Cambridge Particle Meeting

Book of Abstracts

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Cambridge Particle Meeting

Time	Speaker	Affiliation	Title
8:30	**REGISTRATION**		
	Session I (Chair: Jonathan Symonds)		
9:00	Welcome		
9:10	George Biskos	The Cyprus Institute, TU Delft	Towards Lightweight and Cost-effective Tools for Sizing Aerosol Particles
9:30	Arthur Zielinski	University of Cambridge	Submicron Particulate Mass Sensing using Microresonators and Impaction
9:50	Dmitriy Kornilin	Samara State Aerospace University, Russia	In-line sensor for monitoring particles in hydraulic liquids
10:10	Imad Khalek	Southwest Research Institute, Texas	Effect of SMPS Neutralizers on the Accuracy of Particle Size Distribution Measurement
10:30	**BREAK**		
	Session II (Chair: Adam Boies)		
11:00	Suzanne Paulson	University of California at Los Angeles	Closing the ultrafine particle number concentration budget at road-to-ambient scale: implications for particle dynamics
11:20	James Allan	University of Manchester	Real-time emissions of biomass burning aerosol under controlled conditions
11:40	Soheil Zeraati-Rezaei	University of Birmingham	Investigation of SVOC in diesel fuel, engine lubricating oil and diesel engine emissions
12:00	Colin Jenkins	Adaptive Instruments Ltd	Lubricating Oil and Fuel stability and size analysis
12:20	Christopher Tighe	University of Cambridge	Kinetics, changes in particle size and internal structure of two Diesel soots and a carbon black during oxidation in oxygen or nitrogen dioxide.
12:40	**LUNCH & POSTER SESSION**		
	Session III (Chair: Chris Nickolaus)		
13:40	Philip Whitefield	Missouri University of Science and Technology	System-Loss Modelling Challenge Data for Gas Turbine Engine Extractive nvPM Sampling Systems.
14:00	Camille Bilger	University of Cambridge	Sampling of the Velocity Space: An Agenda for Liquid-Sheet Atomisation Analysis
14:20	Kazuhiro Yamamoto	Nagoya University	Flow Dynamics and Pressure Drop during Filtration Process in DPF
14:40	Marc Cyrill Besch	University of West Virginia	Characterization of Atmospheric Dispersing Exhaust Plume during On-Road Operation of Latest Technology Heavy-Duty Trucks
15:00	**BREAK**		
	Session IV (Chair: Christian Hoecker)		
15:30	David Kittelson	University of Minnesota	Particle number measurements: How small should we go?
15:50	Pragalath Thiruvengadam	University of West Virginia	Determination of a Preconditioning Protocol to Stabilize NOx and PN Emissions for Euro VI Engine Certification
16:10	Ting Lao Chung	University of Cambridge	Low-dimensional model for multiple after treatment devices
16:30	Safwan H. M. Murad	University of Oxford	Particulate Matter Emissions from Model M15 Methanol/Gasoline Blends in a GDI Engine
16:50	Paul Maguire	University of Ulster	Chemical reactivity of low temperature plasma treated aerosols
17:10	**END**		

09:10-09:30 – George Biskos
Towards Lightweight and Cost-effective Tools for Sizing Aerosol Particles

George Biskos[1,2]*, Spyros Bezantakos[1] and Konstantinos Barmpounis[1,2]

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The most effective way of sizing aerosol particles is by classifying them based on their electrical mobility using differential mobility analyzers (DMAs). Although DMAs have now become state-of-the-art tools, their high cost and bulky size is limiting for widespread use.

In the first part of this presentation I will describe a simple and cost-effective method for size segregating aerosol nanoparticles by employing tubes made of Electrostatic Dissipative Materials (EDMs). EDM tubes have surface resistivities that range from 10^5 to 10^{12} Ω/sq. Applying a potential difference along the tube creates an electric field of varying strength that has a radial and an axial component. This field affects positively or negatively charged particles (depending on the polarity of the field) passing through the tube in two ways: the axial field decelerates the particles and therefore increases their residence time in the tube and their chance for diffusional deposition to its walls, whereas the radial field removes particles by electrostatic deposition. As a result of these two processes, EDM tubes can be viewed as a combination of a diffusion battery and an electrostatic precipitator (or a crude DMA), with the advantage of being significantly more simple and inexpensive.

In the second part of the presentation I will describe an alternative method for manufacturing DMAs using low-cost and low-density polymers to build their body, and metal coatings for providing conductivity only where required (i.e., on the inner DMA surface). More specifically, I will describe how we have built a DMA using polyurethane and spray-coated the inner surface with a 0.5-mm thick conductive Nickel film (referred to as the PU-DMA). Then I will show measurements demonstrating the performance of the PU-DMA in comparison to that of an identical stainless-steel DMA (SS-DMA). Considering that the weight of the PU-DMA is 95% lower compared to that of its metallic counterpart, while its cost is also reduced substantially, makes the proposed manufacturing method a very attractive alternative for producing DMAs and other similar instrumets.

Combination of the EDM tube classifiers and the PU-DMAs can lead to compact and portable systems for measuring the size distribution and other intrinsic properties, such as hygroscopicity and volatility, of aerosol particles in a cost-effective way. My presentation will close by providing an outlook of different applications for such systems.

09:30-09:50 – Arthur Zielinski
Submicron Particulate Mass Sensing using Microresonators and Impaction

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Current portable small-scale particle detection instruments typically rely on optical methods which are limited to 300 nm diameter particles. However, microfabricated bulk acoustic resonators, when used as mass balances, could take particle detection below this size limit due to their high sensitivity to mass changes. These sensitivities, measured in terms of frequency shifts on the order of Hz/ng, can be increased by reducing the size, and hence mass, of the resonator. Unlike optical methods, which may have sizing capabilities, microresonators require integration of a size speciation mechanism.

This study examines the collection of particles onto piezoelectric bulk acoustic mode resonators from gaseous flows using classical impaction. The resonators are suspended 1.4 mm x 1.4 mm plates with theoretical unloaded resonant frequencies of 3.16 MHz for the tested in-plane mode. They are housed in a new modular impactor stage enabling the adjustment of impactor, resonator, and aerosol properties. Collection of both polystyrene latex (PSL) particles and α-pinene secondary organic aerosol (SOA) particles was examined in terms of the resulting frequency shifts and collection efficiency. Frequency responses were recorded every minute over typical collection periods of one hour with an additional four-hour saturation study to determine the maximum detectable mass. A differential mobility analyser (DMA) was used to size select 300 nm particles prior to impaction onto the resonator.

Experiments were conducted in tandem with condensation particle counters (CPCs) upstream and downstream of the impactor stage. The CPCs provided an estimate for the expected cumulative masses collected on the resonators which strongly correlated with the mass derived from the measured frequency shifts. For the saturation test, a SOA concentration of 70,000 particles/cc (similar magnitude to total number concentration of ambient submicron particles) was introduced to the impactor at 0.7 LPM. During the collection period, a deviation from the linear relationship was observed implying a saturation limit was reached. However, frequency shifts continued to be observed leading to the potential for characterising the effect and quantifying the lifetime of the device.

Additional proof-of-concept testing shows the capability to analyse the chemical composition of collected particles from a resonator surface using Liquid Extraction Surface Analysis Mass Spectrometry (LESA-MS). Confirmed using α-pinene SOA, it allows microresonators to provide similar information to classic filter-based collection with higher time resolution mass measurements. The application of solvents for LESA-MS also verifies the potential for removing organics and reusing resonators. A summary of the experimental setup, results, and their implications will be presented.

09:50-10:10 – Dmitriy Kornilin
In-line sensor for monitoring particles in hydraulic liquids

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Reliability of modern tribological systems (like hydraulic oil systems) is strictly determined by the quality of diagnostic of their technical state. As one of the most effective methods for such diagnostic can be proposed the assessment of the parameters of wear particles that are generated by hydraulic unit during their lifetime. The concentration, size and shape of particles can reveal significant information about the state of entire hydraulic system.

In-line automatic particle counters are widely used in order to determine the parameters of wear particles. The working principle these counter is based on the use of the photoelectric method. This means that when the particle crosses the volume between the source and receiver of light, the value of photocurrent is changed in dependence of particle size. Existing devices detect the presence of particles according ISO (channels 4, 6, 14 and 21 µm), NAS or GOST17216-2001. The concentration of particles in each group of sizes determines the purity class as an integrated indicator of the quality of liquid. However, this information is often not sufficient for diagnostic purposes of the hydraulic unit or the hydraulic system, as it is impossible to determine the specific amount of generated particles in each range of sizes.

In this paper we propose to utilize enhanced automatic particle counter that was developed by authors. It is based on a digital signal processing algorithms and can introduce a histogram of particle contamination in the range of 2 to 200 micrometres with the step as low as 1 micrometres. Such parameters were achieved by implementation of precision analog-to-digital converters and digital signal processor. In addition, the device has a digital system that helps to maintain a constant illumination in the flow channel. The implementation of RS-485 interface on the output of the sensor can help to integrate the sensor into modern control systems. It is also should be mentioned the possibility of multi-point control by connecting several sensors in the network.
The experimental results reflect that the average particle size determined by the sensor relates to the average reference particle size. Therefore sensor can be recommended for scientific studies that examine the relationship between the generation of particles and the state of the entire hydraulic system or its units separately.

10:10-10:30 – Imad Khalek
Effect of SMPS Neutralizers on the Accuracy of Particle Size Distribution Measurement

Imad A. Khalek[1]*, Huzeifa Badshah[1], Vinay Premnath[1] and Robert Giannelli[2]

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The Scanning Mobility Particle Sizer (SMPS) is a widely used instrument in various applications in the aerosol field. Due to its fundamental working principles, this instrument is considered the best reference for number-weighted size distribution measurement in the sub 1 □m size range. There is also a strong interest to use this instrument for higher moments such as surface area, volume, and mass by making the appropriate assumptions. The SMPS is typically used with a Krypton 85 (Kr 85) radioactive source for the bipolar neutralization of particles to a minimum steady-state level in accordance with the Boltzmann distribution of charge.

Due to some restriction and higher expense of the Kr 85 neutralizer, there is interest in using different ionization sources, namely Polonium 210 (PO 210) and Soft X-Ray. In this work, we examined the effect of Kr 85 age on different moments of the size distribution, and compared the performance to that using PO 210, soft X-Ray neutralizers, and no neutralization. Furthermore, we investigated the impact of inlet concentration on the quality of the results. To perform this work, we used a soot generation system coupling a mini-CAST propane flame with a catalytic stripper.

In our presentation, we will report on our findings and will make recommendations on how to best use the SMPS for accurate measurement of the number-weighted size distribution and higher moments using different neutralizer types and ages. We will also provide means to correct the size distribution relative to a fresh Kr 85 neutralizer that the instrument uses for particle neutralization

11:00-11:20 – Suzanne Paulson
Closing the ultrafine particle number concentration budget at road-to-ambient scale: implications for particle dynamics

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Freshly emitted vehicle exhaust particles are diluted quickly as they mix into ambient air, but the contribution of evaporation, coagulation, and/or nucleation of new particles to the number concentration has been the subject of some debate. We analyzed one-second time resolution size distribution data from an early morning field campaign, data collected at a time at which dilution has a smaller (but still dominant; ~70–80%) impact on particle concentrations. Because the plume is diluted over an hour, and a distance of 1500 m, we can constrain particle dynamics processes with higher accuracy. We find that concentrations in the smaller size bins (5.6 to 23.7nm) peak further downwind than the reference particles (42.1 to 562nm), and decay significantly faster than larger particles particularly in the area 100–400m downwind. Comparisons of the cumulative contributions of van der Waals enhanced coagulation, dry deposition, and dilution and the observed decay curves, implies that for up to the first 50–100m there is nucleation and/or growth of particles smaller than 5.6 nm. In contrast, in the ~100–400m region, some of the smaller particles evaporate. In the further downwind areas (> 400m) the particles all appear to decay at rates consistent with the sum of dilution, coagulation and deposition. We also find that a dry deposition parameterization at the low end of those available in the literature is most consistent with the observational data.

11:20-11:40 – James Allan
Real-time emissions of biomass burning aerosol under controlled conditions

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Particulate emissions from biomass burning are known to impact the climate substantially by affecting the atmosphere's radiative balance. In addition, they can cause significant harm to human health. This is of particular concern in tropical regions, where small-scale residential burning, wildfires and agricultural burning introduce vast quantities of polluting aerosol into the atmosphere (Bond *et al* 2013; Venkataraman *et al* 2005).

Biomass burning emissions in models are typically calculated using emission factors taken from large inventories. These are determined from field observations and laboratory tests using a wide variety of fuels. However, due to the huge variation in emissions associated with even small changes to the burning environment, the uncertainty of these measurements can be large (Akagi *et al* 2011).

Previous studies have considered the relationship between emission factors and the fire-integrated combustion efficiency (eg McMeeking *et al* 2009). The difference between flaming and smouldering combustion is often taken into account, but it has, as yet, not been possible to distinguish greater levels of detail. In this study, the Fire Propagation Apparatus was used to strictly control the conditions of combustion in comparison with previous experiments. The burning environment was controlled by a series of infrared heat lamps positioned around the sample and the airflow was adjusted to a pre-defined level. Samples were of similar size, mass and quality in each test. Coupling this system with an Aerosol Mass Spectrometer and a Single Particle Soot Photometer, it was possible to measure real-time particulate emissions of West African wood under well-defined, repeatable conditions.

This methodology produced remarkably repeatable results, allowing aerosol emissions to be mapped directly onto different phases of the combustion. Several details emerged that have not been seen previously: due to pre-ignition heating of the sample, emissions from pyrolysis were visible as a distinct phase before flaming was established. In addition, the flame could be split into a black-carbon-dominant flame and an organic-dominant flame during which very little black carbon was seen. This contradicts previous assumptions that all flaming behaviour is dominated by black carbon emissions. Finally, no particulate emissions at all were measured after the flame extinguished, suggesting that the latter stages of the combustion in these tests was dominated by char oxidation rather than smouldering.

These results clearly demonstrate the importance of understanding the coupling between the combustion processes and the emissions in order to provide a more substantial estimate of the resulting emissions. Using this approach, it has been possible to examine correlations between burning conditions, fire behaviour and aerosol emissions on a fundamental level. Further research would allow the characteristics of different burning states and their associated emissions to be understood more completely. If the conditions under which biomass is burning are known, this approach will allow its emissions to be modelled with more precision than can currently be achieved.

11:40-12:00 – Soheil Zeraati-Rezaei
Investigation of SVOC in diesel fuel, engine lubricating oil and diesel engine emissions

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There are uncertainties regarding the composition of vehicular particulate emissions. Some of these uncertainties are attributed to the limited knowledge relating to the composition of semi-volatile organic compounds (SVOC). SVOC partition between the gas and particulate phase and can have adverse effects on human health and environment. Using comprehensive gas chromatography (GC) coupled to variable electron ionisation time-of-flight mass spectrometry (ToF-MS), the composition of engine SVOC emissions are investigated; identifying a wealth of homologous series from within the unresolved complex mixture (UCM) of the chromatogram.

Fuel and engine lubricating oil are major contributors to engine SVOC emissions. The composition of diesel fuel and engine lubricating oil were investigated. The gas and particulate phase SVOC emissions from a light-duty diesel engine were identified and attributed to originate from the fuel and/or oil. Engine emission samples were collected, at steady state conditions, before and after the diesel oxidation catalyst (DOC) from the exhaust of a 2.2 L four-cylinder diesel engine. Engine exhaust was diluted with clean ambient air and collected using both adsorption tubes and filters, for gas and particulate phase species respectively. Samples were subsequently analysed using thermal desorption (TD)-GC×GC-ToF-MS. Particulate number and size distribution was investigated using a CAMBUSTION DMS500 fast particulate analyser.

A quantification technique for SVOC was developed based on the relation of total ion current to molar quantity or mass. The composition of diesel fuel was dominated by compounds of $<C_{20}$. Preliminary results indicate that high molecular weight alkanes (C_{25}-C_{32}) are present in abundance in the lubricating oil. Differences in composition of engine exhaust before and after the DOC are presented. Compounds identified from the engine exhaust contained n- and branched alkanes, alkyl-cycloalkanes, alkyl-benzenes, various aromatics and polycyclic aromatic hydrocarbons (PAH). Gas phase engine SVOC emissions were similar to those characterised in the fuel ($<C_{20}$), whereas particulate phase engine SVOC emissions were similar to compounds identified in the engine lubricating oil. These preliminary results exemplify the complexity of SVOC emissions from vehicular exhaust emissions.

12:00-12:20 – Colin Jenkins
Lubricating Oil and Fuel stability and size analysis

Colin Jenkins

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- The quick characterisation of any de-mixing phenomena, sedimentation, flotation or consolidation and the calculation of the velocity distribution in a centrifugal field including particle size analysis distribution.

- Particle-Migration Driven by Gravitational or Centrifugal Forces
- Detection by Optical NIR-Technique and Short wave length blue light

- Applications

- Proper Selection of Surfactant Additive Ensures Better Well Stimulation in Unconventional Oil and Gas Formations
- Stability assessments of high active dispersion based Paraffin Inhibitors
- Engine oil additive composition, comprising nano-diamond method preparation.

12:20-12:40 – Christopher Tighe
Kinetics, changes in particle size and internal structure of two Diesel soots and a carbon black during oxidation in oxygen or nitrogen dioxide.

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The rates of oxidation of two Diesel soots in oxygen were measured in an isothermal packed bed of quartz sand at 450 to 550°C, with O_2 concentrations of 2.7 to 24.4 vol. % in argon. Separately, the rates of oxidation of these carbons in nitrogen dioxide (NO_2) were measured at 300 to 550°C, with NO_2 concentrations from 50 to 880 ppm in argon. These soots were collected from the exhaust of an engine, burning either ultra low sulphur Diesel (ULSD) or a blend of 90 vol. % biodiesel and 10 vol. % ULSD. First, the soots were heated in argon to 550°C, then held for 1 hour, to remove volatile matter, during which ~ 5 % of their carbon was lost by reaction with adsorbed oxygen, thus forming CO and CO_2. The rate of oxidation of a carbon black (Printex U) in O_2 was also studied; this was first heat-treated in argon at 900°C, for 1 hour, losing ~ 1.5 % of its carbon.

In O_2, the particles were found to burn in two stages: an initial fast reaction consumed nearly 20 % of the devolatilised soots and 6 % of the heat-treated carbon black. These highly-reactive fractions probably resulted from the pyrolysis of hydrocarbons during heat-treatment. During the second part of their oxidation, the rates of production of CO and CO_2 from the two Diesel soots were consistent with a model of porous particles oxidised uniformly throughout their interiors. The overall oxidation rates in this second stage were half-order with respect to O_2, with an apparent activation energy of 145 ± 8 kJ mol–1. It was demonstrated that the heat-treatment did not affect the rate of oxidation in O_2 or NO_2.

For both Diesel soots, [CO] and [CO_2] in the off-gases decreased, whilst the carbon burned. However, the rate of oxidation of Printex U increased to a second maximum, suggesting these carbon particles have pores, which grow and intersect during oxidation. Their porosity was probably generated by these particles being heated during either the initial devolatilisation or their subsequent oxidation.

The second stage of burning of the two Diesel soots is inherently faster in NO_2 than in O_2. The rate of production of CO and CO_2 is first order with respect to NO_2, with an apparent activation energy of 71 ± 19 kJ mol–1. The result is that soot particles react relatively rapidly with NO_2 mainly on their exteriors.

13:40-14:00 – Philip Whitefield
System-Loss Modelling Challenge Data for Gas Turbine Engine Extractive nvPM Sampling Systems.

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Jet engine exhaust emissions in the atmosphere are causing increasing concern for their environmental impact, particularly their effect on the air quality around airports. The growth of commercial air traffic over the last decade has led to an increased contribution to the local inventory of gaseous and particle emissions from the operations associated with airports and aircraft engines. An accurate assessment requires that the number concentration and size distribution of the aerosols within engine exhaust and aging plumes be understood and well characterized. A recently released certification measurement methodology for gas turbine engine nvPM, relies on extractive sampling, with sample line lengths, between the source and monitoring instrumentation specified to be ~25 meters in length (SAE Aerospace Information Report 6241). Such a sampling line length will result in size dependent nvPM loss which must be accounted for if the instrument data i.e that measured downstream of the sample line, is to be used to estimate source emission characteristics. A procedure for the calculation of sampling and measurement system penetration functions and system loss correction factors (SAE AIR 6504), without using direct size measurement has been under development for several years. The effectiveness of the model can be assessed by challenging the model with representative engine exit plane exhaust aerosols. Penetration efficiencies are determined for any given sample line using a penetration function calculator provided by United Technologies. Research Center (UTRC). Representative exhaust aerosol parameterizations reported in this paper, have been derived from a proprietary archive of some 10 field campaigns where real gas turbine engine exhaust data has been acquired by the authors using the DMS500 instrument. The DMS500 feature that distinguishes single mode from bimodal distributions was exploited to classify the size distribution types observed. These data were acquired during extractive sampling from the exit plane of the exhaust nozzle of a range of in-service commercial gas turbine engines. As may be expected the representative data from the set of engines and operating conditions studied revealed instrument size distributions of variable modality.

14:00-14:20 – Camille Bilger
Sampling of the Velocity Space: An Agenda for Liquid-Sheet Atomisation Analysis

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A novel state-of-the-art numerical capability for efficient modelling of multiphase flows has been developed and applied to primary breakup of liquid sprays. The Robust Conservative Level Set (RCLS) method uses high-order WENO schemes on mixed-element unstructured meshes to solve the transport equation for the level-set variable. The method is implemented within the framework of OpenFOAM, and is fully parallelised. The present study uses the new capability to understand the phenomenology observed during prefilming air-blast atomisation of a planar liquid sheet. In commercial aircraft application, this is essential for effective control of fuel atomisation and cleaner, more efficient combustion processes. We performed a parametric study to make an informed qualitative assessment on the impact of various liquid and air velocities for a fixed prefilmer geometry.

The computations reproduced the transient nature of the fluid dynamics of the phase interface behaviour. The development of surface instabilities is mainly dependent on the shearing intensity exerted by the air on the liquid-sheet. However, the behaviour and development of the liquid-sheet at the prefilmer trailing edge is found to be influenced mainly by the relative inertia of the gas and the liquid, in favour of the liquid.

Results also show the influence of vortex action and shearing effects on the breakup mechanism at the atomiser edge. The results suggest that, in some cases, the atomisation mechanism is not aerodynamic tearing but vortex flapping downstream of the lip. All of these results show that phenomenological analyses are effective to help interpret and correlate the different behaviours of atomisation by varying the operating conditions to map a wide range of gas and liquid velocities. Several graphical classifications of regimes for two-phase flow dynamics have been reported in the literature based on experimental observations: these cover secondary atomisation of liquid drops, jet breakup, diesel-engine fuel injection, non-prefilming liquid-sheet atomisation. Based on the observed physics, the present study proposes a regime mapping for prefilming liquid-sheet atomisation in the form of a matrix of liquid film breakup phenomena.

14:20-14:40 – Kazuhiro Yamamoto
Flow Dynamics and Pressure Drop during Filtration Process in DPF

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A diesel particulate filter (DPF) is used for the after-treatment of exhaust gas. The suitable structure for the particle trap is a well-known monolithic wall-flow filter. In simple explanation of DPF, it removes particles when exhaust gas passes through its porous wall. It has been reported that DPF filtration efficiency can be as high as 99 %. However, the filter is plugged with particles that would cause an increase of filter back-pressure, which must be kept at lower levels, because the higher back-pressure increases fuel consumption and reduces available torque. Thus, we need to reduce the sufficient particle emission at acceptable pressure drop in order not to compromise less fuel consuming of diesel cars.

To optimize the filter structure for better filtration with lower pressure drop, we need to fully understand the phenomena occurring in the filter. However, it is difficult to observe the soot deposition process experimentally. This is because the typical inlet size of the ceramic filter monolith is about 2 mm, and the thickness of the filter wall is only 0.2 mm, where soot particles are removed by the filtration. Alternatively, a numerical simulation has been a powerful tool for investigating the phenomena in such a small scale phenomena.

In this study, we examined the effects of the porous ceramic structure on the filtration performance. The actual filter was obtained by an X-ray computed tomography (CT), which was used as a reference, and other seven types of filters were prepared, in which the porosity was changed systematically. That is, the porosity of the front or rear section of the filter was changed independently, or the surface of a filter was flattened. Using these filters, numerical simulations were performed to investigate the flow field and the process of soot deposition for discussing the transaction between the depth filtration and the surface filtration.

Results show that the initial pressure drop decreases as the average porosity increases, but it is not changed by flattening the filter surface. As for the pressure drop due to the soot deposition, the effect of the porosity in the rear section is small, whereas that in the front section is more prominent. By decreasing the porosity in the front section, the period required for shifting from the depth filtration to the surface filtration is shorter. As more soot is deposited, the flow rate in one channel becomes smaller and smaller, whereas the flow rate of other channel increases. An important finding in the soot deposition process is that the flow preferentially passes through the channel with lower pressure drop. Once the soot layer is formed on the filter surface, the smooth velocity profile appears, showing that the pressure drop is proportional to the thickness of the soot layer. Thus, the non-linearity variation in pressure drop during the depth filtration is caused by the change of the flow field inside the filter.

14:40-15:00 – Marc Cyrill Besch
Characterization of Atmospheric Dispersing Exhaust Plume during On-Road Operation of Latest Technology Heavy-Duty Trucks

Marc Cyrill Besch[1]*, Arvind Thiruvengadam[1], Daniel Carder[1], Pragalath Thiruvengadam[1], Saroj Pradhan[1], Mridul Gautam[2]

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Traditionally, particulate matter emissions data used in emission inventories are collected during engine and chassis dynamometer testing, performed in controlled laboratory environments, whereby natural atmospheric interactions are replicated by means of a full- or partial-flow dilution tunnel that may generate/suppress physical mutations. Several physical processes that may impact particle size distribution and composition of an aerosol occur during exhaust atmospheric dilution. Furthermore, laboratory-based measurements use HEPA filtered dilution air, whereas background air during atmospheric dilution may contain a variety of biogenic aerosols and dust particles that could impact or alter the formation dynamics of nucleation mode particles in the exhaust plume. Studies in a large scale environmental wind-tunnel have identified turbulence intensity (TI) within the dispersing exhaust plume to be a primary driving factor for the formation of nucleation mode particles.

This study was employing a novel experimental methodology that allowed to integrate atmospheric and laboratory PM sampling techniques in a unique setup. In a first phase, particulate matter emissions were measured with WVU's transportable emissions measurement system through a traditional full-flow CVS system while the test vehicle was operated over the road. During the second phase the exhaust plume was allowed to freely disperse and mix with background air after exiting the exhaust stack. A moveable sampling probe setup was installed within the boundaries of the exhaust plume making it possible to extract a partial sample from different locations within the three-dimensional structure of the dispersing plume. The extracted sample was routed through a heated sampling tube to a manifold and subsequently split between different particle measurement instruments, including; i) TSI EEPS® for particle size distributions, ii) CPC for total particle number concentrations, iii) TSI EAD for a proportional measure of particle surface, iv) Dekati DMM and AVL MSS for particle mass information, as well as v) an aethalometer to quantify black carbon content. Additionally, samples were collected on carbon grids for subsequent analysis of the particle's morphology via scanning electron microscopy. Turbulence intensities at the sample extraction points were measured using an omnidirectional hotwire anemometer.

The test articles for both phases included three heavy-duty tractors typically employed for goods movement applications, including a DPF equipped, MY' 2007, a DPF-SCR equipped EPA-2010 emissions compliant, as well as a stoichiometric operating and TWC equipped natural gas engine. Exhaust plume sampling was conducted at three characteristic steady-state vehicle speeds (i.e. 20, 35, and 45mph) and during a transient operation over highway and suburban driving conditions. For the latter, the extraction probe was held at a fixed position, whereas for steady-state experiments the probe was moved through the plume allowing to characterize particle emissions as a function of dilution rate and ratio. Finally, data collected during this study while the vehicle was operated over the road was compared to experiments conducted in an earlier study using an environmental wind-tunnel setup.

15:30-15:50 – David Kittelson
Particle number measurements: How small should we go?

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In the EU "solid" particles larger than 23 nm from Diesel and SI engines (ground vehicles) are regulated. This regulation was originally developed on the assumption that it would apply to diesel vehicles and would force the use of high efficiency particle filters. This happened and now "solid" number emissions from new diesel vehicles are very low. However, other engine technologies that don't use exhaust filters like spark ignition direct injection gasoline and spark ignition natural gas produce significant "solid" particle number emissions - and many of these particles are smaller than 23 nm. "Solid" particle mass (black carbon) and "solid" particle number larger than 10 nm from aircraft turbine engines will be regulated worldwide starting in 2020. Should the lower size cutoff for "solid" particle number emissions from ground vehicles be lowered to 15 nm, 10 nm, or lower? The current EU PMP method will be compared with the proposed aircraft method. Measurement challenges will be discussed.

15:50 - 16:10 – Pragalath Thiruvengadam
Determination of a Preconditioning Protocol to Stabilize NOx and PN Emissions for Euro VI Engine Certification

Arvind Thiruvengadam[1]*, Don Sanfilippo[1], Arvind Thiruvengadam[1], Daniel Carder[1], Mridul Gautam[2], Shirish A. Shimpi[3], Chet Mun Liew[3]

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The purpose of this study is to understand and determine the preconditioning protocol for Euro VI engine certification in order to obtain repeatable NOx and particle number emissions results, specifically for engines equipped with Diesel Particulate Filter (DPF) and Selective Catalytic Reduction (SCR) after-treatment systems. With Euro VI emissions limits being phased in by 2016, more and more engines will be certifying under these standards. The emission limits defined in Euro VI regulations are comparable to US-EPA 2010 emissions standards with the additional introduction of particle number (PN) emissions limits to the regulations. This adds complexity to the engine testing and certification process. Although current model year diesel engines are equipped with diesel oxygen catalyst (DOC) and DPF that have a filtration efficiency of 95 to 99% by mass on an average over an entire particle size distribution, the PN based filtration efficiency of a catalyzed DPF can be as low as 50% after regeneration and up to 80% efficient in filtering, with significant soot loading on the DPF. In addition, engine parameters such as exhaust temperatures, DPF soot loading, as well as exhaust flow rates adds an extra dimension to the problem of obtaining repeatable PN results.

The study was conducted on an MY2016 15 Liter diesel engine equipped with a de-greened DOC-DPF-SCR after-treatment system in a CVS test cell. Although UN ECE's R49 document regulates the use of a newly manufactured engine with a run-in time of up to 125 hours, this study made use of an engine and after-treatment system that had over 125 hours of operation prior to the study. Moreover, three distinct engine calibrations were developed by varying levels of engine-out NOx (EO-NOx) emissions in order to simulate various soot loading rates impacting NOx and PN repeatability. The engine was exercised over 10 repeats of the World Harmonized Transient Cycles (WHTC) followed by 3 repeats of World Harmonized Steady-state Cycles (WHSC) with a 20 min soak in between tests for the three different EO-NOx engine calibrations where the mid-level EO-NOx calibration met 2010 EPA emissions standards. The scope of this study is to obtain a generic engine preconditioning cycle or procedure specifically for engines tested for emissions compliance in the CVS test cells under Euro VI regulations to obtain repeatable NOx and PN results. In addition, another MY2008 6.4 Liter diesel engine equipped with DOC-DPF aftertreatment system was tested at WVU CAFEE's EERL, with an in-use DPF as well as a new de-greened DPF with less than 125 hours of operation. The engine was exercised over a custom designed soot loading cycle. The work done at WVU aims to understand the effects of aftertreatment age on the stability of PN emissions from a catalyzed DPF.

Results obtained from these studies showed that a minimum of three consecutive preconditioning cycles are required before acquiring the stabilized brake-specific NOx and PN emissions for the three different EO-NOx levels. The effect of the duty cycle type used for preconditioning and the age of after-treatment was not found to be significant on number of preconditioning runs required.

16:10-16:30 – Ting Lao Chung
Low-dimensional model for multiple after treatment devices

Chung Ting Lao[1]*, Jethro Akroyd[1], Amit Bhave[2], Markus Kraft[3]

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The after treatment of the exhaust emissions from a 7L diesel engine is modelled using a network of ideal reactors to describe a DOC-DPF-SCR system. The cylinder-out exhaust conditions are simulated using a detailed in-cylinder combustion model. The chemistry in each after treatment device is described via a set of user-defined reactions.

The functionality and consequence of modelling each device in the after treatment model as an ideal reactor was assessed by comparing simulations of each device to data reported in the literature. The ideal reactor models were able to describe the microkinetic surface reactions and able to be evaluated rapidly, and were shown to provide satisfactory agreement with data reported in literature. Particulate cake formation and regeneration were included in the DPF model.

The DOC-DPF-SCR system was simulated at two different engine operating points to demonstrate the effect of the NOx-PM trade-off in the engine operating conditions. The DOC (diesel oxidation catalyst) is responsible for complete oxidation of CO and unburnt hydrocarbons. The DPF (diesel particulate filter) traps particulate matter in the exhaust. Ammonia is introduced into the SCR (selective catalytic reduction) to reduce NOx into N2. The model was used to investigate the effect of changing volume, catalyst loading, reductant flowrate, and configuration of the devices. The main reaction pathways in the mechanism were identified using flux analysis. The performance of the final design was tested under varying inlet flowrate, temperature and composition conditions. The interaction between the individual after treatment devices and the impact of the engine operating strategy on the design of after treatment system is discussed.

16:30-16:50 – Safwan Hanis Mohd Murad
Particulate Matter Emissions from Model M15 Methanol/Gasoline Blends in a GDI Engine

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The influence of oxygenates on particulate matter (PM) emissions from GDI engines has differing reports in the literature. It is hypothesised that these conflicting results can be explained by fuel vaporisation, and its composition in terms of aromatic content and heavy end components. For good control of the experiments M15 fuels have been mixed from pure fuel components and this enables the distillation characteristics to be matched to those of an M15 ULG. Code has been written to predict the vapour pressure of the non-ideal M15 blends; by controlling the fuel temperature experiments can be conducted with flashing and non-flashing fuel sprays. Two contrasting groups of M15 fuels have been used: one 'light' fuels group and second 'heavy' fuels group in terms of the vapour pressure, T50, T90, aromatic content. Rig studies with backlit illumination and Mie scattering have been used for characterization of penetration length, spray angles (and collapse) and bulk evaporation rate. The spray structure is characterized by the pressure ratio (system pressure / vapour pressure). The same fuels have been used in an engine with a full-length optical liner, to study the interaction of spray with cylinder flow and piston impingement. Particulate matter emissions are reported from different optical engine builds for comparison of the PM emissions vs fuel temperature and the effect of quartz vs metal components.

16:50-17:10 – Paul Maguire
Chemical reactivity of low temperature plasma treated aerosols

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We have developed a confined low temperature plasma – aerosol system which creates highly charged droplets through electron and ion bombardment. Since the arriving electrons have almost zero energy, they are likely to be trapped at the surface and induce rapid chemical reactions. Plasma-liquid interactions are complex but offer considerable scope for use in nanomaterials synthesis. The introduction of individual picolitre micro-droplets into a steady-state low temperature plasma at atmospheric pressure, offers opportunities for enhanced scope and control of plasma-liquid chemistry and material properties. The gas-phase droplet system is similar in concept to liquid bubble microfluidics currently under intense research but with enhanced opportunities for scale-up. For nanomaterials and quantum dot synthesis, the addition of a liquid phase within the plasma expands considerably the scope for core-shell and alloy formation. The synthesis and encapsulation within a liquid droplet allows continuous delivery of nanoparticles to remote sites for plasma medicine, device fabrication or surface coating.

Measurement and models indicate a droplet charge lower bound of at least 10^5 electrons for a mean droplet size of 15 $\square$m. Metal nanoparticles have been synthesised within the droplet in flight with rates that are many orders of magnitude higher than reported for colloidal chemistry, radiolysis or high energy electron beam radiations. Chemical modification of water in flight has been measured, transport of plasma activated water downstream has been demonstrated and its interaction with biological cells has been investigated. These results offer interesting prospects for new avenues of research in topics such as catalysis, airborne pathogen decontamination, pollution remediation and plasma medicine.

Poster Session

01	**Brian Graves**	University of Cambridge	Synthesis of carbon nanotube fibres using microwave plasma and a floating catalyst CVD process
02	**C. E. Garcia-Gonzalez**	Imperial College London	Investigating Silica Nanoparticle Formation with Laser Diagnostics
03	**Hamisu Adamu Dandajeh**	University College London	Effect of Degree of Unsaturation of Single Component C2 and C3 Fuel Molecules on the Formation of PAHs in a Laminar Tube Reactor
04	**Jacob W. Martin**	University of Cambridge	Dynamic gas interactions with polycyclic aromatic hydrocarbons
05	**Joshua Lewis**	University of Cambridge	Combining microfluidics and aerosol processing for improved nanoparticle synthesis
06	**Kaiqi Hu**	University of Cambridge	Gas-phase synthesis of bimetallic nanocatalysts for diesel engine after-treatment
07	**Manoel Yohanes Manuputty**	University of Cambridge	Numerical Simulation of TiO2 Synthesis in a Stagnation Flame Reactor
08	**Olalere R. Kayode**	University of Birmingham	Experimental Investigation of Particle Emissions From A Gasoline Fuelled GDI Engine
09	**Robert Nishida**	University of Cambridge	Direct Ultraviolet Photoionization and Charge Recombination of Nanoparticles
10	**Safwan Hanis Mohd Murad**	University of Oxford	Particulate Matter Emissions from Model M15 Methanol/Gasoline Blends in a GDI Engine
11	**Christian Hoecker**	University of Cambridge	A Continuous Gas Phase Process for Carbon Nanotube Synthesis at an Industrial Scale

Poster 02 – C. E. Garcia-Gonzalez
Investigating Silica Nanoparticle Formation with Laser Diagnostics

C. E. Garcia-Gonzalez*, B. Williams, F. Beyrau, G. Neuber, A. Kronenburg

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A significant proportion of man-made air particulate is generated during combustion processes. Also, the use of flames for the production of nanopowders is an established method of chemical synthesis at industrial scale. Yet, the processes responsible for particle formation and their dependence on the characteristics of the flow are not fully understood.

In this work, nanoparticle formation takes place during the oxidation of a silane-laden jet in a "Cabra" burner and is investigated with laser diagnostics. The vitiated co-flow inherent to the "Cabra" geometry has the advantage of providing a controlled environment for the reaction to take place. Hydrogen is used as fuel to avoid soot formation and ensure all particles observed come from the silane reaction, while the silane-silica system provides known chemical kinetics.

At present, suitable conditions of temperature and precursor concentration that lead to particle formation have been identified and an elastic light scattering experiment has been performed. Elastic light scattering is a very sensitive technique for detecting particle formation from the gas phase because signal strength increases with the sixth power of the diameter of the scattering body.

Results show that with a co-flow temperature of 1500K and moderate Reynolds number (10000) only concentrations in excess of 2000 ppm of silane lead to the formation of detectable particles. The reaction completes approximately at 70 mm above the burner. Final particle size depends strongly on the initial concentration of precursor. Assuming a monodisperse particle size distribution, a simple model has been developed to interpret scattered light intensity measurements. Estimates obtained using this model suggest a particle diameter is 65 Å for an initial silane concentration of 3100 ppm.

Upcoming experiments involving thermophoretic sampling and electron microscopy will provide direct measurements of particle diameter to confirm laser measurements. Further research on this system will involve Planar Light-Induced Fluorescence (PLIF) to measure the abundance of the SiO intermediate species and help validate numerical simulations currently under development at the University of Stuttgart. Finally, Laser-Induced Incandescence is being explored as a technique to measure particle size distribution in-situ.

Poster 03 – Hamisu Adamu Dandajeh
Effect of Degree of Unsaturation of Single Component C2 and C3 Fuel Molecules on the Formation of PAHs in a Laminar Tube Reactor

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Engineering systems such as gas turbines usually utilise gases which produce toxic substances when they are burnt. These substances could be emitted either as solid soot particles or as gas phase polycyclic aromatic hydrocarbons (PAHs). The link between soot and PAHs have long been established. Firstly, PAHs assemble themselves into larger structures which are the soot particles themselves. Secondly, they are found mostly, adsorbed on the surfaces of soot particles and form their cancerous components. In order to address the toxicity of soot particles, it is imperative to start from their toxic precursors. This paper presents the results of both gas-phase and particle-phase PAHs generated from pyrolysis of ethane, ethylene, acetylene, propane and propylene in a homogenous laminar flow reactor. Pyrolysis of the five gaseous fuel molecules was carried out within the temperature range of 1050 - 1350°C under oxygen free condition and a fixed fuel concentration of 5,000pm on C_1 basis. Soot sand gas phase samples generated within the reactor were sampled from the exit of the reactor. The PAHs from the samples were then extracted using an accelerated solvent extractor (ASE) and their PAH analysis was implemented using a gas chromatography coupled to mass spectrometry (GCMS).

The experimental results showed that, depending on the temperature at which a fuel is pyrolysed, its degree of unsaturation plays an important role on the type and concentration of PAHs per unit mass of soot and per unit gas volume, which in turn, influenced the overall carcinogenic potential of the effluent species. The amount and type of PAHs were observed to be decreasing with rise in temperature. Larger PAHs were significantly depleted or sometimes completely disappeared at high temperatures. This was believed to be connected with the rates at which they are converted to soot. It was established that the double bonded C_3 propylene (the fuel which produced the highest soot propensity) produced the highest amount of particle-phase PAHs per unit mass of soot and per unit volume of gas. Also, propylene produced the most prolific carcinogenic equivalent sum (CES) per unit volume of gas at all temperatures tested. However, the triple bonded C_2 acetylene produced the highest amount of gas phase PAHs per unit volume of gas when compared with other C_2 and C_3 fuels. It was concluded that increasing the unsaturation of a fuel, increases its gas phase PAHs and the gas phase PAHs mostly dominate the total PAH distribution.

Poster 04 – Jacob W. Martin
Dynamic gas interactions with polycyclic aromatic hydrocarbons

Jacob W. Martin[1]*, Peter Grančič[1], Dongping Chen[2], Sebastian Mosbach[1,3] and Markus Kraft[1,2,3,4]

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The initial formation of soot particles is still poorly understood. A complete description of this process would have widespread implications, from reducing the amount of soot released into the environment to controlling the manufacturing process of industrial carbon particles. The best description to date considers nascent soot particles to be aggregates of small polycyclic aromatic hydrocarbons (PAH) containing 10-20 rings.[1,2] Gas interactions are of primary importance in these early stages of soot formation; pressure affects the aggregation of the particles, acetylene grows and oxidation shrinks the PAH. Understanding how accessible gas species are to these self-assembled PAH clusters becomes of primary importance to describing these early soot precursors.

Chen and co-workers found that there is a size dependent melting phenomenon in PAH clusters which significantly changes the surface topology of the clusters.[3] At low temperatures they forms long turbostratic stacks of molecules held together by Van der Waals interactions. At high temperatures thermal motion breaks apart these structures opening the structure. Previously, the surface reactivity of these clusters were explored by applying a static probe to integrate the accessible surface area for potential chemical reactions using the concept of solvent excluded surface.[4] However, dynamic interactions were not considered and it was not possible to determine whether penetration of the cluster was possible.

We present an investigation of the dynamic interactions between gas-phase molecules and coronene clusters. The study considers temperatures corresponding to both liquid and solid clusters. Nitrogen was used as a probe as it possess similar adsorption properties to reactive species present in soot gas phase reactions (i.e. O_2, NO, C_2H_2). We found two main scattering regimes: specular and diffuse. Specular scattering involved the direct reflection of the nitrogen by the cluster, resulting in a short interaction time. Diffuse scattering led to a significant interaction time between the nitrogen and the cluster surface. The nitrogen was observed to be attracted to the surface and hopped between sites/wells of low potential energy. For solid clusters we found three main sites where the nitrogen spends extended time: hydrogen sites, pockets between stacks and pinned on the top carbon surface of the coronene. Increasing the temperature beyond the melting point of the clusters broke apart the stacks of coronene and allowed nitrogen to penetrate the cluster. We present a dynamic model for the interaction of gas-phase molecules with nascent soot particles. This can be used to improve the modelling of soot oxidation, growth and effect of pressure.

[1] M. L. Botero, D. Chen, S. Gonzalez-Calera, D. Jefferson, M. Kraft, HRTEM evaluation of soot particles produced by the non-premixed combustion of liquid fuels, Carbon 96 (2016) 459-473.

[2] H. Wang, Formation of nascent soot and other condensed-phase materials in flames, Proceedings of the Combustion Institute 33 (2011) 41-67.

[3] D. Chen, T. S. Totton, J. W. J. Akroyd, S. Mosbach, M. Kraft, Size-dependent melting of polycyclic aromatic hydrocarbon nano-clusters: A molecular dynamics study, Carbon 67 (2014) 79-91.

[4] D. Chen, J. Akroyd, S. Mosbach, M. Kraft, Surface reactivity of polycyclic aromatic hydrocarbon clusters, Proceedings of the Combustion Institute 35 (2) (2015) 1811-1818.

Poster 07 – Manoel Yohanes Manuputty
Numerical Simulation of TiO2 Synthesis in a Stagnation Flame Reactor

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The laminar flame synthesis of titanium dioxide nanoparticles from titanium tetraisopropoxide (TTIP) is modelled using a population balance model and 1-dimensional flow approximation implemented in *k*inetics®. The validity of the flow approximation is investigated using cold-flow computational fluid dynamics simulations in OpenFOAM and compared against the experimental data. Two possible solutions are identified to minimize the error from invoking the 1-dimensional approximation. In order to simulate the reactions in the gas-phase, a detailed hydrocarbon combustion mechanism is coupled to simple and widely used one-step decomposition model to describe the formation of TiO_2 particles from TTIP. The population balance model includes nucleation, surface growth and coagulation processes and is closed using the method of moment with interpolative closure (MoMIC). Further work will include using a more detailed TTIP decomposition mechanism. Experimental work will be performed to assess the performance of both models.

Poster 08 – Olalere R. Kayode
Experimental Investigation of Particle Emissions From A Gasoline Fuelled GDI Engine

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Particulate emissions from gasoline engines are important issues. This issue is especially true for direct injection spark ignition (DISI) gasoline engines which have been considered as a bigger contributor to ultra-fine particulate emissions and hence total particulate number. Research evidence shows that particle number (PN) emissions from gasoline direct injection (GDI) engines are similar in level or even higher than those of diesel engines equipped with diesel particulate filters (DPFs). Nanoparticles, despite their negligible contribution to total mass, may also impose a great hazard to both the environment and human beings due to their significant number. In this study the effect of engine fuel injection sweep on the Particulate number emission characteristics was investigated in a DISI engine using DMS500. Experiments were conducted under the engine operating conditions of stoichiometric air–fuel ratio, 1500 rpm engine speed and at engine loads of 4.5, 6.5 and 8.5bar IMEP. The fuel injection timing sweep was from 160 crank angle degrees (CAD) bTDC to 320 CAD bTDC using unleaded gasoline (ULG) RON 95 fuels. It was observed that the particle size of most of the PN emissions across the three loads were in the range of about 10nm to 100nm which could be described as nanoparticle. The peak PN emissions recorded during the late injection timing of 160 CAD bTDC was due to inadequate homogeneous mixture formation. The peaks PN emissions recorded during the early injection 320 CAD bTDC was due to piston wetting. The optimal fuel injection timing for PM emission across the loads was observed around 260 to 280CAD bTDC. An increasing number of the accumulation mode was noticed as the load increases. The reduced PN emissions noticed as the loads increases were due to the increasing combustion flame temperature which helps in unburned particle post-oxidation.

Poster 10 – Safwan Hanis Mohd Murad
Particulate Matter Emissions from Model M15 Methanol/Gasoline Blends in a GDI Engine

SAFWAN HANIS MOHD MURAD[1]*, JOSEPH CAMM[1], MARTIN DAVY[1], RICHARD STONE[1,] DAVE RICHARDSON[2]

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The influence of oxygenates on particulate matter (PM) emissions from GDI engines has differing reports in the literature. It is hypothesised that these conflicting results can be explained by fuel vaporisation, and its composition in terms of aromatic content and heavy end components. For good control of the experiments M15 fuels have been mixed from pure fuel components and this enables the distillation characteristics to be matched to those of an M15 ULG. Code has been written to predict the vapour pressure of the non-ideal M15 blends; by controlling the fuel temperature experiments can be conducted with flashing and non-flashing fuel sprays. Two contrasting groups of M15 fuels have been used: one 'light' fuels group and second 'heavy' fuels group in terms of the vapour pressure, T50, T90, aromatic content. Rig studies with backlit illumination and Mie scattering have been used for characterization of penetration length, spray angles (and collapse) and bulk evaporation rate. The spray structure is characterized by the pressure ratio (system pressure / vapour pressure). The same fuels have been used in an engine with a full-length optical liner, to study the interaction of spray with cylinder flow and piston impingement. Particulate matter emissions are reported from different optical engine builds for comparison of the PM emissions vs fuel temperature and the effect of quartz vs metal components.