Cambridge Particle Meeting

Book of Abstracts

15th June 2018

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Cambridge Particle Meeting

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Time	Name	Affiliation	Title
09:00	**REGISTRATION**		
	Session I (Chair: Jonathan Symonds)		
09:30	Welcome		
09:40	Roy Harrison	University of Birmingham	Studies of Nanoparticles in Diesel Exhaust and Ambient Air
10:00	David Booker	Sensors Inc.	Performance and Operational Demands for low-cost Particle Number Measurements for Periodic Technical Inspection
10:20	Douglas Booker	NAQTS	Integrating a CPC into a "low cost" air quality monitoring device: challenges & opportunities
10:40	Siddharth Gumber	Vellore Institute of Technology	Turbulent mixing and generation of short lived climate forcers from an Asian Mega City: The Soot and Black Carbon Conundrum
11:00	**BREAK**		
	Session II (Chair: Adam Boies)		
11:30	Paul Quincey	National Physics Laboratory	Bringing metrology to measurements of aerosol particle light absorption: the EMPIR Black Carbon Project
11:50	Roger Teoh	Imperial College London	Methodology to Relate Black Carbon Particle Number and Mass Emissions
12:10	Dumitru Duca	Université de Lille	Determining the adsorption energy of aromatic compounds onto carbonaceous surfaces from the signal decay in two-step laser mass spectrometry
12:30	Martin Irwin	Paul Scherrer Institut	Towards accurate aerosol absorption measurements using particles with truly monodisperse size distributions
12:50	**LUNCH & POSTER SESSION**		
	Session III (Chair: Simon Payne)		
13:50	David Kittelson	University of Minnesota	Does the trimodal size distribution adequately describe aerosols from modern engines?
14:10	Caro Hosier	Ford	Activities of the UN PMP (particle measurement procedure) group – exhaust and non-exhaust particle emissions
14:30	Chung Ting Lao	University of Cambridge	Modelling Particulate Emissions during the Active Regeneration of Diesel Particulate Filters
14:50	Hongming Xu	University of Birmingham	Soot formation and particulate characteristics in the cylinder of a Gasoline Direct Injection (GDI) engine
15:10	**BREAK**		
	Session IV (Chair: Brian Graves)		
15:40	Philip Whitefield	Missouri University of Science and Technology	Tandem DMA approach for Real Time Measurements of Deliquescence and Volatility of Plume Processed Jet Engine PM Exhaust
16:00	Lukai Zheng	University of Sheffield	Experimental Investigation on Fuel Properties Impacts on Soot Formation Using a Gas Turbine Combustor
16:20	Tianyi Hu	Imperial College London	Experimental Investigation of Pore Growth in Carbonaceous Nanoparticles during Low Temperature Combustion in O2
16:40	Leonid Nichman	Boston College	Optical characterization of neutral dimers of soot and dioctyl sebacate formed by charged coagulation
17:00	**END**		

Posters

Group 1: Ambient Air, Emissions

1.1	**Markus Bainschab**	Graz University of Technology	First results of vehicle technology effects on sub-23nm exhaust particle number emissions using the DownToTen sampling and measurement system
1.2	**Carl Desouza**	King's College London	Reducing NOX emissions from generators in London, using SCR technology and hybridization of the fleet
1.3	**Chris Nickolaus**	Cambustion	Investigation of brake wear particle emissions from various friction couples in an enclosed brake dynamometer
1.4	**Christopher Chinedu Ogbunuzor**	University College London	In-cylinder sampling and quantification of PAH during combustion of fossil diesel and oxygenated fuels
1.5	**Prahlad Rajhans**	VIT University	Quantifying adaptive thermal comfort levels and PM2.5 removal rates using living green drapes for the regeneration of the Cuffe Parade region of central Mumbai.
1.6	**Matthew Wright**	Centre for Radiation, Chemical & Environmental Hazards	Aerosol measurements from e-cigarette devices in an in vitro Air-Liquid Interface (ALI) cell exposure system
1.7	**Chenjie Yu**	University of Manchester	Characterizing mass-resolved mixing state of black carbon in Beijing using morphology-independent measurement method

Group 2: Fundamentals, Nanotechnology

2.1	**Georg Brunnhofer**	CTR AG	Concept for Holographic Particle Detection
2.2	**Tyler Johnson**	University of Cambridge	Agreement between Different Aerosol Classifiers using Spherical Particles
2.3	**Clémence Le Cornec**	Imperial College London	Development of a virtual soot sensor based on artificial neural networks
2.4	**Paul Maierhofer**	Graz University of Technology	Deposition of micrometric particles on a capacitive sensing area

Group 3: Combustion, Chemistry

3.1	**Jochen Dreyer**	University of Cambridge	Experimental study of the soot particle size distribution inside a vapour-fed co-flow diffusion flame
3.2	**Carlos Garcia**	Imperial College London	In-situ sizing of silica particles in a reacting jet
3.3	**Laura Pascazio**	University of Cambridge	Degree of crosslinking in combustion carbons

09:40-10:00 – R. M. Harrison
Studies of Nanoparticles in Diesel Exhaust and Ambient Air

Roy Harrison*, Mohammed Salim Alam, Ruixin Xu, Christopher Stark, Ajit Singh, Soheil Zeraati Rezaei, Hongming Xu, Rob MacKenzie, Xiaoming Cai, Irina Nikolova, Jian Zhong

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The ERC-funded FASTER project is studying many aspects of the semi-volatile particle emissions from automotive diesel engines. The various facets of the project include the following:

- Collection of particulate matter and associated vapour emissions from a diesel engine using fuels of differing quality and different engine oil lubricants, sampling both before and after a diesel oxidation catalyst and a diesel particle filter [1].
- Chemical analysis of the semi-volatile content (comprising mainly hydrocarbons of C12-C35) using 2-dimensional gas chromatography with Time-of-Flight Mass Spectrometry detection [2, 3].
- Laboratory measurements of the vapour pressures of relevant n-alkanes.
- Field experiments in London in which the evolution of particle size distributions as air advects from a busy roadside into an urban park, and mixes upwards to an elevated sampling point are measured.
- Numerical modelling studies designed to simulate the behaviour of the particles with a high semi-volatile content [4].

Recent highlights of the study will be shown including the characterisation of composition and the behaviour of particles in engine exhaust as measured in the urban atmosphere.

[1]   Alam MS, Rezaei SZ, Stark CP, Liang Z, Xu HM and Harrison RM, Faraday Discuss., 189, 69-84 (2016).

[2]   Alam MS and Harrison RM, Chem. Sci., 7, 3968-3977 (2016).

[3]   Alam MS, Stark C and Harrison RM, Anal. Chem., 88, 4211-4220 (2016).

[4]   Nikolova I, MacKenzie AR, Cai X, Alam MS and Harrison RM, Faraday Discuss., 189, 529-546 (2016).

10:00-10:20 – D. R. Booker
Performance and Operational Demands for low-cost Particle Number Measurements for Periodic Technical Inspection

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With the anticipated widespread introduction of a light-duty Particle Number (PN) Periodic Technical Inspection program in Europe in the near future, Sensors Inc. has been developing a low cost Automotive Particle Bench (APB) for OEM integration and a complete Automotive Particle Analyzer (APA). The unique requirements of operating in the demanding PTI environment require the complexities of performing such measurements to be addressed with specific regards to operation, service and cost of ownership whilst endeavoring to maintain close links to the EU PN established measurement regulations.

This presentation will cover the extensive testing of these products with specific attention on both robustness, ease-of-use and calibration. In particular, metrology studies examining the complexity of calibration in the framework of the resulting measurement uncertainties has been used to provide both value engineering requirements and a potential simplified lower-cost calibration methodology.

Metrology studies of multiple units (both theoretical and experimental) have been used to determine measurement uncertainties for the individual components and the full system. Internal data has been supplemented by external third-party ULAC accredited laboratory data. The data has been used to define and potentially simplify the calibration and setup requirements for potential large-scale deployment of these products into PTI markets. For example, particle size / measurement efficiencies of the devices have been fully characterized from 10-200nm. This data has facilitated the assessment of measurement uncertainty for different engine / after-treatment technologies by simplification of the calibration methodology.

The metrology studies examined flows, pressures, temperatures, size-related particle counting efficiencies, particle losses and system demands.

The results provide clear "value engineering" information by balancing the complexity of the calibration methodology with the calculated and measurement uncertainties. The results clearly suggest that a much simplified calibration methodology, compared with, for example, ISO 27891:2015, could be adopted with only a small increase in the uncertainty budget. Furthermore, potential field calibration and daily check standard operating procedures, to maintain and validate the in-use devices, have been identified.

10:20-10:40 – D. Booker
Integrating a CPC into a "low cost" air quality monitoring device: challenges & opportunities

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National Air Quality Testing Services (NAQTS) has developed an integrated air quality monitor (NAQTS V1000) incorporating the latest developments in low-cost sensor technologies, alongside a regulatory grade Condensation Particle Counter (CPC), thermal desorption tubes (TD), and other environmental measurements. Users can interact with the device using a HTML GUI and a database management system that can be directly uploaded to the cloud. The NAQTS V1000 unit is a portable air quality monitoring station designed to be easy-to-use for high-volume, low-cost measurements, facilitating a holistic understanding of indoor and outdoor air pollution.

The NAQTS V1000 measures Particle Number (CPC - d50 15nm), CO_2 (NDIR), CO, NO_2, and VOCs (electrochemical and metal oxide) and is also fitted with Temperature, Pressure and Relative Humidity measurements. External GPS and Noise measurements are available through USB ports on the back of the equipment. NAQTS' regulatory compliant CPC allows users to measure ultrafine particles, whilst keeping fluid consumption low due to an integrated solvent recovery system. The novel integration of TD tubes for GC-MS into a real-time air pollution monitoring device allows low-cost sensors to be used as triggers for VOC speciation, adding another layer to potential analyses.

This presentation will introduce the community to this new technology, and discuss the challenges and opportunities of integrating a CPC into a "low-cost" air quality measurement device, and making high quality air quality monitoring affordable to everyone. The presentation will also briefly cover some of the main research projects that are using the equipment. Including:

- Indoor Air Quality & Energy Efficiency- Developing models for assisting building design and modification whilst ensuring energy efficiency and good indoor air quality. Investigating the relationship between real-time temporal TVOC concentrations and speciation of VOCs by TD GC-MS.

- Vehicle Interior Air Quality – simultaneous measurements of inside-outside four vehicles to understand *Ingress Ratio* (how much ambient pollution is getting into the vehicle cabin) and *Stuffiness* (how well the vehicle is ventilating CO_2).

- Environmental Justice - Are certain groups more likely to be exposed to poor IAQ? Previous research has suggested that "air pollution follows the poor", however, this was based on outdoor air pollution, despite the fact that we spend 90% of our time indoors.

- Citizen Science - Capturing real-time pollution levels during school drop off/pick up times. Measurements taken by students.

10:40-11:00 – S. Gumber
Turbulent mixing and generation of short lived climate forcers from an Asian Mega City: The Soot and Black Carbon Conundrum

Siddharth Gumber[1], C.R. Sathish Kumar[1,2], Sat Ghosh[1,3]*, Jacob Varghese[1,4]

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This paper delineates the process of activation of soot and black carbon particles over Chennai City into actual cloud droplets. These particles are "short term climate forcers" because their effects last for only up to a few days. They contribute significantly to the aerosol semi-direct and indirect effects. Chennai being a coastal city also receives marine sea salt aerosols comprising of both film and jet modes blown over by horizontal winds. The city is also known for its notorious traffic conditions where non-stringent regulatory mechanisms result in the copious release of soot and black carbon particles from a high traffic density. Archaic wood-fired cook stove emissions from shanty slum hutments also add up to the PM emission loads. The experimental determination of the source strengths of stoves was done in a controlled manner with considerations for the equipment and particulate collection rate. Grab sampling method was adopted and particle segregations were effected through Fine Particulate Sampler which segregated particles less than of size 10μm diameter with adjusted flow rate. This was followed by a UV-Spectrometry analysis to ascertain the presence of soluble sulphates in the collected samples. The presence of inorganic sulphates in Chennai's aged aerosols ensured that some of these particles are activated into droplets. It is clear that when strong up draughts blow the aerosol up into Chennai's turbulent boundary layer, the resulting signature is very complicated. The novelty of this paper lies with a clear quantification of the percentage of activated nuclei using a sophisticated chemical parcel cloud model. The first results show that 80% of such partciles are activated as haze and very small low-lying cloud droplets hovering over Chennai's lower boundary layer and adding to its ever deteriorating air quaility index (AQI). This happens because the resultant droplet size spectrum is biased to a single humped spectrum inhibiting stochastic coalescence to promote autocoversion to rain droplet formation.

11:30-11:50 – P. Quincey

Bringing metrology to measurements of aerosol particle light absorption: the EMPIR Black Carbon Project

Paul Quincey*, Heli Raitanen, Francois Gaie-Levrel, Andreas Nowak, Kostas Eleftheriadis, Thomas Mueller, Ernest Weingartner, Konstantina Vasilatou, Martin Gysel

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Measurements of dark carbonaceous particles produced by incomplete combustion, loosely called "soot", have long been made using simple optical techniques, This Black Carbon (BC) is widely recognized as the foremost particulate absorber of solar radiation in the atmosphere and has been associated with the detrimental health effects of air pollution. The atmospheric-science community has developed an array of technologies for monitoring BC concentrations based on light absorption measurements. In general, the absorption is interpreted as a mass concentration of Equivalent Black Carbon (EBC) by using a standard mass absorption cross-section. The most common field instruments collect the aerosol particles onto a filter, which greatly complicates their optical properties. Various options are available for the calibration of such instruments, based on substantial efforts from the community. However, there is a lack of SI traceability for absorption measurements where no filter is involved, and a lack of standardized calibration methods for filter-based instruments.

The EMPIR Black Carbon project, *Metrology for light absorption by atmospheric aerosols (2017 – 2020)*, aims to establish SI traceability for atmospheric aerosol light absorption measurements for filter-free methods such as extinction minus scattering, photoacoustic, and photothermal interferometry, and standardised calibration methods for filter-based instruments. To this end, its specific scientific objectives are to (1) develop a traceable and primary method for measuring aerosol absorption at specific wavelengths, with defined uncertainties, (2) recommend well-characterized reference aerosols suitable for challenging filter-based instruments, and (3) develop a validated method for the in-situ calibration of filter-based field instruments.

This presentation aims to summarize the goals and early progress of the EMPIR project, in order to encourage and invite contributions from the wider community.

11:50-12:10 – R. Teoh
Methodology to Relate Black Carbon Particle Number and Mass Emissions

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Black Carbon (BC) Particle Number (PN) emissions from various sources contribute to the deterioration of air quality, adverse health effects, and anthropogenic climate change. In particular, BC PN emissions contribute to the formation of contrails and is a critical input parameter for contrail models. However, BC mass measurements and models are more commonly available than PN data for aviation emissions and other applications such as remote sensing measurements for vehicles and health studies. Previous methodologies used to estimate aviation BC PN emissions also relied on simplified assumptions.

This research critically reviews fractal aggregate theories that describe aggregate properties including mass, diameter and morphology to develop a methodology in relating BC PN and mass emissions. The new methodology, named as the FA model accounts for the differences in particle size distribution and aggregate morphology. It is validated with three distinct BC emission sources: an internal combustion engine, an inverted burner, and two aircraft gas turbine engines. Validation results show that the estimated BC PN emissions is in good agreement with the measured value. R^2 values range from 0.68 to 0.99, while Normalised Mean Bias (NMB) values are in between -10.6% and +41.5%. Uncertainty and sensitivity analyses show that the FA model estimates have an uncertainty range of ± 52% (1.96σ) and are most sensitive to uncertainties in the geometric standard deviation of the BC particle size distribution. Given the improved performance in estimating BC PN emissions from various sources, we recommend the FA model to quantify BC PN effects on health and climate, where measurements of PN are scarce.

12:10-12:30 – D. Duca
Determining the adsorption energy of aromatic compounds onto carbonaceous surfaces from the signal decay in two-step laser mass spectrometry

Dumitru Duca[1]*, M. Vojkovic[1], Y. Carpentier[1], M. Ziskind[1], A. Faccinetto[2], C. Focsa[1]

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Global extensive emission of fine and ultra-fine carbon-based particulates presents a well-known health risk and raises significant environmental concern. The toxicity of carbonaceous particles, soot in particular, is mainly determined by their surface composition and reactivity. It is thus important to have information on the actual interaction (physisorption, chemisorption) of adsorbates with the particle surface, and if possible to have an estimation of the adsorption energy. This can be an arduous task for a "real-world" soot particle bearing a multitude of molecular compounds on a (usually) full-of-defects surface. Selective monitoring of individual compounds in mass spectrometry can be useful in this context. Among the variety of molecules which can be encountered on a soot particle surface, the Polycyclic Aromatic Hydrocarbons (PAH) are of paramount importance, both for fundamental mechanisms (crucial role in soot nucleation and growth) and for toxicology issues (proven carcinogenic effect).

We propose in this study an original method for measuring the adsorption energy of PAHs onto a carbon surface. This method is using the pulse-to-pulse signal decay in a Two-step Laser Mass Spectrometry (L2MS) approach, developed in our lab over the last decade to specifically probe the chemical composition of soot particles with high sensitivity and selectivity [1]. For this initial study, "synthetic" soot samples were produced in the laboratory by adsorbing a well-determined amount of selected pure PAHs onto commercial black carbon particles, thus allowing us to work in controlled conditions in terms of adsorbate surface concentration.

The new method proposed here is based on the assumption of quasi-thermal desorption at low laser fluences. Two approaches are derived and used for the measurement of the adsorption energy. For the first one, the signal for the PAH of interest is measured for a multitude of successive desorption laser pulses. The data is then fitted with a pseudo-exponential decay (number of desorbed molecules vs number of applied laser pulses). The second method consists in recording the 'fluence characteristic', which denotes the variation of the signal intensity with the desorption laser fluence. The signal corresponding to the first laser shot was recorded for a multitude of laser fluences and enabled us to, once again, retrieve the adsorption energy of different PAHs onto the black carbon surface. These two different approaches complement each other, thus helping to obtain a more precise result by reducing the uncertainties induced by possible non-homogeneous surface concentration and/or fluctuations in laser fluence.

First results on common interest PAHs, such as pyrene and coronene, will be presented. These results show good agreement with adsorption energies reported in the literature, thus providing a proof-of-concept for the new method.

[1]   A. Faccinetto *et al.* (2015), *Environ. Sci. Technol.*, 49, 10510, doi: 10.1021/acs.est.5b02703.

12:30-12:50 – M. Irwin
Using particles of truly monodisperse size distributions to improve the accuracy of in situ aerosol absorption measurements

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Aerosol light absorption contributes to the earth's radiative forcing budget through the absorption of solar radiation and subsequent heating of the absorbing aerosol layer (direct effect). Beyond the direct effect, this heating can effect cloud formation and longevity (secondary effects). Black carbon (BC) dominates aerosol light absorption in the atmosphere, with significant but poorly constrained influences from brown carbon and mineral dust. Sources of these absorbing aerosols include numerous combustion processes such as biomass burning and power generation, as well as from dust entrainment.

For particles much smaller than the wavelength of incident light, absorption is directly proportional to the particle volume and mass (Rayleigh regime). For particles at or larger than the wavelength of incident light absorption, still approximately proportional to volume and mass, can be calculated with Mie theory for spherical particles and with more complicated numerical methods for other particle shapes.

However, quantitative measurement of aerosol light absorption is still a challenge. Filter based techniques are prone to multiple measurement artefacts (e.g. concentration dependence, changes to filter behaviour due to particle deposition, scattering interference). In situ absorption measurements include photoacoustic, refractive index-based, incandescence-based, and extinction minus scattering (EMS) techniques. Applications of the EMS technique most commonly used two separate instruments measuring scattering and extinction; each propagating their own errors through to the derived absorption. The relatively recent CAPS PMSSA uses a cavity enhanced absorption technique to achieve an extremely long path length (order of several km) thus improving extinction sensitivity, and as such is one of the first instruments to simultaneously measure ambient extinction and scattering for the same aerosol sample. Extinction is measured due to a phase shift in the laser cavity due to the presence of aerosol, and scattering measured using an integrated sphere and PMT.

However, no technique is without its limitations, and one such limitation with the CAPS PMSSA is that as the particle diameter approaches the wavelength of the laser, the forward scatter-component increases in magnitude and more light is lost through the exit of the integrating sphere than for a much smaller particle following Rayleigh scattering principle. This "truncation effect" increases with particle diameter. Coupling the CAPS PMSSA to the Aerodynamic Aerosol Classifier (AAC; which supplies a monodisperse aerosol free from multiple charging artefacts), accurate quantification of this truncation effect across a wide particle size range (70nm – 5µm) has been performed for PSL and Ammonium Sulphate aerosols, with the aim of reducing uncertainties and constraining models for use alongside improved ambient measurement.

13:50-14:10 – D. Kittelson
Does the trimodal size distribution adequately describe aerosols from modern engines?

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Engine exhaust size distributions generally are well described by trimodal lognormal distributions with 2 submicron modes, the nucleation mode and the accumulation (or soot) mode; and a third mode, typically consisting of particles larger than about 0.5 μm, the coarse mode. However, this description may not adequately describe size distributions produced by some modern engine configurations. The coarse mode is not directly produced by combustion so only submicron particles are considered here.

Common practices that hide the modal structure include using heated dilution which often largely eliminates the nucleation mode and averaging instrument response over an entire test cycle leading to overlapping and merging of modes. However, other cases may be less obvious.

Modes may be incorrectly identified, interpreted. For example, size distributions from well mixed low temperature combustion engines operating with near soot free combustion often show a single submicron mode in the accumulation mode size range that is sometimes identified as an accumulation (or soot) mode because of its size. In this case, it really a mode formed by nucleation and growth semi-volatile materials, which in the absence of soot to adsorb semi-volatile material, grows into the accumulation mode size range.

Apparently lognormal distributions, on close examination may not be lognormal. For example, size distributions measured in the exhaust exit plane of aircraft gas turbines typically exhibit a single submicron mode consisting mainly of carbonaceous soot particles. Superficially the mode appears to be lognormal but closer examination reveals that it is much more accurately described by two, closely spaced, nearly overlapping soot modes.

In some cases, nearly no modal structure is evident. Recent work with a gasoline direct injection engine running in lean and stoichiometric modes shows significant departures from typical lognormal size distributions, instead showing very broad flat size distributions. There does not appear to be a clear modal structure.

These examples and others will be discussed along with possible reasons for departures from the lognormal structure.

14:10-14:30 – C. Hosier
Activities of the UN PMP (particle measurement procedure) group – exhaust and non-exhaust particle emissions

C. Hosier[1]*, G. Martini[1,2], T Grigoratoros[2]

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The PMP (particle measurement procedure) group operating under the auspices of the United Nations in Geneva continues to make progress on globally harmonised particle measurement regulation procedures. In the most recent mandate period, PMP activities include developing a robust particle number measurement method to include more of the sub-23nm non-volatile particles and revisiting the calibration materials. PMP is leading the global activities with an expanded mandate to also include non-exhaust emissions – in particular brake particles and tyre/road wear particle measurement. The presentation will provide a short overview of the current status of the PMP activities and expected timeline of next steps.

14:30-14:50 – C. T. Lao
Modelling Particulate Emissions during the Active Regeneration of Diesel Particulate Filters

Chung Ting Lao[1]*, Jethro Akroyd[1], Nickolas Eaves[1], Alastair Smith[2], Neal Morgan[2], Amit Bhave[3], Markus Kraft[1,4]

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A numerical model has been developed to describe the size-dependent effects that are responsible for transient particle mass (PM) and particle number (PN) emissions observed during experiments of the active regeneration of Diesel Particulate Filters (DPFs). The model uses a population balance approach to describe the size of the particles entering and leaving the DPF, as well as those accumulated within the DPF. The population balance model is coupled to a unit collector model that describes the filtration of the particles in the porous walls of the DPF. In addition, a reactor network model is used to describe the geometry of the DPF. Two versions of the unit collector model were investigated. The original version, based on current literature, and an extended version, developed in this work, that includes terms to describe both the non-uniform regeneration of the cake and thermal expansion of the pores in the DPF. Simulations using the original unit collector model were able to provide a good description of the pressure drop and PM filtration efficiency during the loading of the DPF, but were unable to adequately describe the change in filtration efficiency during regeneration of the DPF. The extended unit collector model has shown to be able to describe both the timing of particle breakthrough and the final steady filtration efficiency of the regenerated DPF. Further work is required to better understand the transient behaviour of the system and improve the predictive power of the model. In particular, we stress the importance that future experiments fully characterise the particle size distribution at both the inlet and outlet of the DPF.

14:50-15:10 – Y. Mei

Soot formation and particulate characteristics in the cylinder of a Gasoline Direct Injection (GDI) engine

Yuanzhuo Mei, Yusong Yu, Hongming Xu*

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Soot formation and particulate characteristics in the cylinder of a Gasoline Direct Injection (GDI) engine are investigated using modelling and experimental approaches. The spatially zero-dimensional model -Stochastic Reactor Model (SRM Engine Suite) is used for the simulation, and the experimental results are obtained from a single-cylinder, four-stroke GDI research engine. Detailed information on the soot morphology and associated bulk quantities, such as particle number concentration, mass concentration and particle size distribution are examined. In the first step, the SRM is calibrated by experimental data obtained under late injection and stoichiometric operating condition. The in-cylinder pressure profile and heat release rate profile are matched with the experimental data. Then the in-cylinder soot formation with different injection timing strategies are simulated. Results obtained from the simulation are compared with those from experiments, and reasonable agreement can be observed. The results show that there is a significant increase in the particle number concentration as the injection timing retards as a result of insufficient time for spray vaporization and mixing. In addition, the rates of associated processes to form soot aggregates are obtained as a function of crank angle, including Coronene inception, Coronene condensation, coagulation. It can be found that the injection timing affects the Coronene inception rate, which is believed to be directly related to the soot formation.

15:40-16:00 – P. D. Whitefield
Tandem DMA approach for Real Time Measurements of Deliquescence and Volatility of Plume Processed Jet Engine PM Exhaust.

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Soluble Mass Fraction (SMF) and Volatile Mass Fraction (VMF) measurements were made on PM emissions from a stationary aircraft-mounted CFM56-2C1 gas turbine engine. The engine was operated at several power levels, burning JP-8, and two sustainable renewable jet fuels: a coal-based Fischer-Tropsch (FT) fuel, and a Tallow-based Hydroprocessed Renewable Jet (HRJ) fuel. In addition, blends of JP8 and HRJ and FT with 1000 ppm sulfur added (THT) were also studied. Emission samples were extracted at the engine exit plane (1m), in the near field (30m), and in the advected plume (145m). Condensation particle counters and electrical mobility-based size spectrometers were used for number and size distribution measurements. Volatility and deliquescence measurements were conducted on the downstream samples, using a thermal denuder operating at 300 C and a tandem differential mobility analyzer with saturator, to determine the aerosol's SMF and VMF. The performance of the measurement system will be discussed as will the fuel/engine operating condition-specific data acquired.

16:00-16:20 – L. Zheng
Experimental Investigation on Fuel Properties Impacts on Soot Formation Using a Gas Turbine Combustor

Lukai Zheng*, Bhupendra Khandelwal**

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Diversified fuel supplies and the stringent environmental pollution regulations in the aviation sector promoted the development and prosperity of the alternative fuels industry. The chemical and physical properties of those diverse fuel substitutes lie outside the historical experience. Therefore, the combustion behaviour cannot be judged by the outdated research of petroleum-derived jet fuel. A large scale experimental testing is essential to improve our understanding of alternative fuel effects on the combustion performance and environmental impact.

The aim of this study was to evaluate the impact of fuel properties and composition on the particulate matter (PM) emissions characteristics and flame sooty tendency profile on a Rolls-Royce Tay gas turbine combustor. 16 kinds of alternative fuels have been tested under stable burning and lean burning conditions. PM emissions were measured via DMS 500 and soot propensity profile was analysed using an innovative visual method based on flame luminosity high-speed imaging.

The results show that the high value of aromatics is main leading factor for insufficient burning and heavier soot formation. In addition, fuel with higher density, cyclo-paraffin content and surface tension may also have potential to induce soot promotion to some extent. On the contrary, the fuel with high hydrogen content can perform much more environmental friendly. Furthermore, it was observed that the results of PM emission measured by DMS 500 and sooting tendency computed via imaging method correlated particularly good for all the tested fuels and conditions in this study. These soot emission monitoring methods can be used as mutual inspection, supplement and support. The imaging detection method can be considered an alternative evaluation method for qualitative soot emissions.

16:20-16:40 – T. Hu

Experimental Investigation of Pore Growth in Carbonaceous Nanoparticles during Low Temperature Combustion in O_2

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Diesel engines are a significant source of particulate matter (PM), which is a major air pollutant threatening human health. An effective solution is using a diesel particulate filter (DPF), which reduces PM emissions by trapping soot and then removing it through a regeneration process. During regeneration, the soot is either burned periodically with O2 at a raised temperature or continuously oxidised over a catalyst at the exhaust temperature. This study investigated the burning mechanism of a surrogate soot, Printex U, and developed both experimental and theoretical methodologies to explore the microstructural changes of carbon particles during oxidation in O2. The experimental results showed a second maximum in reaction rate, which suggested that the reacting surface area of carbon spherules increased at the early stage of burning. This phenomenon contradicted the uniform shrinkage framework, where a carbon particle's surface area will decrease as exterior oxidation progressed. It was postulated that O2 accessed the interiors of carbon spherules while they were burning, causing pore growth and intersection within the spherules and resulting in an increase of the reacting surface area. To verify this assumption, a random pore model which can describe such behaviour was fitted to experimental data, with two parameters in the model being adjusted by applying an effective optimisation algorithm. Sensible agreements between the model and experimental data were obtained, and values for the two parameters were physically meaningful. This observation not only agreed with the spherules' internal structural change of pore growth and intersection during burnout in O2, but also supported some researchers' findings that through a process called graphitization during heat treatment, the outer surface of particles formed graphenelike layers which were more ordered but less reactive, compared with the disordered but highly reactive core. The apparent activation energy was found to be 134.3 27.5 kJ mol-1, which was consistent with literature findings and suggested no diffusional limitation in the system, since otherwise a much lower apparent activation energy should have been observed. This also indicated that O2 had no preference to surface reaction at the spherule's exteriors.

Various measuring instruments and experimental methods were applied in this study. It was found that thermogravimetric analyser (TGA) measurement had a significant mass transfer limitation at a high temperature, while the packed bed reactor with a Fourier transform infra-red (FTIR) spectrometer can achieve reasonably accurate measurements in terms of the mass balance and reaction rates. For an appropriate deconvolution of the measured results to eliminate effects such as delay or concentration change during real measurement, it was found that an FTIR gas cell can be modelled as a first order lag and it is recommended to use a fast-response mass spectrometer (MS) to obtain residence time distribution in a FTIR gas cell for certain gas flowrates. Measurements of the surface areas of carbon particles during combustion at different conversions are being carried out using a sensitive BET surface analyser, to further investigate and elucidate this burning mechanism.

16:40-17:00 – L. Nichman
Optical characterization of neutral dimers of soot and dioctyl sebacate formed by charged coagulation

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Black carbon (BC) is produced from the incomplete combustion of biomass and fossil fuels, and consists mostly of elemental carbon monomers that are aggregated into more complex structures that strongly absorb light across the visible spectrum. The size distributions of BC-containing particles evolve in plumes due to coagulation of soot along with deposition and/or evaporation of a variety of atmospheric organic compounds. [1].The resulting internal mixing state of the BC particle with other species can have a core shell structure (concentric) or an eccentric dimer structure. The formation of internally mixed eccentric dimers can be enhanced by coagulation between oppositely charged particles produced in the process of particle generation or by atmospheric ionization.

The absorption of light by BC is typically enhanced beyond the bare particle case due to organic coatings. Although such organic coatings themselves do not absorb light, the coated black carbon particles present a larger optical cross section resulting in a phenomenon called "lensing" that enhances the absorption of light by the BC. Laboratory and modelling studies have shown that the addition of non-black-carbon materials to black-carbon particles may enhance the particles' light absorption by 50 to 60% due to refraction and reflection of light. Evidence from field studies for this 'lensing' effect is scant and conflicting, showing that absorption enhancements can be less than 5% or as large as 140% for the same amount of organics in the particle [2,3]. Laboratory and field measurements of absorption enhancement discrepancies could be partially attributed to particle population diversity in composition, and particularly the configuration of coagulated dimers [4]. If the soot and organic particles coagulate without merging into a core shell configuration, absorption enhancement would not be expected.

To test this hypotheses we developed a controlled method to generate and characterize the neutral dimer formed in the coagulation process of positive and negative charge monodisperse distributions of nanosized soot and dioctyl sebacate aerosols. Two differential mobility analyzer (DMA) systems in tandem with centrifugal particle mass analyzer (CPMA) enabled the identification of the mass of the neutral dimer formed in an 8 L mixing volume, while uncoagulated charged particles were removed with an electrostatic precipitator. The dimer was then mass selected and its optical properties were measured in the Cavity Attenuated Phase Shift single scattering albedo (CAPS-PMssa) monitor, and single particle soot photometer (SP2).

Our results demonstrate the efficiency of charged coagulation and its role in the explanation of the discrepancies observed in the mean measurement of ambient environment compared to the single

particle information obtained in laboratory experiments. We discuss the efficiency and the limitations of this technique and present the absorption enhancement for different internal mixing ratios of the dimer.

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Poster Presentations

Poster 1.1 – M. Bainschab

First results of vehicle technology effects on sub-23nm exhaust particle number emissions using the DownToTen sampling and measurement system

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Introduction

Modern and near-future combustion engine vehicle technology may emit notable levels of particles below the current particle size threshold (23 nm) of the European Particle Number (PN) emission standards. Studies suggest that sub-23 nm particles might be even more harmful to humans than larger particles. The Horizon 2020 funded project DownToTen (DTT) is developing a sampling and measurement methodology to characterize exhaust aerosol emissions down to at least ten nanometers. The focus is on the newest generations of direct injection gasoline and diesel engines under real world conditions. Based on detailed investigations of the nature and characteristics of these particles, DownToTen is evaluating a variety of sub-23 nm PN measurement instruments and sampling approaches, using rigorous criteria under conditions of challenging aerosol from a variety of sources. This study presents the first prototype of a Portable Exhaust Particle Sampling system (PEPS) developed in the framework of the project together with preliminary results from the assessment of different vehicle technologies.

Methodology

The performance of the DTT PEPS was first assessed in comparison to commercial regulation compliant sampling systems. The double porous tube dilution system exhibited an excellent linear correlation with commercial systems across four orders of magnitude, when considering measured particle concentration data from conventional >23 nm particle counters. Particle Concentration Reduction Factors (PCRF), accounting for losses and dilution, measured in two laboratories from

the DTT system both with and without an optional tertiary dilution stage (ejector dilutor), were consistent with production systems in the size range >23 nm, and fully compliant with current regulatory requirements. This indicates that the DTT prototype in its present configuration would be compliant with current, requirements for Constant Volume Sampling (CVS)-based PN sampling, while also providing measurement of <23 nm with low particle losses.

After initial laboratory characterization, two DTT systems were employed to preliminarily survey existing and development vehicles for the presence and magnitude of both sub-23 nm PN, measured primarily with 10 nm d50 particle counters, and the current regulatory range, nominally "PN23" emissions.

Results & Conclusions

The evaluations indicated that when standard emissions cycles are considered, the majority of emissions were below the Euro 6c limit value of 6×10^{11} #/km for >10 nm PN. Drive cycles containing Diesel Particulate Filter (DPF) regenerations showed elevated PN emissions above the limit value, but when the contribution of these events is adjusted for the frequency of regenerating to non-regenerating tests, even >10 nm results fall back below the current regulatory particle number emissions limit. Some gasoline vehicles, both with and without Gasoline Particulate Filter (GPF), and diesel applications including Lean NOx Trap (LNT), also had PN emissions close to but above the limit, for >10 nm, and occasionally, >23 nm particles. This indicates development immaturity of these emissions control technologies.

Based on these preliminary findings, work in the project continues towards the assessment of the latest engine, emission control technologies and fuels under real drive emissions conditions.

Poster 1.2 – C. Desouza

Reducing NO$_X$ emissions from generators in London, using SCR technology and hybridization of the fleet
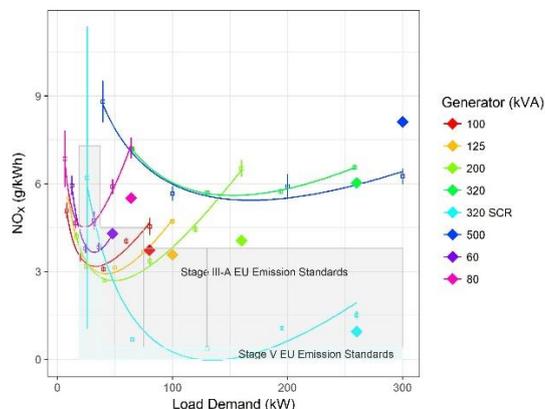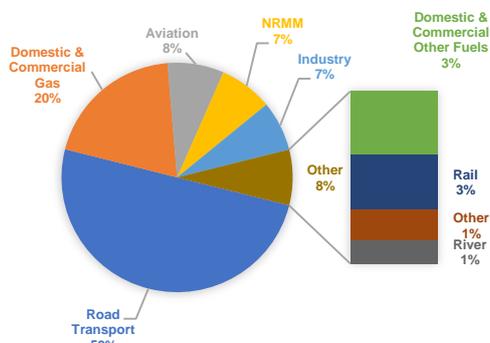
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Background

The London Atmospheric Emissions Inventory attributes 7%, 11%, and 2% to NO$_X$, PM$_{2.5}$, and CO$_2$, respectively, to non-road mobile machinery (NRMM) in London [1]. Generators are one of the most commonly used types of NRMM on construction sites, and the register of construction machinery for London [2] quantifies generators as the 4th most common NRMM type, which is 6% of the fleet. They therefore contribute significantly to NO$_2$ and PM$_{2.5}$ pollution problems in London, which is a major concern for public health. This study aimed to compare the emissions from diesel generators with and without exhaust after-treatment, and diesel-battery hybrid systems, during operation.

Sources of NO$_X$ emissions[1] (tonnes/year) in London during 2013

Measured generator NO$_X$ emissions v/s load demand

Methods

Emission factors of seven generators with different capacities (60, 80, 100, 125, 200, 320, and 500 kVA) were measured using a portable emissions measurement system (PEMS). The engines used by the generators varied in age, engine size, and operational hours. The ISO 8178 standard D2 cycle was used to test the generators, which were all Stage III-A. Selective catalytic reduction (SCR) was trialed as an exhaust gas after-treatment, for the 320kVA generator, and the emissions factors were compared with the pre-SCR trial emissions factors.

Results

Measured emission factors showed that minimum NO_X emissions were recorded at 25-50% engine operation. The measured emission factors were coupled with the register of construction machinery and activity data, to quantify the emissions from generators in London. This resulted in emissions of 186.08t NO_X. The SCR emission factors were applied to the >100kVA generators. This resulted in emissions of 54.32t NO_X.

Conclusions

If hybridization were rolled out to the <100kVA generator fleet in London, it would decrease emissions by 2.9% for NO_X. If SCR were implemented to >100kVA generator fleet in London, it would decrease NO_X emissions by 70%.

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Poster 1.3 – C. Nickolaus

Investigation of brake wear particle emissions from various friction couples in an enclosed brake dynamometer

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The ongoing reduction in particle mass & number emissions from engine exhaust have meant that brake wear particle emissions are coming increasingly into focus within the automotive and brake industry. There is active research into emissions reduction by advances in friction materials, regenerative braking and even filtration. As yet, no common agreement exists for the way in which particles emitted by the brakes are to be measured.

TMD Friction's current study in collaboration with Cambustion and MS4 demonstrates a well-suited method for measuring brake emissions on an enclosed inertia dynamometer, using a CVS approach with a sophisticated air flow concept and sampling design. By using this methodology the potential of various friction couples to reduce brake emissions can be investigated; particle size, total number and mass are measured during a test schedule comprising urban and extra-urban sections. It will be shown that total number emissions are generally dominated by high demand braking events when a certain temperature threshold (dependent on friction material) is exceeded, leading to high concentration releases of sub-20 nm particles.

Poster 1.4 – C. Ogbunuzor

In-cylinder sampling and quantification of PAH during combustion of fossil diesel and oxygenated fuels

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Polycyclic Aromatic hydrocarbons (PAHs), a class of hydrocarbons which are toxic, carcinogenic and mutagenic to humans, made up of two to six benzene rings joined together in different arrangements, are emitted from a range of combustion sources (including IC engines) and are of serious concerns to human health as PAHs are transported into the human body when particulate matter is inhaled. Low molecular weight PAHs, which consist of two to four benzene rings, exist mainly in the gaseous phase while high molecular weight PAHs, which consist of five to six benzene rings, exist mainly in the solid phase, adsorbed onto soot particles (also referred to as particulate matter) and are 100-1000 times more toxic than light molecular weight PAHs. Previous studies have shown an influence of both conditions during combustion and fuel composition on levels and species of PAH emitted; however, the extent to which, for example the presence of fuel-bound oxygen, impacts on the formation route of individual PAHs produced during combustion is not well known. In designing fuels for the future, understanding how the composition of the fuel determines the formation of specific PAH during combustion, and thus the toxicity of the particulate matter emitted from the engine exhaust, is essential for achieving clean burning fuels. Therefore, this project experimentally investigated the speciation of PAHs and its precursors during combustion in a modern diesel engine when fuelled with fossil diesel and fossil diesel-oxygenated fuel blends via in-cylinder and engine exhaust sampling. Prior to the engine tests, the PAHs present in the liquid fuels were identified and quantified using GC-MS. Particulate matter and gas phase PAHs were collected using quartz filter papers and XAD-2 resin respectively during the combustion cycle at four sampling points (370, 385, 400 and 415 CAD) with a fast sampling valve and at the engine exhaust, with subsequent analysis of these samples by GC-MS. GC-MS analysis of the liquid fuels prior to combustion showed that fossil diesel had the highest PAH content which was predominantly naphthalene, with lower amounts of Acenaphthalene, Fluorene and Pyrene while unblended SME biodiesel and methyl decanoate had a negligible PAH content. During combustion, at 370 CAD, M20 produced the highest total (gas phase and soot-bound) amount of PAH species relative to fossil diesel and B20. At 385 CAD, following the end of the premixed combustion phase, a significant decrease in total PAH species present occurred for all the fuels tested, attributable to increased oxidation rates as in-cylinder temperature increased. From 385 CAD through 400 CAD to 415 CAD, the total level of PAH species increased slightly due to accumulation and as a result of decreased oxidation rates. In the case of all the fuels tested, the abundance of PAH decreased significantly prior to sampling from the exhaust, with pure diesel fuel emitting twice the level of PAH emitted by the oxygenated fuel blends on a per volume of exhaust gas basis.

Poster 1.5 – P. Rajhans

Quantifying adaptive thermal comfort levels and PM2.5 removal rates using living green drapes for the regeneration of the Cuffe Parade region of central Mumbai

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There are striking similarities in the sky line of both Hong Kong and the Cuffe Parade region of Central Mumbai. Both have high-rise complexes, housing up to 180 office workers per floor with buildings crammed within a narrow strip of land. The building density of both cities are respectively 104.3 and 101.5 per square km. Whilst the former boasts of enviable levels of thermal comfort albeit using excessive HVAC loads, the latter i.e. Mumbai is fast succumbing to the pressures unleashed by unsustainable surges of migrant populations from the rest of the country. Although both cities receive a mixture of marine and continental aerosol particles, Mumbai's PM2.5 and PM10 pollution levels are alarmingly high. The AQI for PM2.5 over Mumbai stands at 330. The main cause is attributed to the very high PM2.5 and PM10 particles generated from auto rickshaws, trucks and busses totaling a staggering 27.81 Kg/Day in the Cuffe Parade area.

This first design study proposes the use of Hedera helix or English Ivy brought over to Mumbai during the British Raj. This study shows how the same creeper can be used as a sustainable green drape to cleanse a 32 storeyed skyscraper from the menace particulate pollution generated by the above mentioned sources. Thence, we also show how a frame mounted drape clad with Hedera helix also increases the adaptive thermal comfort levels inside. This study performs new calculations on estimating the U value (thermal transitivity) of this drape to work out the heat transfer rates across open plan office spaces. It is found that the depth of the passive zones increases by a sizeable fraction causing a concomitant decrease in the HVAC loads. The Complex airflow patterns mediated by the process of displacement ventilation are modelled through a suite of CFD codes including the effects of shear generated turbulence within the said space. This provides a comfortable air changes per hour without any extra HVAC loads and results in substantial energy savings in an overstretched Mumbai city.

Poster 1.6 – M. Wright

Aerosol measurements from e-cigarette devices in an in vitro Air-Liquid Interface (ALI) cell exposure system

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Whilst assessment of the potential public health impact of e-cigarette use suggests a reduction in harm relative to smoking conventional cigarettes, risk assessments are at present still based on limited knowledge. E-cigarette emissions contain a range of gas-phase and aerosol components with varying properties and respond very strongly to changes in humidity, dilution and temperature conditions, meaning that different measurement techniques result in, for example, very different particle size distributions. Hence, in any experimental setup, the dose estimate and assessment of toxicological response induced by e-cigarette aerosol depends critically on the conditioning and measurement processes.

Here, an experimental setup to examine the effect of e-cigarette aerosol exposure to human bronchial epithelial cells in vitro in an Air-Liquid Interface (ALI) system is presented, designed to replicate aerosol thermodynamic behaviour along the path from device-to-lung in 'real-world' use. The ECAG (e~Aerosols, USA) is used to generate aerosol from a 3rd-generation e-cigarette using the CORESTA 81 vaping cycle (3 s puff of 55 ml every 30 s). Emissions (gases and aerosol) are passed to a Cultex ALI exposure system heated to 37°C with a water bath. Dilution flow is humidified to > 90% through a bubbler system and maintained at 1.7 litres per minute, approximating the dilution taking place during an average breath of tidal volume 750 ml (~15:1). Aerosol-associated nicotine concentration deposited in the Cultex is determined by washing 'blank' exposure wells with 1 ml milli-Q water and assessed using UHPLC-HESI-OrbiTrap (Thermo), and elemental composition via ICP-MS (iCAP Q, Thermo). Particle number concentrations (PNC) are assessed using a CPC (TSI 3075) at the exhaust outlet, after dilution at ~150:1 (Palas VKL100).

PNC is variable from puff to puff despite supposedly identical generation conditions, a result also seen in previous studies. Typical peak concentrations (corrected for dilution) are 3.0×10^8 cm-3 (S.D. $\pm 0.4 \times 10^8$ cm-3) while cumulative particle number passing through each ALI exposure chamber over a 10-puff exposure is 5.7×10^9. Some variability in nicotine concentration was observed over the three Cultex exposure chambers (200, 200, 286 ng respectively for 10-puff exposure to 18 mg ml-1 nicotine e-liquid) highlighting the need for continued assessment of deposition efficiency within the ALI system. Initial analysis of the elemental components within the aerosol via ICP-MS suggest the presence of some metals (Fe, Ni, Cr, Mn, Co, Cu, Sr, Ba, Pb, Ti, Zr, Zn, Mo, Sn) at a range of abundances.

Ongoing work includes a) exposure of HBEC-3KT immortalised human bronchial epithelial cells to a range of nicotine concentrations followed by rt-qPCR to measure changes in the expression in genes involved in the bioactivation of tobacco specific nitrosamines (TSNAs), cell viability (Alamar blue assay) and cytotoxicity (LDH assay), and b) particle size distribution measurement by SMPS and DMS and direct sampling and quantification of metals, TSNAs and other constituent

components of aerosol collected under different generation and conditioning parameters (RH, dilution, e-liquid) to investigate their effect on physicochemical properties of the e-cigarette aerosol.

Poster 1.7 – C. Yu

Characterizing mass-resolved mixing state of black carbon in Beijing using morphology-independent measurement method

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The mixing state of black carbon (BC) significantly determines its absorbing efficiency and may modify its regional and global radiative forcing impact and may also influence toxicology. Here, with the aim of identifying the mixing state of BC, an experiment was devised as part of a large joint UK-China project investigating air quality in Beijing, Air Pollution and Human Health-Beijing (APHH-Beijing). During this experiment, we successfully applied a morphology-independent mass measurement of BC for intensive measurements in both winter and summer. We directly selected the particle mass using a Centrifugal Particle Mass Analyser (CPMA, Cambustion Ltd) and passed these monodisperse particles to a single particle soot photometer (SP2, DMT inc.) to characterize refractory BC mass for each single BC-containing particle. The coupling of CPMA-SP2 can thus quantify the mixing state of BC without assuming any particle morphology. The CPMA-SP2 results have been applied to a recently published inversion algorithm to derive the full distributions of particle number according to total mass and rBC mass, and this is the first time we applied this inversion method developed by the University of Alberta to the field work. Such detailed mass-resolved BC mixing information could be used as optical model input to estimate the optical properties, and also the micro-scale processing model to investigate the atmospheric processing of BC.

Poster 2.1 – G. Brunnhofer

Concept for Holographic Particle Detection

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The determination of aerosol particle number concentrations is commonly done with Condensation Particle Counters (CPC). CPCs consist of a Condensation Nucleus Magnifier (CNM) unit to make nanoparticles optically detectable and a counting unit. Default counting units rely on a nozzle to separate the droplets condensed around the particles and count them through a consecutive scattered light sequence. The decisive limitation is the rising probability of coincidence of consecutive particles at higher particle densities (>20.000 #/ccm).

The herein presented concept broadens the spatial distribution of particles to reduce coincidence probability, detect multiple particles at once and obtain multiple information by operating in an In-Line Holographic Setup. An imaging system – containing a sampling cell, a laser, a lens system and a Charge Coupled Device (CCD) camera - is set on top of the CNM particle outlet. As a result from the optical setup the camera records a hologram where circular fringe patterns are caused from each single particle, containing full 3D information. Where "shadowed" particles are invisible in state of the art detection units and have to be taken into account by means of coincidence correction, holography enables the possibility to separate objects in all spatial dimensions. The fringe patterns do not only allow a better separability but also include information about the particle positions, trajectories and speed of motion. As the camera requires a minimum exposure time the interference patterns of the particles are convolved with its motion vectors, leading to elliptic shaped fringe patterns. The eccentricity and orientation of the patterns can be used to recover that information. Based on the knowledge of the particle position its original object plane may be reconstructed to determine the particle size.

The described concept was first modelled for aiding both the design of a functional demonstrator and the development of a detection and counting approach. The aerosol particle model simulates a synthetic hologram plane which resembles an aerosol volume with the aforementioned attributes. Based on that model output an algorithm was developed focusing on the detection of regular fringe patterns. These consist of a set of concentric fringes sharing a common feature, namely the common midpoint. A customized Hough Transform is applied to extract circles where the accumulation of common circle centers is high. The detection result of the Hough Transform directly correlates to the particle number in the recorded sample volume.

A functional demonstrator was realized to verify the feasibility of the concept in terms of particle detectability, respectively the imaging quality and the performance of the described detection method.

Poster 2.2 – T. Johnson

Agreement between Different Aerosol Classifiers using Spherical Particles

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Due to health and environmental consequences, nanoparticles are often characterized using an aerosol classifier, such as a Differential Mobility Analyzer (DMA), Centrifugal Particle Mass Analyzer (CPMA) or Aerodynamic Aerosol Classifier (AAC). The DMA, CPMA and AAC select particles based on their electrical mobility (i.e. electrostatic to drag force ratio), mass-to-charge ratio (i.e. centrifugal to electrostatic force ratio) and particle relaxation time (i.e. centrifugal to drag force ratio) respectively. For each instrument, only particles that induce the correct force ratio follow the trajectory required to pass through its classifier.

This study investigates the agreement between Tandem AAC-DMA and AAC-CPMA measurements using spherical DOS (Bis-2-ethylhexyl sebacate) particles. The AAC was set at a constant setpoint (from 40 to 600 nm) and selected particles based on their aerodynamic diameter from a polydispersed aerosol generated using a BGI Collison nebulizer. The monodispersed aerosol produced by the AAC was then diluted, charged using a Kr85 radioactive neutralizer and split between a stepping DMA and stepping CPMA in parallel. The particle number concentration of each twice classified aerosol was recorded as a function of the DMA or CPMA setpoint using a Condensation Particle Counter (CPC). At each AAC setpoint, the effective particle density was independently determined from each tandem configuration by fitting the theoretical tandem transfer function [1][2] to the experimental data using chi-squared minimization. The AAC classification was also compared against standardized polystyrene latex (PSL) particles and found to agree within 8.6% difference across ten different mobility diameters from 29 nm to 2.02 μm.

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Poster 2.3 – C. Le Cornec

Development of a virtual soot sensor based on artificial neural networks

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Diesel exhaust particulate matter (PM) is composed of a solid carbon fraction (soot) and a soluble organic fraction (SOF). PM (mainly composed of soot) has a mutagenic action associated with adverse health and environment effects including lung cancers, asthma and increased mortality rate [1]. Increasing concerns about these effects lead to stringent new emissions standards (from 0.14 g/km for Euro 1 to 0.005 g/km for Euro 6) which motivated the development of PM control technologies such as a diesel oxidation catalyst (DOP) in combination with a diesel particulate filter (DPF).

Real-time modelling of soot emissions is an interesting way to evaluate the effectiveness of PM control technologies. Soot formation is a highly complex process and consequently difficult to describe purely mathematically [2]. Empirical and semi-empirical models are easier to implement but are generally limited to specific operating conditions and are not able to generalize accurately [2]. One promising method is the use of Artificial Neural Networks (ANNs) which are able to model highly non-linear relationships. ANNs are trained on a representative dataset to adequately generalise for new data. Long-short term memory (LSTM) networks are a variant of ANNs where each node (called a memory cell) is a complex unit with gates controlling which information is passed through [3]. LSTM networks are able to capture time dependencies [3] and are known to perform well when dealing with time series data. Python 3.6 and TensorFlow are used for development.

Soot measurements for two Euro 5 heavy-duty diesel vehicles equipped with Selective Catalytic Reduction (SCR) but without DPF [4] are used to develop soot predictions models. The 1Hz measurements of particle size distributions from a Cambustion DMS500 cover various operating conditions (including steady-state and transient tests). Data from the on-board diagnostic device (OBD), including engine RPM, throttle position, engine out temperature, engine pre-aftertreatment temperature and post-aftertreatment temperature are used as an input to the neural network. The developed algorithm is able to predict with PM mass, number and size distribution. A robustness analysis is conducted to identify the limits of the model.

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Poster 2.4 – P. Maierhofer

Deposition of micrometric particles on a capacitive sensing area

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We characterize a novel micro-sensor with pairs of interdigitated combs of microelectrodes designed to detect particles in air. We evaluate the sensor's response to 1 µm Polystyrene Latex (PSL) particles experimentally and crosscheck the results with simulations. Experiment and simulation show good consistency. Based on the promising results we propose a redesign of the capacitive particle sensor with respect to PM2.5.

We have built a setup for selective deposition of well-defined spherical particles in order to evaluate the performance of a microsensor for the capacitive detection of particulate matter in air. The deposition setup consists of an atomizer in combination with a diffusion dryer, which disperses PSL particles of defined size, shape, and dielectric constant in air. A nozzle is used to accelerate the particles towards the sensor in order to use impaction as a means of depositing. Particles induce a sudden change in capacitance when deposited on the sensor's surface. Width and spacing of the electrodes is 1 µm which allows 1 µm particles to be deposited both onto the electrodes as well as in between them. The capacitive change depends on size, shape, dielectric constant, and the exact position of the particles. Since the dispersed particles are uniform within an experiment, the only influence left is the position of the particles relative to the surface structure of the sensor. Deposited particles are detected both optically using a digital microscope, and utilizing the described sensor effect. The experiment is also simulated using Comsol. We observe a relatively broad distribution of capacitive jumps caused by monodisperse 1 µm particles which stems from the exact position of the particles relative to the microelectrodes. A particle on top of the electrodes will lead to a weaker signal compared to a particle in between the combs. Since the electrodes protrude over the SiO2, particles are more likely to be deposited onto the electrodes rather than in between them. Experiment and simulation agree reasonably well.

As particles of larger diameters than the distance between two electrodes cannot fall between the electrodes, the sensor can operate in two regimes: large particles are detected at the surface, smaller ones are detected in between the electrodes. This can be used as a feature to tune the size range of detectable particles. A redesign of the sensor should focus on this effect in order to optimize e.g. for PM2.5. We propose to reduce the spacing between the electrodes as far as to 0.5 µm, which we assume is the limit for the size of detectable particles on top of the electrodes. Particles smaller than 0.5 µm can then be detected in between the electrodes. Therefore, the microsensor can be used as a sensor for PM2.5.

Poster 3.1 – J. Dreyer

Experimental study of the soot particle size distribution inside a vapour-fed co-flow diffusion flame

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Soot emission caused by the incomplete combustion of hydrocarbon fuels poses a serious environmental risk and health hazard. Examples are the role of soot in global warming and respiratory problems and cardiovascular diseases associated with aerosol inhalation.

Soot mitigation requires a fundamental understanding of the chemical and physical processes governing its formation. Here, we present a newly developed experimental set-up for studying liquid hydrocarbon combustion in the well-established Yale burner. The liquid fuel delivery and evaporation system enabled us to study fuels regularly encountered in real combustion processes and to investigate the correlation between fuel structure and its sooting propensity. Soot samples were taken from within the flame using a newly developed quartz probe and the soot particle size distributions (PSDs) were measured with a DMS500.

The addition of toluene (0, 5, 10, and 15 mol%) to heptane moved soot inception to lower heights above the burner (HAB). The earlier inception extended the soot growth zone in the toluene-laden flames, leading to larger soot primary and agglomerate particles. The earlier inception is hereby suggested to be caused by much higher rates of PAH formation in the presence of toluene. Toluene addition had little influence on the maximum soot number density, indicating that increases in soot volume fraction can mainly be attributed to the observed increase in particle size.

Poster 3.2 – C. Garcia

In-situ sizing of silica particles in a reacting jet

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In this work, nanoparticle formation is studied during the oxidation of a silane-laden jet that is issued into a vitiated co-flow, using a "Cabra" burner. Various laser diagnostic techniques have been used as multiple validation of the LES model. The vitiated co-flow inherent to the "Cabra" geometry has the advantage of providing a controlled environment, and hydrogen is used as fuel to avoid soot formation, thus ensuring that all particles come from silane oxidation.

Previously, OH-PLIF and elastic light scattering (ELS) experiments were performed in the turbulent jet. These two techniques were successful at retrieving qualitative information about OH abundance and particle formation in the jet. However, ELS suffers from an inherent ambiguity between particle size and particle number density.

In order to overcome this challenge, Multi-Angle Light Scattering (MALS) is employed as an alternative for in situ particle size measurement. The technique has been proven to be suitable to measure large aggregates and simulations suggest it should be suitable to measure particles starting from ~10 nm. Additionally, since MALS measurements are based on intensity ratios rather than absolute intensity measurements, the technique is, in principle, insensitive to variations in number concentration.

In this poster we present results of particle size measurements in a reacting jet. MALS measurements are compared with particle sizes determined from electron microscopy images of samples extracted from the jet. MALS results are promising, however, further development of the technique is needed before it can be fully relied upon.

Finally, SiO-PLIF is currently being explored as a means to measure the abundance of the SiO radical and help validate numerical simulations currently under development at the University of Stuttgart.

Poster 3.3 – L. Pascazio

Degree of crosslinking in combustion carbons

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In this work, the presence of covalent bonds between soot aromatic constituents was investigated studying the mechanical properties of cross-linked polycyclic aromatic hydrocarbons (PAHs) using reactive force field molecular dynamics simulations (MD).

Electron microscopy has revealed soot particles are constituted by aromatic layers generally organized in a turbostratic structure. These layers have been interpreted as the stacking of large PAHs. On the other side, MD studies have shown that the binding energy between medium-sized PAHs is not strong enough to stabilize the dimer or trimer from evaporation at high temperatures. Nanoindentation experiments have also shown that the hardness value of nanocrystalline graphite, known to be an uncrosslinked structure made of mobile PAH molecules, is very low and hardness values of mature soot and carbon black are found to be close to a hard crosslinked carbon such as charcoal. These results suggest that mature soot and carbon blacks are carbonised and crosslinked, and aliphatic chains and bridge formation between aromatic parts can play an important role in soot formation.

In this work, we estimated the degree of crosslinking within mature soot particles and carbon blacks, making use of reactive force field MD simulations of the mechanical properties of crosslinked PAHs.

Representative systems of PAHs (pyrene, coronene and ovalene) with density similar to nascent soot and with varying degrees of crosslinking were built. MD simulations of uniaxial tensile tests on these PAH boxes were made. The yield stress and hardness of each sample were calculated and the results were compared with nanoindentation experiments of soot particles. The results clearly show that the soot structure must present cross-links between its constituent PAH molecules to have a comparable value of the hardness found experimentally. The results give also information on the possible degree of crosslinking within soot particles.

These results present the first simulations of mechanical properties of cross-linked PAH structures and can help further understanding of soot formation and growth processes.