Cambridge Particle Meeting

Schedule (LR0)			
Time	**Speaker**	**Affiliation**	**Title**
09:30	Welcome and coffee		
09:50	Opening remarks		
10:00	Una Trivanovic	METAS	Lower cost particle counters for traffic related emissions.
10:30	David Kittelson	University of Minnesota	How should we define ultrafine particles?
10:50	Zayne Zaman	Brunel University	Characterisation of Particle Number and Size from a Hydrogen DI SI Engine: Operating Sensitivities and Filtration Effect.
11:10	Siriel Saladin	University of Cambridge	Chemical Origin of Tyre Nanoparticles in a Tube Furnace.
11:30	Jacob T. Varghese	Saintgits College of Engineering	Assessment of particulate emissions (PM<2.5) at elevated motorways and the cleansing efficacy of vegetative retrofits.
11:50	Coffee break and posters		
12:05	Pádraig Meehan	University of Oxford	Comparing Retrieval Methods for Size and Refractive Index from Broadband Scattering Spectra of Single Aerosol Particles.
12:25	Chi Wang	University of Cambridge	Model, design and measurements of an extinction-based condensation particle counter.
12:45	Alireza Darzi	Imperial College	Nanoparticle Formation via Aerosol Spray Pyrolysis: A Molecular Dynamics Study
13:05	Haia Al-Assaf	Aston University	Nitrogen-assisted particle fluidization for dry coating of high-dose inhalable powders: Impact on particle micrometrics.
13:25	Lunch break and posters		
14:25	Paul I. Williams	University of Manchester	Life beyond nvPM number and mass: Characterisation of other particulate and gaseous emissions from a range of engines.
14:55	Joel Ponsonby	Imperial College	Review of UK facilities for laboratory-based contrail research.
15:15	Graeme Nott	FAAM Airborne Laboratory	Impact of Airframe Flow Distortions on Aerosol Measurements - the SAFIRE CPCMATEX Campaign.
15:35	Coffee break and posters		
15:50	Jan Goeing	Technische Universität Braunschweig	Emission Characterization: TU Braunschweig Full-Scale Research Turbofan Engine – Current & Future Campaigns.
16:10	Flavio Quadros	TU Delft	Air quality measurements at airports: results from a campaign at Rotterdam The Hague Airport.
16:30	Thomas Truscott	University of Southampton	What level of modelling is sufficient for predicting ice particle growth in aircraft exhaust?
16:50	Closing remarks & reception		

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Posters		
No.	**Author**	**Title**
1	Nick Kateris	Two-dimensional quantum dot theory for polycyclic aromatic hydrocarbon molecules, ions and radicals
2	Durre Nayab Habib	Tracing Photochemical Aging in Biomass Burning Aerosols Using Stable Carbon Isotopes
3	Durre Nayab Habib	Carbon Isotopic Composition of Anthropogenic Aerosols in Atmospheric Pollution Research
4	William Klipstine	Ex Situ Synthesis of Elemental Iron Nanoparticles for Enhanced Catalyst Activation in CNT Production
5	Alireza Darzi	Nanoparticle Formation via Aerosol Spray Pyrolysis: A Molecular Dynamics Study
6	Tan Yong Ren	The effects of non-premixed hydrogen on soot formation in an ethylene-fuelled lab-scale rich-quench-lean combustor

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List of attendees	
Name	**Affiliation**
Simone Hochgreb	University of Cambridge
Una Trivanovic	METAS
Paul I. Williams	University of Manchester
Tim Watling	Johnson Matthey
David Unitt	ENVEA UK
Andrew Akiba Nathanson	Ford Motor Company
Andrew York	University of Cambridge
Dr Tony Collier	Retiree
David Kittelson	University of Minnesota
Sofia Medina Cassillas	University of Cambridge
Leven Davies	PhD student Cambridge
Haia Al-Assaf	PhD Candidate
Mushtari Saidikova	Yusuf Hamied Department of Chemistry, Cambridge University
Brian Barney	Peritus Consulting Ltd
Anton Souslov	University of Cambridge
Lukas Knowles-Wilkinson	TU Braunschweig - Institute of Internal Combustion Engines and Fuel Cells
Durre N. Habib	Center for Physical Sciences and Technology (FTMC)
Lauretta Rubino	VERT Association
Ying Teng	University of Cambridge, Department of Engineering
Jan Goeing	Technische Universität Braunschweig
Zayne Zaman	Brunel University London
Sayed Esmatullah Torabi	Prince of Songkla University
Pádraig Meehan	University of Oxford
Graeme Nott	FAAM Airborne Laboratory
Samiah Qamar	University of West London
Nick Kateris	University of Cambridge
Dr Jacob Thottatil Varghese	Saintgits College of Engineering (Autonomous)
Durre N. Habib	Center for Physical Sciences and Technology (FTMC) Vilnius Lithuania
Mark Brend	Loughborough University
Antonino La Rocca	The University of Nottingham
Edward Richardson	University of Southampton
Yashar Shoraka	Department of Aeronautical and Astronautical Engineering, University of Southampton
Siriel Saladin	University of Cambridge
Thomas Truscott	University of Southampton
Tan Yong Ren	Cambridge CARES Ltd
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Anthony Dufour	CNRS Nancy France & University of Cambridge
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Lewis Reeves	ENVEA
Astron Gerov	M2M Pharma
Dr Mark Giles	Consultant
Angus Millar	Imperial College London
Colin Jenkins	Adaptive Instruments Ltd
Wiktor Jakubas	University of Cambridge
Dr Jonathan Symonds	Cambustion
Daisy Thomas	3DATX Corporation
Vidhi Sharma	University of Cambridge
Alex Vasiliou	Caterpillar
Georgia May Gamble	Imperial College London
Rachel Schwind	University of Edinburgh
Zain Robson	University of Cambridge
Dr Flavio Quadros	TU Delft

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3	Durre N. Habib	Tracing Photochemical Aging in Biomass Burning Aerosols Using Stable Carbon Isotopes
4	Jan Goeing	Emission Characterization: TU Braunschweig Full-Scale Research Turbofan Engine – Current & Future Campaigns
5	Zayne Zaman	Characterisation of Particle Number and Size from a Hydrogen DI SI Engine: Operating Sensitivities and Filtration Effect
6	Pádraig Meehan	Comparing Retrieval Methods for Size and Refractive Index from Broadband Scattering Spectra of Single Aerosol Particles
7	Graeme Nott	Impact of Airframe Flow Distortions on Aerosol Measurements - the SAFIRE CPCMATEX Campaign
8	Nick Kateris	Two-dimensional quantum dot theory for polycyclic aromatic hydrocarbon molecules, ions and radicals
9	Dr Jacob Thottatil Varghese	Assessment of particulate emissions (PM<2.5) at elevated motorways and the cleansing efficacy of vegetative retrofits.
10	Durre N. Habib	Carbon Isotopic Composition of Anthropogenic Aerosols in Atmospheric Pollution Research
11	Siriel Saladin	Chemical Origin of Tyre Nanoparticles in a Tube Furnace
12	Thomas Truscott	What level of modelling is sufficient for predicting ice particle growth in aircraft exhaust?
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14	William Klipstine	Ex Situ Synthesis of Elemental Iron Nanoparticles for Enhanced Catalyst Activation in CNT Production
15	Alireza Darzi	Nanoparticle Formation via Aerosol Spray Pyrolysis: a Molecular Dynamics Study

16	Mridul Majumder	Morphological Characterisation of Dry Powder Inhalation Formulations: A Response to the US FDA Guidelines
17	Tan Yong Ren	The Effects of Non-Premixed Hydrogen on Soot Formation in an Ethylene-Fuelled Lab-Scale Rich-Quench-Lean Combustor

1. How should we define ultrafine particles?

David Kiitelson[1*], R. Giannelli[2], J. Kinsey[2], J. McDonald[2], J. Stevens[2] and I. Khalek[3]

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[3] SWRI

At present there is no clear epidemiological evidence linking adverse human health effects to ultrafine particles (UFP), arguably because there is no universally agreed upon UFP definition. A commonly used definition is either particle number below 100 nm or total particle number, but without an agreed upon lower cut point. For example, a lower cut point of 3 nm compared to 10 nm could result in a substantially higher count. Another definition for UFP is total particle mass but without a commonly agreed upon aerodynamic diameter upper cut point, e.g., below 100 nm, 200 nm, 300 nm, etc. Yet another definition is lung deposited surface area weighted by lung deposition fraction, found mainly in the particle mobility diameter range from 20 to 400 nm. It is clear from these definitions that there are inconsistencies in the way UFP is used and defined in the literature. Sometimes these metrics are well correlated, sometimes not.

In this presentation we suggest three new metrics: UFP-N, UFP-M, and UFP-S, that we believe will add clarity. These metrics represent total number, mass, and surface area below 500 nm, respectively. For surface area and mass, the 500 nm cut point can be either aerodynamic or mobility diameter depending upon measurement methodology. For all metrics, this cut point captures nearly all of the primary particle emissions from mobile sources. Furthermore, UFP-N would include a lower cut point of 3-6 nm and would not require an upper size cut point because there is very little particle number above 500 nm or even above 100 nm. Thus, our definition of UFP-N is consistent with the current definition of ultrafine number except for, importantly, the specification of a lower cut point. These new metrics are not necessarily intended to be used for regulatory tailpipe measurements, but rather for characterization of ambient exposures, and for linking them to acute and chronic health effects in epidemiological studies. They may also be useful for formulating new regulatory ambient standards to complement existing PM10 and PM2.5 standards.

When formulating these new definitions, size and other properties of particles on or near roadways must be considered as this is where the highest exposures to submicron particles occur. Since modern vehicles under normal operating conditions have very low particle emissions, these particles will mainly come from older and malfunctioning vehicles as well as modern vehicles with failed or disabled exhaust aftertreatment systems. Consequently, particle emissions from such vehicles which are expected to dominate roadside exposures have been considered in the formulation in the suggested new metrics. Modern roadside measurements show particle size and modal structures similar to historical measurements going back as far as the early 1970s but at much lower concentrations.

2. Nitrogen-assisted particle fluidization for dry coating of high-dose inhalable powders: Impact on particle micrometrics

H. A. Al-Assaf[1], A. Rahman[2], R. Badhan[1], D. Kirby[1] and A. R. Mohammed[1]

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High-dose inhalable powders present persistent formulation challenges due to increased particle aggregation, poor flowability, and reduced dispersibility, which ultimately compromise aerosol performance (Sibum et al., 2018). Conventional blending approaches often provide limited control over particle surface properties in high drug-content inhalable formulations. Building on recent advances in high-dose powder manufacturing (Al-Assaf et al., 2023), this study investigated isothermal dry particle coating (iDPC) – a low-shear process employing nitrogen-assisted particle fluidization – to modulate particle micrometrics relevant to pulmonary delivery, with a focus on changes in surface area, surface accessibility, and particle layering.

Fluticasone propionate (FP) and lactose (Respitose® SV001) were used to prepare high-dose formulations (50% w/w FP) using iDPC at 1500 rpm for 10 min and nitrogen flow rates of 0 $L{\cdot}min^{-1}$ (F1) and 20 $L{\cdot}min^{-1}$ (F2). Particle properties were analyzed for particle surface properties using BET (Brunauer-Emmett-Teller) (Micromeritics TriStar II Plus), and particle size distribution by laser diffraction (PSD) (Sympatec HELOS).

The iDPC process resulted in a high powder yield (F1: 98.63%; F2: 98.73%) confirming negligible material loss during powder processing. Marked differences in surface and particle micrometric properties were observed between unprocessed materials and dry-coated formulations prepared with and without nitrogen airflow. FP exhibited high surface area (SA) (10.82 m^2/g), indicative of a highly energetic API surface, whereas lactose had a surface area of 0.23 m^2/g, consistent with a smooth, low-energy carrier. Airflow-assisted processing (F2) produced an 8.76% increase in surface area (SA (m^2/g): F1: 3.88; F2: 4.22) and 7.41% larger pore diameter (Pore size (Å): F1: 45.08; F2: 48.42) relative to F1. High-dose inhalable powders present persistent formulation challenges due to increased particle aggregation, poor flowability, and reduced dispersibility, indicating surface alteration and the formation of porous structures due to adsorption of fine FP particles. Particle size distribution analysis showed a clear shift in coated formulations relative to lactose (D90 = 218.90 µm), with higher D90 values observed for F1 (302.48 µm) and F2 (297.92 µm), confirming FP deposition onto the carrier surface. The slightly lower D90 for F2 compared to F1 indicates more compact and stacked multilayer FP assemblies under nitrogen-assisted fluidization rather than randomly distributed coating.

Similarly, the higher BET constant observed for F1 (127.73) compared to F2 (103.05) indicated a more heterogeneous surface resulting from irregular FP attachment, whereas the reduced BET constant for F2 suggests a more uniform surface energy distribution. Such homogenization of surface energetic sites has been associated with improved particle rearrangement and coating uniformity in dry powder systems.

These findings show that the process of dry coating using iDPC (20 $L{\cdot}min^{-1}$ of N2) induces particle fluidization, promoting rearrangement of the powder bed. In contrast, dry coating in the absence of airflow relies primarily on mechanically driven particle movement, which can result in uneven FP distribution and heterogeneous surface coverage. The integration of nitrogen-assisted fluidization therefore represents a key mechanistic advantage of iDPC in achieving controlled multilayer deposition for high-dose inhalable powders.

References:

Al-Assaf, H. A., Papadimitriou, S. A., Rahman, A., Badhan, R., & Mohammed, A. R. (2025). Advanced Manufacturing Methods for High-Dose Inhalable Powders. Pharmaceutics, 17(3), 359. https://doi.org/10.3390/pharmaceutics17030359

Sibum, I., Hagedoorn, P., de Boer, A. H., Frijlink, H. W., & Grasmeijer, F. (2018). Challenges for pulmonary delivery of high powder doses. International journal of pharmaceutics, 548(1), 325–336. https://doi.org/10.1016/j.ijpharm.2018.07.008

3. Tracing Photochemical Aging in Biomass Burning Aerosols Using Stable Carbon Isotopes

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Carbonaceous aerosols from biomass burning emissions are major contributors to atmospheric particulate matter and play a critical role in air quality, climate, and human health. Stable carbon isotopic composition ($\delta^{13}C$) provides a powerful tool for identifying emission sources and evaluating the influence of atmospheric processing on source signatures. This study applies $\delta^{13}C$ analysis of three-step OC to assess the impact of photochemical aging on biomass burning aerosol isotopic characteristics.
Aerosol samples (PM1) from the combustion of twenty different biomass fuels were collected during the biomass burning experiment. Of the twenty biomass burning samples, six were selected for photochemical aging experiments based on their organic carbon mass, which exceeded the minimum detection and precision requirements for $\delta^{13}C$ analysis across all three thermal OC fractions. Samples with lower carbon mass were excluded from aging to avoid increased analytical uncertainty associated with low signal-to-noise ratios. The isotopic composition of total carbon and organic carbon before and after aging experiment will be presented.

OH-aged samples showed no significant isotopic shifts relative to un-aged samples, although minor variations in total carbon mass were observed at higher temperature fractions, likely related to filter loading heterogeneity. In contrast, UV-aged samples exhibited systematic depletion in ^{13}C across three temperature steps (200 °C, 350 °C, and 650 °C). The 350 °C fraction generally displayed the highest $\delta^{13}C$ values among UV-aged samples, indicating distinct isotopic fractionation during photochemical processing. For example, $\delta^{13}C_{OC}$ values for wood pellet emissions changed from −25.6 ‰, −25.7 ‰, and −25.4 ‰ in un-aged samples to −25.3 ‰, −25.1 ‰, and −25.0 ‰ after UV aging at 200 °C, 350 °C, and 650 °C, respectively. Photochemical aging (particularly UV exposure) reveals systematic modifications to biomass burning isotopic signatures. These findings support the use of stable carbon isotopes for robust source apportionment of carbonaceous aerosols and for interpreting atmospheric observations influenced by photochemical aging.

4. Emission Characterization: TU Braunschweig Full-Scale Research Turbofan Engine – Current & Future Campaigns

Jan Goeing *[1,2], Steven Rogak[2], Lukas Knowles-Wilkinson[1], Daniel Lieder[1], Patrick Kirchen[2], Sina Kheirkhah[2], Federica Ferraro[1], Peter Eilts[2] and Jens Friedrichs[1]

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[2] University of British Columbia

The full-scale research turbofan engine at Technische Universität Braunschweig is a unique research infrastructure in Europe. From a university perspective, it is currently the only fully operational high-bypass turbofan engine, serving as an exceptional platform to set up digital twins and analyze the impact of different jet fuels on engine performance, gaseous emissions, and particulate matter.

The Research Platform

The engine is a V2500 turbofan, originally designed for the Airbus A320 family, capable of generating up to 110 kN of thrust. It features a bypass ratio of 5.6 and a turbine inlet temperature exceeding 1700 K. The engine is equipped with over 100 additional measurement probes in both cold and hot sections, enabling detailed in-engine diagnostics. Additional interfaces for emissions and particle measurements are available at multiple locations, including the turbine exhaust case. Previously used to characterize performance and establish digital twin models, the engine's major components and secondary systems (cooling air and lubrication) are well-characterized across the entire mission range. Building on this, the facility is now increasingly used for studies on the emission characteristics of sustainable aviation fuels (SAF).

The VLAME Project

Supported by MTU, Lufthansa Technik (LHT), the University of British Columbia (UBC), and SASOL, the project VLAME (Validation of a Low-Emission Fleet Management) aims to validate a model-based toolchain to predict engine performance and emissions as a function of jet fuel properties. Unlike empirical approaches, this toolchain uses physical models to enable transferable predictions across different operating conditions. Extensive experimental campaigns are conducted across three platforms:

- TU Braunschweig V2500 engine,
- MTU's test facility in Hannover,
- The CFM56 research engine at Lufthansa Technik in Hamburg.

Several Fischer–Tropsch synthetic paraffinic kerosene (FT-SPK) fuels are investigated to assess the influence of fuel composition. Emissions (PM, nvPM, CO2, CO, NOX, and soot precursors) are measured both inside and outside the engine. High-fidelity Large-Eddy Simulations (LES) of the combustor complement the experiments, providing insights into flow, mixing, and soot formation.

Collaborative Research and Scalability

In collaboration with UBC, Boeing, and SAF producers, the turbofan engine is also used to develop a low-budget test platform based on a micro turbojet engine. This low-budget test platform aims to screen candidate jet fuels using only a few hundred liters. A central research question is the scalability of results from micro-scale to full-scale aero-engines. Particular attention is given to:

- Ice-nucleation potential of soot and lubrication oil
- Soot morphology and particle properties
- Impact on contrail formation.
- Impact on performance (power density, combustion temperature etc)

These activities establish the TU Braunschweig research turbofan as a vital link between fundamental, low-cost testing and full-scale validation, advancing the understanding of aviation's environmental impact.

5. Characterisation of Particle Number and Size from a Hydrogen DI SI Engine: Operating Sensitivities and Filtration Effect

A.Harrington[1] J.Hall[1], Z.Zaman[2], X.Wang[2], H.Zhoao[2], Y.Zou[3] and C.Nickolas[3]

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[2] Brunel University of London

[3] Cambustion Ltd

Hydrogen internal combustion engines (H2ICE's) promise near-zero carbon operation, yet particle number (PN) emissions primarily from lubricant oil pyrolysis promoted by hydrogen's short quench distance remain less well understood than NOx emissions. This study characterises exhaust particles from a spark-ignition, single-cylinder research engine (MAHLE Powertrain) at Brunel University of London across a wide variety of operating conditions, comparing gasoline with hydrogen direct-injection strategies (central vs side) and assessing sensitivity to operating parameters (speed, load, λ, rail pressure, spark timing). PN and particle size distribution were measured using Cambustion's DMS500 coupled to a catalytic stripper to focus on solid particles. To probe the role of the engines mechanical condition, a worn configuration with ~30% cylinder leakage was contrasted with a newly overhauled engine state (~5% leakage). Finally, a production Euro 6 gasoline particulate filter (GPF) was evaluated with hydrogen combustion to gauge its efficiency for the small particles typically reported for H2ICE operation. The results show that hydrogen produces markedly smaller particles than gasoline, with PN strongly modulated by the injection strategy, lambda, and rail pressure and engine wear further elevates PN, consistent with increased oil ingress. Compared with gasoline, hydrogen's PN is shifted to smaller diameters, underscoring the relevance of sub-23 nm regulation and measurement practice for H2ICEs. The GPF assessment indicates practical PN mitigation potential under hydrogen operation, while also highlighting that injection mode and calibration must consider the predominance of ultrafine modes. Overall, these findings map the operating and design levers that govern PN from hydrogen DI engines and provide evidence to support SPN10/SPN23 compliance strategies and filtration choices for durable, low-emission H2ICE powertrains.

6. Comparing Retrieval Methods for Size and Refractive Index from Broadband Scattering Spectra of Single Aerosol Particles

Pádraig Meehan *[1], Aidan Rafferty[2] and Michael Cotterell[1]

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Aerosols contribute substantially to Earth's radiative balance, with aerosol radiative forcing representing one of the largest uncertainties in projecting future climate. Aerosol refractive index is a key parameter required in calculations of this radiative forcing, with refractive index strongly dependent on the wavelength of light. Accurate and precise optical characterizations of atmospheric aerosols, and how their refractive indices vary with wavelength, are therefore crucial for improving aerosol radiative forcing estimates. We use a counter-propagating laser beam optical trap for single aerosol particle levitation, with particle analysis provided by cavity ringdown spectroscopy (CRDS) and broadband light scattering (BLS). BLS enables retrievals of wavelength-dependent refractive indices over a broad spectral range, while CRDS allows for determinations of refractive at a specific wavelength with high sensitivity. We provide a quantitative evaluation of two different methods for retrieving refractive index from BLS spectra for single aerosol droplets: a peak position-based retrieval, and a full-spectrum fitting method. These two methods are applied to aerosol particles comprised of 1,2,6-hexanetriol, a benchmark organic aerosol with well-characterised refractive index. Comparison with concurrent CRDS measurements of single particle extinction cross-sections reveals a systematic bias in the BLS retrievals that depends on particle radius. These results establish a robust foundation for characterising the broadband optical properties of atmospherically relevant aerosol species and extending the approach to light absorbing species.

7. Impact of Airframe Flow Distortions on Aerosol Measurements - the SAFIRE CPCMATEX Campaign

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SAFIRE, the French facility for airborne research, operate an ATR 42 atmospheric research aircraft. The ATR 42 can be operated with underwing and fuselage-mounted instruments for the measurement of cloud particles and aerosols. The ideal for every airborne measurement is that the data collected perfectly reflects the ambient parameters under study, however perturbations due to the aircraft itself are difficult to avoid and characterise. In September 2025 a short measurement campaign, CPCMATEX, was run out of Toulouse which focused on characterising the impact of instrument installation location on cloud particle and aerosol measurements. Six flights were conducted over the south of France, mainly within the boundary layer and in clear air and (liquid) cloud. Multiples of the same instruments, measuring cloud droplets (sizes 2–50 μm) and aerosols (sizes 60 nm–3 μm) were assembled and strategically moved around the installation positions over different flights.

In this work, results for the Passive Cavity Aerosol Spectrometer Probe (PCASP), a commonly used optical particle counter for the measurement of aerosol size distributions from 0.1 to 3 um, are presented. Two FAAM PCASPs were calibrated in the laboratory before and after the campaign to account for differing instrument sensitivities and then deployed simultaneously on each flight. Between flights the instruments were moved to different positions on the aircraft; underneath the forward fuselage, above the forward fuselage, and in one of three locations on an underwing pylon. The optical alignment of each was checked with each move although full calibration facilities were not available during the campaign. An initialisation flight, where the two PCASPs were located symmetrically on the aircraft, was used to obtain a ratio of in-flight instrument sensitivities and this was then used to quantify differences in the measured aerosol size distributions. This factor was applied to all subsequent flights and a size-dependent scaling factor calculated to quantify the different perturbations of the ambient air and aerosol flows due to the airframe at all instrument mounting positions.

Results from the campaign will be presented along with recommendations for future experiment design to characterise the effect of an airborne platform on similar aerosol measurements.

8. Two-dimensional quantum dot theory for polycyclic aromatic hydrocarbon molecules, ions and radicals

Nikolaos Kateris *[1], Andrea Nobili[2], Manasa Raghuraman[3], Amitesh S. Jayaraman[2] and Hai Wang[2]

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A two-dimensional-Quantum Dot (2D-QD) theory is proposed to describe the HOMO–LUMO gaps of large polycyclic aromatic hydrocarbons (PAHs) and a range of PAH-derived species, including molecules with/without OH-, CH3- and CF3-functionaliσation, radical cations, σ-radicals, and π-radicals, all of which belong to the circumpyrene and circumcoronene families of PAHs. The theory is composed of two terms: a universal quantum confinement term and an electronic structure-specific term. The quantum confinement term is derived from the energy of an electron-hole pair of effective mass 0.115 in a circular well of size equal to the diameter of the species and a well depth of 582 eV. The structure-specific term scales linearly with the HOMO–LUMO gaps of the smallest available species in each family of PAH-derived species. The HOMO–LUMO gaps of PAH-derived species are calculated using density functional theory; the results are used for testing the 2D-QD theory.

9. Assessment of particulate emissions (PM<2.5) at elevated motorways and the cleansing efficacy of vegetative retrofits.

Jacob Thottathil Varghese *[1], Adithyan Suresh[1,2], Amal Shaji[1,2], Arjun Krishna R.[1,2], Derik Shaji Joseph[1,2] and Diyan Reji Alex[1,2]

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The ending years of the current decade will definitely witness the extent of effectiveness concerning the accomplishment of sustainable cities and communities, and climate action: respectively the 11th and 13th Sustainable Development Goals of the United Nations (SDG11 & SDG13). Since the global climatic conditions have become alarmingly erratic, all targets and indicators of both these SDGs are being mended with utmost priority at all possible junctures. This piece of research is one such mentored multiphase work by a senior-level student project group. While the initial phase of this continual research specifically addresses SDG13.2.2 (total Greenhouse Gas emissions) through SDG11.6.2 (particulate emissions: PM2.5 & PM10), the latter stages reveal the projected bio-assisted removal of atmospheric pollutants. Since vehicular exhausts are one of the main contributors to GHG emissions in the suburbs of Kerala state, India, a part of the recently built 6-lane elevated motorway (NH66: ~18km Thalassery–Mahe Bypass) was analysed segment-wise to determine the spewed pollutant concentrations and the connected atmospheric chaos. Along the entire traffic corridor, two portable mini-meteorological stations (systematically separated ~6km apart from start and exit) captured the levels of CO2 emissions (major constituent in total GHGs: nearly 75%) and respirable particulate matter (PM<2.5). At three specific time slots (06:00, 12:00 & 18:00 IST), both traffic density throughout the entire route and the mid-way traffic volumes were recorded manually. The PM<2.5 concentration stayed higher (~4 times) towards noon time (~23 μg/m3) than the mornings and evenings (~5 μg/m3 to 6 μg/m3). A similar pattern was observed for the CO2 levels as well: it spiked to a value > 680ppm at 12:00 noon and stayed between 400ppm and 430ppm at 06:00 & 18:00. Having learnt the diurnal pollutant concentrations, a unique and scientifically corroborated contaminant removal mechanism was proposed. The cleansing process is completely biological and can improve the regional air quality index (AQI) to promote safe and environmentally friendly road transport corridors [1]. The sustainably viable initiative led to the proposal to construct vertical vegetative façade retrofits (maximum height = 1.5m) alongside the entire road median (divider). Interestingly, the natural efficacy of living walls draped with Dolichandra unguis-cati (common name: Cat's claw creeper-cc) and Vernonia Elaeagnifolia (common name: Curtain plant-cp) has already been investigated and proven for both small-scale green façade trellis and extended green walls [2]. It not only curtails the unsafe visual delusions caused by oncoming traffic flow but also removes the hazardous respirable atmospheric pollutants (gaseous & particulates) through the stomatal openings at the dorsal and ventral of leaf foliage (stoma-wise uptake rate of cp: day ~1.085x10-6 & night ~1.27x10-7). Therefore, the construction of an interleaved large area green retrofit trellis (with Dolichandra and Vernonia) is one of the sustainable alternatives to promote a secure and clean environment alongside elevated motorways in tropical climes. Furthermore, it remains and serves as an operable iconic means to envisage a climate-resilient future at all times.

References

[1] Joshi Saumitra, V. and Sat. Ghosh (2014). On the air cleansing efficiency of an extended green wall: A CFD analysis of mechanistic details of transport processes. Journal of Theoretical Biology, 361(21), pp 101-110

[2] Varghese, J. T. (2017). Mass and energy transfer process in high-rise green facade structures (1st ed.). LAP LAMBERT Academic Publishing, Berlin.

10. Carbon Isotopic Composition of Anthropogenic Aerosols in Atmospheric Pollution Research

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Carbonaceous aerosols from anthropogenic sources, including biomass burning (BB) and vehicular emissions, are a major component of fine particulate matter and play an important role in air quality, climate forcing, and human health [1]. However, uncertainties remain in identifying their sources and understanding how their chemical signatures evolve during atmospheric processing. Stable carbon isotopic composition ($\delta^{13}C$) of organic carbon (OC) offers a promising tracer to address these challenges. This study investigates the applicability of $\delta^{13}C$ in anthropogenic atmospheric pollution research through two independent experimental approaches.

Firstly, laboratory aging experiments were conducted on aerosols produced from the combustion of six different biomass fuels to examine isotopic changes during photochemical processing. $\delta^{13}C$ of OC was measured across three thermal fractions (200 °C, 350 °C, and 650 °C). OH-aged samples showed minimal isotopic change, in contrast to consistent ^{13}C depletion following UV aging. The intermediate-temperature OC fraction (350 °C) was generally enriched in ^{13}C compared to other fractions after UV aging. For example, wood-pellet emissions showed $\delta^{13}C$ values of −25.3 ‰, −25.1 ‰, and −25.0 ‰ for the 200 °C, 350 °C, and 650 °C fractions, respectively, compared to −25.6 ‰, −25.7 ‰, and −25.4 ‰ in un-aged samples.

Secondly, $\delta^{13}C$ of three-step OC was characterized for vehicle exhaust aerosols(un-aged) collected from eleven in-use vehicles. Substantial variability in isotopic composition was observed among vehicles and thermal fractions, with most values clustering between −26 ‰ and −28 ‰, alongside notable deviations in specific samples.

Overall, the results demonstrate that $\delta^{13}C$ of OC is sensitive to both photochemical aging and source-specific emission characteristics, supporting its use as a tracer for anthropogenic aerosol source apportionment and atmospheric pollution studies.

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11. Chemical Origin of Tyre Nanoparticles in a Tube Furnace

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Since the 1970s, it has been hypothesised that airborne nanoparticles from tyre wear originate from heat-driven evaporation and condensation of an unidentified tyre component. Tyre extender oil has long been suspected as a source. Here, we revisit this hypothesis and provide a mechanistic characterisation of tyre nanoparticles generated from cryomilled tyre tread under controlled thermal conditions in a tube furnace. Removal of extractable components such as extender oil substantially reduced nanoparticle formation. These results suggest that volatile organic additives, rather than the rubber itself, are the primary source of the tyre nanoparticles in our study. Experiments with tyre extender oil confirmed its ability to emit ultrafine particles when heated to similar temperatures. Nanoparticles collected from both tyre tread and extender oil were chemically characterised using NMR spectroscopy and found to consist predominantly of saturated hydrocarbons, closely matching the pristine extender oil. These findings provide the first experimental confirmation linking tyre nanoparticle chemistry to tyre extender oil, offering a mechanistic basis to interpret tyre nanoparticle emissions and support risk assessments.

12. What level of modelling is sufficient for predicting ice particle growth in aircraft exhaust?

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Predicting contrail ice formation is important for understanding how aircraft affect climate. The way ice particles grow and freeze in engine exhaust jets determines their size and how long contrails last. To make good decisions about aircraft operation, fuel development, and aircraft design, models of contrails need to be accurate enough—but it is not clear how detailed they must be. Existing modelling approaches vary widely. At one extreme, highly detailed methods such as Large Eddy Simulations (LES) with particle tracking are accurate but very expensive to run. At the other, simplified "box models" are fast but ignore important features like uneven mixing in the plume and often neglect variation in particle sizes. The gap between these approaches has not been well explored. In this study, we systematically examine how different modelling assumptions affect predictions of ice particle growth in young contrails. We assess whether turbulent fluctuations captured by LES affect ice growth, meaning simpler Reynolds-averaged models may be sufficient. We also assess whether two-moment models with simple closure assumptions can predict overall growth well compared with more detailed methods. Finally, we introduce a new one-dimensional modelling approach that efficiently captures ice growth in a three-dimensional exhaust jet. This method works by transforming the problem into composition space, allowing much lower computational cost while maintaining good accuracy. Further simplification into a zero-dimensional box model introduces substantial error.

13. Air quality measurements at airports: results from a campaign at Rotterdam The Hague Airport

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A seven-week field campaign was conducted in summer 2025 at Rotterdam The Hague Airport (RTHA) in the Netherlands to characterise particulate and gaseous emissions during airport operations. Instruments were deployed at two runway-side locations and in the former airport fire station, measuring particle size distributions, number concentration, and gas concentrations at high time resolution.

At the runway side, aircraft attributable plume events were identified at each measurement location, with peak particle number concentrations frequently exceeding 10^5#/cm^3. Average particle diameters during peaks were below 20 nm, consistent with expectations. Farther, at the fire station, UFP concentrations showed order-of-magnitude fluctuations. Together, these results illustrate the highly variable nature of airport air quality and the importance of high time resolution measurements for capturing emission events.

14. Ex Situ Synthesis of Elemental Iron Nanoparticles for Enhanced Catalyst Activation in CNT Production

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The properties of carbon nanotube (CNT) materials have promise as a low-carbon alternative material to widely used metals and alloys. Their synthesis via methane pyrolysis is of interest as a means of hydrogen production with a 75% reduction in GHG emissions relative to unabated steam methane reforming from which most hydrogen and an accompanying 980 Mt of CO2 emissions presently derive. CNTs can be synthesized in a floating catalyst chemical vapor deposition (FCCVD) process that employs aerosolized metallic particles as the catalyst. The higher quality CNTs obtained from this technique are more valuable for their engineering properties than those grown in fluidised bed and substrate-based reactors, yet the current mass yield of FCCVD reactors relative to their volume (< 1 kg/h/m3) lies some two orders of magnitude below that typical of industrial processes and inhibits industrial scaling of the method. It is known already that the content of sulfur in the catalyst controls the transition between single and multi-walled nanotubes, however the mechanisms by which it affects the mass production rate of FCCVD reactors are less understood and are of interest to this study. As < 1% of iron catalyst nanoparticles are observed to be catalytically active in manufactured material, new methods for producing and delivering the catalyst are worthy of investigation for their potential to improve catalytic activity. In this study, new routes for catalyst particle synthesis with a heated particle generator are evaluated for their feasibility. The particle size distribution and number density of particles is studied as a function of their chemical composition, and the potential of the synthesized aerosol for use in FCCVD processes is investigated.

15. Nanoparticle Formation via Aerosol Spray Pyrolysis: a Molecular Dynamics Study

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Gas-phase nanoparticle synthesis methods, such as aerosol spray pyrolysis (ASP), are attractive for large-scale production due to their scalability, rapid processing and cost-effectiveness. An important question pertains to the size and morphology of the resulting nanoparticles and how these are governed by parameters including precursor concentration, chemical composition and temperature. The objective of this study is to investigate this question using classical molecular dynamics (MD) simulations. In particular, we investigate the evaporation of water nanodroplets containing iron nitrate or iron chloride, leading to iron-containing nanoparticles. Analysis of the radial ion number density reveals two distinct morphologies: a hollow structure in the nitrate system, where ions accumulate near the droplet surface, and a dense spherical structure in the chloride system, where ions remain uniformly distributed within the droplet. Surface tension calculations indicate that the lower surface tension of the nitrate solution drives ion enrichment at the interface. Analysis of evaporation rate and molecular diffusivity reveals that evaporation-diffusion competition is the second factor that contributes to the formation of distinct morphologies. Although the evaporation rates are comparable for nitrate and chloride droplets, the ionic diffusivity is lower in the nitrate case, limiting ion transport towards the droplet core and thereby reinforcing the formation of hollow particles. A sensitivity analysis on gas-phase temperature, droplet size and initial precursor concentration shows that higher gas-phase temperature promotes hollow structures by enhancing surface evaporation, while higher initial concentration suppresses hollowness by favoring uniform, bulk crystallisation over surface-driven crystallisation. Hollow morphologies are observed across all droplet sizes studied. Consequently, despite the smaller droplet sizes used in the simulations compared with real systems, the mechanistic insights and morphological trends reported here are expected to be relevant to experimentally accessible scales.

16. Morphological Characterisation of Dry Powder Inhalation Formulations: A Response to the US FDA Guidelines

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The behaviour of active pharmaceutical ingredient (API) and excipient particles influences product performance and, in turn, dictates formulation efficacy. Manufacturing and process challenges are related to the particle size and surface morphology and influences the formation of aggregates, drug dispersion and deposition [1]. Morphologi 4 ID (Malvern Panalytical), also called morphology directed Raman spectroscopy (MDRS), is a widely used technique for studying the morphological characteristics and identification of powder particles. Food and drug administration (FDA) guidelines recommend using MDRS for comparative characterisation study as a technique to understand particle morphology of emitted dose for various dry powder inhalation (DPI) formulations [2]. The objective of this study is to understand similarities between the morphological characteristics displayed by APIs and excipient particles in two different marketed DPI formulations using MDRS. This study aims to form a foundation for generic product development and provides background information for novel drug product development in the DPI domain.

Two marketed DPI formulation products, Product 1 (Fobumix Easyhaler® 320µg Budesonide /9µg Formoterol Fumarate Dihydrate) and Product 2 (WockAIR® 320µg Budesonide /9µg Formoterol Fumarate Dihydrate) were selected for particle morphology analysis. The entire contents of a unit dose equivalent were transferred onto a spool and dispersed using the sample dispersion unit (SDU) of the MDRS. Each sample was analysed at two different magnifications (5x and 50x) to bring the API and the excipients in adequate focus.

Data analysis included measurement of particles by the optical microscope of MDRS and analysis using Morphologi software. Particle size distribution (PSD) and morphological characteristics, namely aspect ratio, convexity, solidity, elongation and High sensitivity (HS) circularity were measured.

The graphical presentation of PSD data shows Class 1 and Class 2 distributions for both the products. A shift in PSD values can be seen at the two different magnifications likely due to the resolution limits, which bring the larger excipient or Class 1 particles in focus at 5x and 50x resolving the smaller sized or Class 2 particles. In addition, Figure 3 shows values for Class 1 and Class 2 matching with the expected values showing D90 of <10 µm for APIs and ca. 130 µm for the excipients as cited in literature. A close similarity was observed between the predicted morphological trend and the observed trend for both the products at 50x and 5x magnifications. The values obtained by MDRS for both products, Product 1 and Product 2 demonstrated higher values for aspect ratio, HS circularity, solidity and convexity for Class 1 than Class 2. On the other hand, lower elongation values were observed for Class 1 than Class 2 for both products. Based on the data obtained by MDRS, the API and excipients' morphological characteristics for both the marketed DPI products appear to align with the predicted morphological trend data. The morphological trend presented in this study establishes a reference for the particle characteristics of API and excipient in DPI formulation.

This study demonstrates morphological profile data for APIs and excipient by MDRS which is evidenced by two marketed formulations. It proposes to reduce the testing and comparative analysis of test batches and with reference batches during product development. This study aims to act as a time-saving and cost-effective approach for product development scientists and companies to accelerate their bioequivalence studies.

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17. The Effects of Non-Premixed Hydrogen on Soot Formation in an Ethylene-Fuelled Lab-Scale Rich-Quench-Lean Combustor

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This work investigates the effects of hydrogen blending on soot formation and flame structure in a laboratory-scale Rich-Quench-Lean (RQL) burner using ethylene-hydrogen mixtures (0-50 vol.% hydrogen) at constant carbon mass flow rate. Laser-induced incandescence and single-ring and multi-cyclic polyaromatic hydrocarbon (PAH) planar laser-induced fluorescence were employed to quantify soot and PAH distributions respectively, while $OH*$ chemiluminescence was used to detect the flame structures and reaction zone location. Hydrogen addition progressively reduced soot by c.a. 9, 36, and 68% at 10, 30, and 50 vol.% blending, respectively, with multi-cyclic PAHs decreasing more than single-ring aromatics. The single-ring aromatics were confined to the early parts of the fuel jet, while the multi-cyclic PAHs spread more downstream. Increasing the percentage of air flowing through the dilution jets results in significant shortening of the flame and reduction in soot, irrespective of the hydrogen content, and to a smaller difference between single-ring aromatics and multi-cyclic PAH distributions, possibly due to the reduction of the residence time in rich mixtures. An additional case with helium instead of hydrogen helped to isolate chemical effects from aerodynamic effects. The results suggests that the chemical effects of hydrogen addition dominate over thermal effects. This study shows that hydrogen addition can control particulate emissions. The dataset enables validation of turbulent combustion models for soot.