main defenses against the climate crisis and a crucial tool for reducing carbon emissions. This presentation will explore the methodology, accuracy, and implications of the tree inventory, providing a comprehensive overview of its potential applications in environmental management and policy.

**Authors**

Anna Zenonos

# Condensation Particle Counter for Extended Unsupervised Use

**Joonas Purén**
Airmodus Oy

## Introduction

Here we present results of the Airmodus A20 and A30 condensation particle counters (CPC) using a Propylene glycol (PG) as the working fluid. PG is an odourless, non-harmful fluid, with low flammability suitable also for indoor air measurements (ECHA, 2023). A CPC using PG can run more than 10 times longer than a butanol CPC with a given amount of working fluid.

## Results

PG has been used in particle counters e.g. in Model 3851 manufactured by Kanomax and been tested by Iida et al. (2009) as a "booster" for activating sub-2 nm particles but has not seen extensive use in the field in CPCs. PG has considerably lover vapor pressure compared to butanol (10.6 Pa vs. 639.6 Pa @ 20 ºC), resulting in lower PG consumption, enabling the longer operation.

Compositional effects on particle activation are a well-known property of all CPCs for all working fluids. Water, Butanol and DEG for instance activate organics, silver, and sodium chloride, respectively, more poorly than ammonium sulphate (Wlasits et al., 2020). PG, likewise, has a compositional effect, but based on a recent study appears to be smaller than for butanol CPC's (Wlasits et al., 2024, preprint).

## Conclusions

We have presented an CPC with an alternative working fluid, without the drawbacks of butanol including toxicity, strong odour, high consumption, and flammability. The change of the working fluid has not affected the cut-off or the concentration response of the CPC according to our preliminary results. PG would appear suitable for long-term monitoring stations, and remote location where high butanol consumption can be problematic, as well as for indoor air studies.

## References

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Iida et al., (2009), Aerosol Science and Technology,43:1,81—96

Wlasits et al., (2020), Atmos. Meas. Tech.,13,3787–3798.

Wlasits et al., (2024). Aerosol Research Discuss. [preprint], https://doi.org/10.5194/ar-2024-2, in review

**Authors**

J. Purén (né Enroth), J. Vanhanen, A. Pajunoja

**Twst Cloud Properties Sensor**

**Zachary Payne**
Aerodyne Research Inc

Clouds play a major role in the Earth's radiation budget. Improving our ability to model Earth's climate requires a better understanding of clouds, cloud processes, cloud-aerosol interactions, and associated feedback mechanisms. Ground-based shortwave (SW) spectral measurements, including ultraviolet, visible, and near-infrared spectral ranges that make up the solar spectrum, provide important observations of clouds and aerosols that provide insights into climate-related processes and help constrain climate models.

The Aerodyne TWST Cloud Properties Sensor measures absolute spectral radiances from 400-1665 nm and provides derived Cloud Optical Depth (COD), droplet effective radius (Reff), and cloud thermodynamic phase with a rapid time response (1 second) for a narrow field of view (1/2 degree zenith). This low-cost, autonomous instrument was developed for cloud-based research, validation of satellite, high-resolution model radiation and cloud property outputs, and solar energy research, with the ability to be distributed in sub-grid networks.

Here we present updates on instrument reliability, calibration accuracy, and cloud property retrievals from data collected at DOE ARM's Southern Great Plains (SGP) Facility and as part of the DOE ARM's SAIL project. Observed cloud properties from both sites will be presented and compared with co-located measurements. Preliminary results from an in-field calibrator development will be presented.

**Authors**

Zachary Payne, Benjamen Moul, Stephen Jones, Timothy B. Onasch

**Deducing the Composition of Aerosol and Cloud Particles with the Autofluorescence Nephelometer (AFN)**

**Darrel Baumgardner**
DMT

The composition, size and shape of aerosol and cloud particles impact weather and climate yet they are a complex mixture in the atmosphere that remain under-characterized, largely due to a lack of sensors that can measure these properties. A newly developed spectrometer, the single-particle autofluorescence nephelometer (AFN), is specifically designed to address uncertainties associated with the asphericity and complex refractive indices of atmospheric particles. The AFN projects a collimated, focused, linearly polarized, 440 nm wavelength laser beam through a window of an aircraft, uncrewed or crewed, into the airstream and measures the polarized components of some of the light that is scattered by individual particles that pass through the laser beam. The AFN also measures fluorescence from those particles that contain material that fluoresces when excited at a wavelength of 440 nm and emits at 470–520 nm. Fluorescence is expected from some organic molecules if present in the particles. The dual polarization feature of the AFN, not only provides a quantification of particle asphericity, but the complex refractive index can also be estimated, from which particle composition can be deduced.

The very small volume, weight and power of the AFN (< 125 cm3, 900g, < 100W), and its capabilities to provide detailed particle properties over a size range of 2 – 20 µm, make it an ideal candidate for installation on UxS platforms.

**Authors**

Darrel Baumgardner, Ted Fisher, Roy Newton, Pat Zmarzly, Chris Roden and Ben Kamen

**The Portable Ice Nucleation Experiment Pine: A New Online Instrument for Automated Long-Term Field Observations and Laboratory Studies of Ice-Nucleating Particles**

**Benjamin Murray**
University of Leeds

There is an increasing evidence that ice-nucleating particles are of first order importance for a range of climatically important cloud types. For example, INPs define the balance between ice and water in mid- to high-latitude boundary layer oceanic clouds, which is critical for their albedo and climate-feedback. Historically, it has been very challenging to routinely measure these particles, hence we set about developing an INP counter based around an expansion chamber – PINE (Portable Ice Nucleation Experiment) – that can be used in both the field and laboratory settings. PINE makes use of the first law of thermodynamics, mimicking cloud formation on reducing pressure under controlled conditions. PINE then counts ice crystals based on their size using an optical particle counter at the outlet.

PINE is now commercially available and has been deployed in 17 campaigns around the world ranging in length from ~1 month to multi-year. The acquired data reveal variations in INP concentrations on a range of temporal scales, from changes associated with synoptic weather patterns through to seasonal cycles. These data are being used to challenge the predicted global INP distribution in a climate model (the Met Office Unified Model), revealing biases that are helping to define the foci of future measurement efforts.

In addition to measurements of atmospheric INPs, PINE has also proven to be a powerful instrument for laboratory-based characterisation of the ice-nucleating ability of a variety of samples. For example, a study of aerosolised high latitude dusts reveals substantial differences between samples from the Copper River Valley in Alaska and the Kangerlussuaq valley in Greenland at temperatures below –20 °C, despite their ice-nucleating activity being remarkably similar at higher temperatures. We also used PINE to demonstrate that hydrophobic jet engine lubrication oil droplets activate to droplets and ice crystals above water saturation under conditions relevant for contrail formation, illustrating PINE's suitability for studying contrail processes and the non-CO2 impacts of aviation. Furthermore, we show that the ice-nucleating ability of aerosol in certain environments (laboratory and field) is sensitive to the methodology employed, with PINE revealing greater INP concentrations than other measurement techniques. We suggest that, because cloud formation is mimicked in PINE, the higher INP concentrations reported by PINE are more relevant for clouds in the atmosphere.

**Authors**

Benjamin J. Murray, Larissa Lacher, Franziska Vogel, Jens Nadolny, Romy Fösig, Nicole Büttner, Pia Bogert, Achim Hobl, Naruki Hiranuma, Leon King, Mark D. Tarn, Ross J. Herbert, Joseph Robnson, Joel Ponsonby, Marc E.J. Stettler and Ottmar Möhler

**Traceable Calibration for In-Situ Aerosol Absorption Instrumentation**

**Griša Močnik**
Haze Instruments d.o.o

Few direct methods for in-situ aerosol absorption measurement include photothermal interferometry and photo-acoustic spectroscopy. In-situ absorption instruments use different calibration schemes. NO2 is used for calibration in the visible range and can be traceable to SI units. Particles, on the other hand, allow calibration without wavelength limitations. Water soluble nigrosin is a candidate calibration material, forming spherical particles when nebulized. Mie calculations can be used to determine absorption coefficients. Calibration with monodisperse aerosols provides lower uncertainties compared to polydisperse ones.

We compare different calibration schemes in light of their measurement uncertainty and ease of implementation. Aerosol absorption was measured with a photothermal interferometer PTAAM-2λ (Haze Instruments). NO2 calibration was performed using a SI-traceable mobile reference gas permeation generator based (METAS), pre-prepared NO2 mixtures in cylinders or ambient NO2. Monodisperse nigrosin was selected from the nebulized sample using a centrifugal particle mass analyser (CPMA, Cambustion) and an electrostatic classifier (EC 3082, TSI) in series, removing multiply charged particles and neutral particles from the sample stream. Particle number concentration was quantified using a condensation particle counter (CPC 3750, TSI). The refractive index of nigrosin was determined by using an ellipsometer (Acurion).

The experimental results and a comparison with the Mie model monodisperse nigrosin aerosols show that mass-based parameters are more suitable for the modelling rather than mobility-based ones. The Mie calculation is based on measured particle number, measured nigrosin refractive index and either on particle mobility diameter (SMPS) or mass derived diameter (CPMA). Error bars represent method uncertainty. The Mie model using the mass derived diameter shows better agreement with the measurements, resulting in aerosol absorption coefficient uncertainty of 5%.

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# 3D Plume Mapping with UAVs And Lidar Technology

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In the framework of the European research program EDU4Climate – Horizon, we aim to calibrate a novel ground-based remote-sensing lidar using UAV-based atmospheric measurements. This study focuses on stack emission locations in Cyprus, specifically targeting major air pollution hotspots such as power plant stacks, cement plant stacks, harbors, and urban areas. These diverse sites offer a robust testing ground for our instrument, enabling the measurement of particle concentrations from various emission sources, including industrial facilities, marine vessels, and natural sources.

The core of our research involves the calibration process, which will be carried out through multiple flights of an unmanned aerial system (UAS) in close proximity to the lidar instrument. The lidar under calibration, the PMeye from RAYMETRICS, is the first commercially available lidar-based aerosol remote sensing solution capable of 3D mapping of particulate matter (PM) over several kilometers. This advanced capability allows for more accurate quantification of PM across extensive emission areas.

The Climate and Atmosphere Research Center of the Cyprus Institute (CyI), in collaboration with RAYMETRICS, aims to enhance the accuracy of the PMeye retrieval algorithms for both 3D and 4D PM monitoring. Calibration and validation of PM retrievals will be performed against data from ground-based sensors and CyI's UAV-sensor systems, facilitating real-time 3D monitoring of PM concentrations. This comprehensive approach ensures the reliability of our measurements and the effectiveness of our monitoring techniques.

By integrating advanced lidar technology with UAV-based measurements, our project aspires to deliver more precise and comprehensive 3D monitoring of particulate matter. This will significantly contribute to improved air quality management and pollution control strategies.

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# Aerosol Retrievals and PM2.5 Concentration Estimations from Nephelometers Using Grasp Algorithm and Machine Learning Method

**Chong Li**
GRASP SAS

This study demonstrates the capability of characterizing aerosol optical and microphysical proper-ties as well as estimating PM2.5 concentration using measurements from different types of nephe-lometers developed by AirPhoton using GRASP (Generalized Retrieval of Aerosol and Surface Properties) algorithm in combination with a machine learning method.

The 3-wavelength polarized imaging nephelometer (PI-Neph) allows the accurate measurement of phase function and degree of polarization, while the 3-wavelength integrating nephelometer (IN-Neph) measures forward and backward scattering, with the capability to adjust the size bin cut-offs by controlling inlet flow rate. GRASP algorithm is a next generation open-source algorithm devel-oped for aerosol retrievals which has been applied in diverse in-situ and airborne instruments such as sun-radiometer, lidar, satellite sensors etc. [Dubovik et al., 2011; Torres et al., 2014; Lopatin et al., 2021]. In our study, the capability of GRASP for advanced aerosol characterization from different types of nephelometers have been demonstrated.

For PI-Neph [Espinosa et al., 2017], aerosol optical and microphysical properties were retrieved with high accuracy for both synthetic data and real measurement data obtained in Granada, Spain. For IN-Neph, the results have shown that the aerosol size distribution and refractive index can be retrieved with rea-sonable accuracy while size-bin cut-off information is provided. The IN-Neph with PM2.5 and PM10 size-cutoffs with high temporal resolution were deployed over SPARTAN network together with sampling stations as well as other instruments. By combining gravimetric measurements from sampling station filters and nephelometer measurements, SPARTAN has estimated hourly PM2.5 which has been validated and shown reasonable accuracy [Snider et al., 2015]. In this study, we combined the GRASP algorithm with a machine learning (ML) method, gradient boosting (GB), to estimate PM2.5 mass concentrations from IN-Neph measurements from the SPARTAN network. The comparison between GRASP/ML retrieved PM2.5 concentrations with SPARTAN PM2.5 hourly estimates has shown good consistency. In addition, the new method combines aerosol retrieval algorithm with machine learning model, offers additional retrieved parameters such as aerosol size distribution and complex refractive index, which can provide a better understanding of the aerosol types and characteristics over monitoring sites.

**Authors:**

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# Cavity Attenuated Phase Shift (CAPS) Instrument for Simultaneous Measurement of $NO_x$ And $NO_2$

**Zachary Payne**
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Nitric oxide (NO) and nitrogen dioxide (NO2), the sum of which is referred to as NOX, are important trace gas pollutants whose chemistry controls the concentration of tropospheric ozone (O3), a key component of photochemical smog. As such, accurate quantification of NOX is critical in implementing coherent pollution control strategies. Currently, NOX is widely monitored using NO chemiluminescence (CL) techniques, which measure photons emitted by electronically excited NO2 upon reaction of NO with O3. This technique is prone to a wide variety of interferences, most notably from volatile organic compounds (VOCs) and other nitrogen containing species, which can lead to incorrect conclusions in air quality and chemical kinetic models.

Aerodyne Research Inc. has a long history of providing instruments for the measurement NO2 by the cavity attenuated phase shift (CAPS) technique, whereby square modulated light from a 450 nm LED is fed into a high finesse optical resonator with a small fraction of light coupled out to a photodiode. The difference in the cotangents of the phase shifts detected in the output signals with and without the presence of NO2 is proportional to the number density of absorbing species. We have extended the capability of this monitor to simultaneously measure both NOX and NO2 with high time resolution and excellent precision.

Our CAPS NOX-NO2 monitor deploys two separate sample cells, one for the measurement of NO2 and the other for total NOX. To measure total NOX, we first convert NO to NO2 using photolytically generated ozone before it is sent to the optical cavity. The NO2 measurement in the NOX channel is shifted to 405 nm to avoid a significant ozone interference. This technique has several benefits over the traditional CL method: (1) it measures the primary toxic pollutant (NO2), (2) it measures both NO2 and NOX simultaneously, allowing for the resolution of plumes which may be missed by lower frequency techniques, and (3) it is free of the numerous interferences in CL measurements (e.g., long-lived reactive nitrogen species, VOCs, etc.)

Our CAPS NOX-NO2 instrument has 1s precision (1σ) of <100 ppt, with 60s precision approaching sub-10 ppt over a range of 0-1000 ppb NOx. The prototype instrument has been deployed on several research campaigns alongside CL and TILDAS (Tunable Infrared Laser Differential Absorption Spectroscopy) measurements. Our NOX measurement compared favorably with the sensitivity and chemical specificity of the TILDAS technique. Additionally, this work highlighted the strengths of our monitor relative to the NO CL technique, with a commercially available CL instrument reporting NOX values significantly higher than ours (even at sub-10 ppb concentrations) due to the presence of long-lived reactive nitrogen species. Widespread adoption of the CAPS NOX-NO2 instrument will help develop a clearer understanding of trace reactive nitrogen oxides and their role in air pollution.

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**Particulate Matter Concentration Evaluation of Vaisala's AQT560 Against Multiple Equivalence Reference Methods**

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Vaisala

Airborne particulate matter (PM) poses a substantial threat to public health and the environment, leading to the implementation of regulatory measures for monitoring and controlling its levels.

To meet the requirements of the EU Air Quality Directive for measuring mass concentrations of PM, instrumentation varies from the reference methods specified in the directive, to typically employed automated continuous measurement systems (AMS) utilizing technologies such as oscillating microbalances, ß-ray attenuation, or in-situ optical methods. This contribution delves into the comparison between the compact Air Quality sensor AQT560 (Vaisala, Finland) and AMS systems, considering diverse aerosol types and climate conditions.
Vaisala AQT560 is a compact air quality sensor that can be had in various configurations for measuring particulate matter, various gaseous pollutants, or both. For the measurement of PM, AQT560 utilizes a completely renewed laser particle counter (LPC) with an excellent detection efficiency and a steady airflow ensuring reliable and accurate operation in various environmental conditions.

Three AQT560 units were deployed at each of the four sites in various climate types ("Cfb," "Dfb," and "Bsk", Köppen classification) paired with distinct equivalent reference methods (oscillating microbalance, TEOM; β-attenuation, two BAM units; in-situ optical method, FIDAS 200S). To assess variations between the AQT560 and AMS in diverse monitoring conditions, we employed a range of analytical techniques. Descriptive statistics, regression analysis, correlation analysis, and uncertainty calculations were employed to quantify differences and provide a comprehensive understanding of the performance across various scenarios.

The outcomes of our study reveal a high level of agreement between the measurements obtained for particulate matter sizes PM1, PM2.5, and PM10 using the AQT560 and the equivalence reference method. This agreement underscores the reliability and accuracy of the AQT560 in effectively capturing and quantifying particulate matter concentrations across different size fractions in various climates.

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**Improving Low-Cost Optical Sensors Accuracy Using Machine Learning**

**Marianna Chaves**
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Air quality monitoring is important to ensure that pollution levels do not exceed regulated standards, in order to avoid or minimize the harmful effects of pollutants to human health. Optical sensors are an alternative for monitoring particulate matter (PM) in cities and their associated low cost makes it possible to create sensor networks spread over several points, increasing the available information regarding the concentration of this pollutant.

An important aspect of using optical sensors is the reliability of their measurements, so that they can be used in research and to develop effective air quality control strategies. In this sense, studies have focused on the calibration of sensors in field and laboratory experiments, but accuracy is still a critical factor for using optical sensors in monitoring. In recent years, machine learning has been used to estimate the concentration of PM with good results since it takes into account non-linearity and other characteristics such as seasonality and the correlation of variables, offering a better alternative to traditional statistical methods.

The Random Forest algorithm is one of the most common models used for PM estimation and it makes it possible to select variables of interest that can influence the concentration of PM, calculating the importance of each one in the model and classifying them. Studies using Recurrent Neural Networks (RNN) and their variations for air quality forecasting are being used, and among them the long short-term memory (LSTM) takes into account the temporal dependencies in PM concentration records and has been increasingly applied.

The aim of this work is to use Machine Learning to improve the accuracy of optical sensors so that the algorithms can correct the sensor's reading based on meteorological variables, providing final values close to those of reference equipment. This work corroborates in developing software technology for more reliable air quality monitoring networks.

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**Sensor-Based Air Quality Systems for Accurate Emissions Monitoring**

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Industry and transport pollution significantly impact both populations and ecosystems, imposing substantial societal costs estimated by the European Environmental Agency to range between €268-428 billion in 2024. In response, considerable advancements have been made in emission control technologies and processes over the past few decades. A critical first step in improving air quality management involves understanding and controlling emissions through cost-effective and robust methods. Sensor-based air quality systems have emerged as a viable solution, providing real-time monitoring and comprehensive spatial coverage. However, it is well-known that low-cost sensors have limitations related to environmental conditions, cross-sensitivities, and drifts over time. In this context, Kunak has been working to mitigate these effects, increasing data accuracy and reducing errors compared to reference instruments without using external data or any post-processing models based on Machine Learning or AI. This enables accurate detection of pollutants and contributes valuable data for identifying pollution trends, hotspots, leaks, and emission sources.

This study presents two case studies involving the deployment of Kunak Air monitoring systems in industrial and transport settings: (i) air quality networks in ports, and (ii) multipollutant monitoring in a landfill. The Port Authority of Balearic Island deployed 25 Kunak Air Pro devices across five ports, facilitating the assessment of port activities' impact on air quality and serving as early warning tools. On the other hand, the use of a multipollutant sensor-based system with an integrated anemometer allowed for the identification of emission sources in a landfill in Portugal, distinguishing between pollution originating from the landfill and external sources.

The results underscore the utility of sensor-based air quality systems in providing reliable, real-time data on industrial and transport emissions. These systems enhance public health protection and worker safety by delivering actionable insights for pollution management and mitigation strategies.

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