2012 Cambridge Particle Meeting

Program abstracts

18 May 2012

Lecture Room 4, Engineering Department,
Cambridge University, Trumpington Street

Chairmen:

Adam Boies and Jacob Swanson (University of Cambridge)

Jon Symonds (Cambustion)

Particulate Mass Measurement: A Statistical Study

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Although particle number has been introduced as a new tailpipe emissions metric for Europe, the particle mass limit remains and is the only measure of regulating vehicle tailpipe emissions in other markets. This method involves capturing a dilute sample onto a filter paper and measuring the change in mass of that filter.

This presentation focuses on the repeatability of measuring filter masses and propagates this component of measurement uncertainty through both the Federal and European emissions calculations to express as mg/mile and mg/km, respectively.

A Fully Coupled Simulation of PAH and Soot Growths with a Population Balance Model

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We present a detailed soot population balance model in which soot nanoparticles are described by primary particles made up of individual PAH molecules. This model improves on a previous PAH-PP model (Sander et al., 2011, Proceedings of the Combustion Institute. 33, 675-683) as it accounts for particle rounding due to sintering and surface growth, and it fully couples the evolution of PAH and soot particles. The model is described in detail and is used to simulate a variety of flames. From the detailed numerical solution, mass spectra and particle size distributions (PSDs) are extracted and compared with experiments. By using a new counting method and a simple collision efficiency model, experimental mass spectra have been qualitatively reproduced and the results fit well with the experimental PSDs of the various flames.

Dynamics of Fractal-like Aerosols During Sintering

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Gas-borne nanoparticles undergoing coagulation and sintering form irregular or fractal-like structures (agglomerates and aggregates) affecting their transport, light scattering, effective surface area and density [1]. The (real-time) characterization of these structures and their constituent primary particles is necessary for continuous monitoring of aerosol manufacturing and airborne pollutant particle concentrations. Significant advances have been made in characterization of agglomerates (physically –bonded particles) by employing fractal theory and relating agglomerate structure to its generation pattern through the fractal dimension, D_f. What might have been overlooked in characterization and simulations of fractal-like particles is that the above D_f values have been developed for agglomerates of *monodisperse* primary particles. For coagulating aerosols, however, this needs to be carefully examined as Brownian coagulation leads to polydisperse particles [2]. Furthermore, once coalescence or sintering starts between these primary particles, sinter necks are formed between them converting the agglomerates to aggregates [3]. Accounting for primary particle polydispersity is important as the characteristic sintering time depends strongly on primary particle size [4]. These properties may also affect their health impact [5], e.g. agglomerates may undergo restructuring & break-up [6] and release constituent primary particles.

Here, the formation of aggregates (chemically- or sinter-bonded particles) by viscous flow sintering of amorphous materials (silica, polymers) [3] and grain boundary diffusion sintering of crystalline ceramics (titania, alumina) or metals (Ni, Fe, Ag etc.) is investigated [7] by multiparticle sintering simulations. A scaling law is discovered between average aggregate projected area and equivalent number of constituent primary particles during sintering: from fractal-like agglomerates to aggregates and eventually compact particles. This is a relation essentially independent of time, material properties and sintering mechanisms. The surface area mean primary particle diameter determined by (on-line) differential mobility analyzer (DMA) and aerosol particle mass (APM) analyzer measurements and this power law for aggregates. This is in good agreement with the primary particle diameter obtained by nitrogen adsorption and particle counts from microscopic images.

References:

[1] P. Meakin, Fractal aggregates, *Adv. Colloid Interface Sci.* 28 (1988) 249.

[2] M.L. Eggersdorfer, S.E. Pratsinis, The structure of agglomerates consisting of polydisperse particles, *Aerosol Sci. Technol.* 46 (2012) 347.

[3] M.L. Eggersdorfer, D. Kadau, H.J. Herrmann, S.E. Pratsinis, Multiparticle sintering dynamics: from fractal-like aggregates to compact structures, *Langmuir* 27 (2011) 6358.

[4] M. Sander, R.H. West, M.S. Celnik, M. Kraft, A detailed model for the sintering of polydispersed nanoparticle agglomerates, *Aerosol Sci. Technol.* 43 (2009) 978.

[5] L.K. Limbach, P. Wick, P. Manser, R.N. Grass, A. Bruinink, W.J. Stark, Exposure of engineered nanoparticles to human lung epithelial cells: Influence of chemical composition and catalytic activity on oxidative stress, *Environ. Sci. Technol*. 41 (2007) 4158.

[6] M.L. Eggersdorfer, D. Kadau, H.J. Herrmann, S.E. Pratsinis, Fragmentation and restructuring of soft-agglomerates under shear, *J. Colloid Interface Sci.* 342 (2010) 261.

[7] M.L. Eggersdorfer, D. Kadau, H.J. Herrmann, S.E. Pratsinis, Aggregate morphology evolution by sintering: Number & diameter of primary particles, *J. Aerosol Sci.* 46 (2012) 7.

Soot Production and the Importance of Molecular Structure of Novel Diesel Fuels

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Efforts to stem global climate change and dwindling supplies are resulting in a shift away from the exclusive use of fossil fuels in diesel engines and towards that of more sustainable alternatives. For the most appropriate fuels derived from renewable sources, such as cellulosic material and microalgae, to be selected and developed it is important to understand how the molecular structure of such fuels impacts on combustion characteristics and the production of emissions.

To this aim, a number of engine studies have been undertaken to investigate the influence of a particular feature of fuel molecular structure on heat release and the formation of particulate and gaseous emissions. These were performed in a single-cylinder direct injection diesel engine equipped with a novel ultra low volume fuel system, which facilitated the combustion of small samples (~100 mL) of single and binary component fuels at typical common rail injection pressures. To separate the effects of fuel structure from those of combustion timing, these experiments were repeated at constant injection and constant ignition timings. Furthermore, to isolate the effect of ignition delay, an ignition improving additive was utilised to conduct further experiments with differences in ignition delay between fuels removed.

Several features of molecular structure were found to have a significant impact on the level of exhaust particulate emissions. These included: the carbon chain length of an n-alkane, the position of a single double bond in an alkyl chain, the presence of methyl branches and the straight carbon chain length of the alcohol moiety of a fatty acid ester, the alkyl chain length of a carbonate and the percentage of toluene present in blends with n-heptane. Where ignition delay was not found to be the primary driver by which the production of particulates was influenced by molecular structure, physical properties, such as boiling point, were also found to be important.

Closed Crankcase Ventilation: Inline Measurements of Oil Aerosols

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Oily emissions of the crankcase are mainly aerosols. Particle size measurements normally show a droplets size in the area of 1 micron range. These small particles are generated mainly in the piston area. Condensation, atomization at rotating shafts and spraying out of the lubricating circuit can also be the origin of the emission of these oil aerosols. In turbo charged engines, small particles can reach the crankcase via the oil return of the turbocharger. In the crankcase the particle size distribution is affected by secondary effects like decomposition or coagulation of droplets, interactions of the droplets with the wall or sedimentation. In spite of the oil mist separators used, closed crankcase ventilation systems are relevant for the total oil consumption of reciprocating engines. Due to the mandatory closed crankcase ventilation, contaminations of valves and intercoolers is possible with the consequence of reduced engine life and less cooling efficiency. Oil components in combustion also effect particle filters and catalytic converters. Regarding the total oil consumption per operation point of less than 10 g/h per day, the crankcase ventilation is becoming more and more important in engine tests.

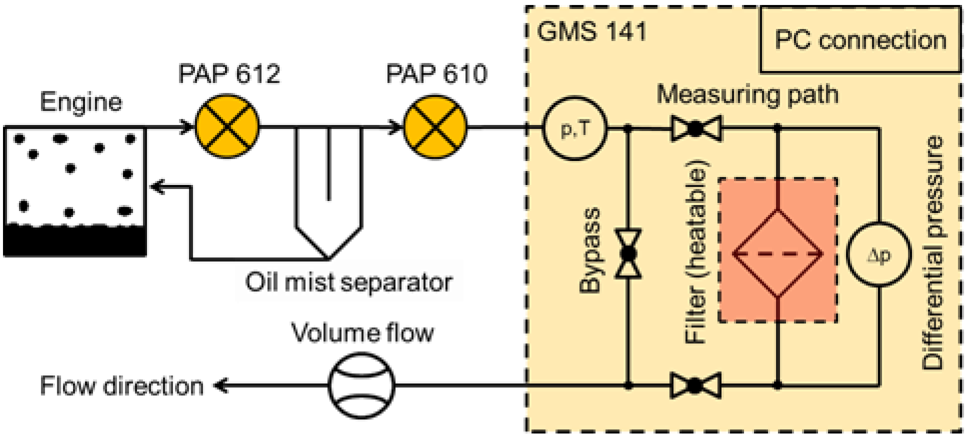

Figure 1: Schematic of the Topas/Adaptive oil blow-by measurement system.

Particle Emissions from a Soot Free Engine

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Abstract to come shortly.

Particle Size and Number Emissions from Dual-Fuel Reactivity Controlled Compression Ignition

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Many concepts of premixed diesel combustion at reduced temperatures have been investigated over the last decade as a means to simultaneously decrease engine-out particle and NO emissions. The main difficulty of these premixed concepts has always been to manage the relatively low volatility and high ignitability of the diesel fuel in order to sufficiently reduce its maximum local fuel-air equivalence ratio in the combustion chamber before the start of combustion. A well-known consequence of employing various means (exhaust gas recirculation, very early or late injection timing, etc.) to achieve premixed diesel combustion (with diesel fuel) has been a reduction in combustion efficiency and increased power-specific fuel consumption.

To overcome this trade-off between low particle and NO emissions and high "diesel-like" combustion efficiency, a new dual-fuel technique called Reactivity Controlled Compression Ignition (RCCI) has been established. In this study, particle size distributions were measured from RCCI for four gasoline-diesel compositions from 65%-35% to 84%-16%, respectively. Previously, fuel blending (reactivity) had been carried out by a port fuel injection of the higher volatility fuel and a direct (in-cylinder) injection of the lower volatility fuel. With a recent mechanical upgrade, it was possible to perform injections of both fuels into the combustion chamber. Thus particle size distributions were measured at four different gasoline injection timings for each fuel reactivity blend, while the ignition-controlling diesel injection timing remained constant. In addition, effects of heated primary dilution ratio on the particle size distribution from one of the "standard" RCCI engine operating conditions was measured to provide some information of the particles' volatility and how high of dilution ratio would be necessary to ensure stable measurements. Finally, for better understanding, some brief comparisons are made with particle size distribution measurements from within the premixed diesel low temperature combustion regime (running solely on diesel fuel). Please find a sample of the RCCI particle size distribution fuel proportion and gasoline injection timing study in Figure 1.

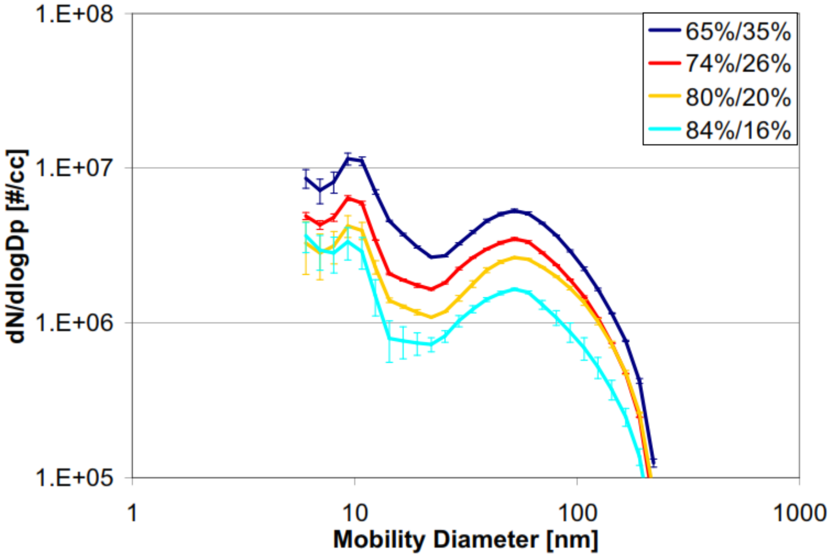

Figure 1: Particle Size Distribution Measurements from 65%-35% to 84%-16% Gasoline-Diesel Proportioning at Fixed Gasoline and Diesel In-Cylinder Injection Timings.

The Effect of Fuel Volatility and Aromatic Content on Particulate Emissions

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Direct injection spark ignition (DISI) engines produce a greater number of particulate matter (PM) emissions than Port Fuel Injected (PFI) engines, but their greater specific output and lower CO_2 emissions have led to their widespread use. Concern over the health effects of PM emissions, and forthcoming European legislation to regulate them from gasoline vehicles has led to an increased interest in the study of PM formation, measurement, and characterisation.

A model has been developed by Aikawa et al. correlating PM emissions with fuel composition. PM emissions are thought to be linked both to the vapour pressure and the Double Bond Equivalent (DBE) of the fuel components. However, there was no independent control of these parameters. Also, this work was undertaken on a PFI engine and experiments have been conducted extending the model to DISI engines.

Fuels were designed using UNIFAC (with careful consideration of octane number) such that the DBE and vapour pressure of the fuel could be varied independently. The fuel design was such that the components would co-evaporate upon injection, ensuring a homogeneous mixture at ignition.

Engine tests were conducted at a matrix of test points, independently varying the DBE and the vapour pressure of the fuel. PM emissions from a single cylinder optical engine have been analysed and these results used alongside observations of the combustion to determine the effect of vapour pressure and the DBE of the fuel components on PM emissions.
These tests have been reinforced by tests using commercially available fuels on a thermodynamic engine. These results show that the index holds under these circumstances too. Varying the DBE and the Vapour Pressure of the fuel caused results that matched the theoretical predictions closely.

References:

Aikawa, K., Sakurai, T. and Jetter, J.J. Development of a Predictive Model for Gasoline Vehicle Particulate Matter Emissions. *SAE International Journal of Fuels and Lubricants*, 2010, **3**(2), 610-622.

Demonstration of an Aerospace Recommended Practice for measuring Non-volatile PM Emissions from Gas Turbine Engines using a Prototype System

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The US FAA, the US EPA and the European Aviation Safety Agency, and the Swiss Federal Office of Civil Aviation (FOCA) have committed to underwrite studies that address research needs identified by SAE's E31 (Aircraft Exhaust Emissions Measurement) Committee that must be resolved if an Aerospace Recommended Practice (ARP) for aircraft non-volatile particulate matter (PM) is to be established. The SAE E31 committee has defined an ARP sampling system concept to capture an exhaust PM sample at the engine exit plane and transport it to a PM instrument package located at a safe distance from the engine. The instrument package is designed to measure PM number and mass concentrations. The ARP sampling system was sufficiently complex that it was important to establish the reproducibility of results from different replicas of the same sample train.

In December 2011, a version of the ARP sampling system was built by Missouri University of Science and Technology (MST) was deployed at SR Technics maintenance facility in Zurich, Switzerland and compared with the prototype sample train which had already been built and installed there by FOCA. The primary objective of this test was to compare the performance of the MST and FOCA systems in terms of PM number, mass, size and composition to assess sampling system variability. Additionally, inter-comparison of the performance of like pairs of instruments, and evaluation of the impact of 10nm vs. 23nm CPC size cutoff could also be performed with this dataset. A secondary objective of the test was to explore the impact of volatile PM removal using a catalytic stripper. Emissions from several different engine types (CFM56-5C, CFM56-7B and PW4060) were measured during the study. This paper will present a description of the sampling and measurement systems, and the major results and conclusions of the study.

New Measurements of Clusters and Nanoparticles: Implications for Atmospheric Nucleation & Growth Models

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The formation of new particles from “extremely minute quantities of matter” (John Aitken, 1911) contributes significantly to the global concentrations of atmospheric particles and cloud condensation nuclei (CCN). Through their role as CCN, these particles affect the earth’s radiation budget, so it is important to account for them in climate models. Challenges in this work involve identifying the trace species that participate in nucleation and growth, measuring their concentrations (typical mole fractions are 10^{-14} to 10^{-11}), and understanding the chemical mechanisms by which particles are formed from gases and subsequently grow. This presentation will describe our progress at developing suitable measurement methods and using this new information to gain insights about the chemical and physical processes that determine nucleation and growth rates. Evidence will be shown that the smallest stable particles contain just a few (two to four) sulfuric acid molecules, and that in the atmosphere (but not always in chamber studies) uptake of sulfuric acid vapor for particles larger than this is collision-limited.

Colleagues who have contributed to this work include James N. Smith and Fred Eisele (NCAR), David Hanson (Augsburg College), Kelley Barsanti (Portland State University) and Modi Chen, Mari Titcombe, Coty Jen, and Jun Zhao (University of Minnesota, Department of Mechanical Engineering).

Effects of Combustion Modes on Gaseous and Particulate Matter Emissions in a 2/4-Stroke Switchable Direct Injection Gasoline Engine

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Since their introduction around a century ago, internal combustion engines have been operated in Spark Ignition (SI) or Compression Ignition (CI) combustion mode. However, in recent decades, serious concerns have been raised with regards to the environmental impact of the gaseous and particulate emissions arising from operations of these engines in these combustion modes. As a result, ever tightening legislation, that restricts the levels of pollutants that may be emitted from vehicles, has been introduced by governments around the world. In addition, concerns about the world's limited fossil fuel energy reserves and, more recently, by Particulate matter and CO2 emissions that affects human health and climate change has lead governments in Europe and other countries of the World to introduce high taxation on duty on fuel and strict legislation on emissions.

These challenges have prompted powertrain researchers and engine builders to seek alternative combustion modes. Over the last decade, an alternative combustion mode commonly known as homogeneous charge compression ignition (HCCI) or controlled auto-ignition (CAI) combustion, was developed that has the potential to achieve efficiencies in excess of GDI units and approaching those of current CI engines, but with levels of raw NOx emissions up to two levels of magnitude lower than either, and with little or no smoke emissions. The HCCI/CAI combustion has a lot of potential benefits over the conventional SI and CI combustion but it has its own challenges, such as difficulty in controlling the combustion phasing, a restricted operating range, and high hydrocarbon emissions.

Direct Injection Gasoline engines are staging a come-back because of its potential for improved fuel economy through principally the engine down-sizing by boosting or 2-stroke operation, and possibly stratified charge combustion or Controlled Auto Ignition (CAI) at part load operations. Due to the limited time available for complete fuel evaporation and the mixing of fuel and air mixture, locally fuel rich mixture or even liquid fuel can be present during the combustion process and high short circuiting rate in 2-stroke mode. This causes significant increase in Particulate Matter (PM) emissions and hydrocarbon from direct injection gasoline engines compared to the conventional port fuel injection gasoline engines, which are of major concerns because of its health implications. In this paper, the Gaseous and Particulate Matter emissions of different combustion modes were measured from a unique direct injection gasoline engine that could be operated in both spark ignition and CAI combustion modes in either 4-stroke and 2-stroke cycle. Gaseous emissions was sampled directly from the exhaust pipe using Horiba Mexa 7100DEGR. Particulate Matter emissions was sampled directly from the exhaust pipe and DMA. The effects of operating the engine using 2 and 4 strokes SI, CAI on Gaseous and Particulate Matter emissions in various operational modes are presented and analysed.

Reduction of DPM and NOx using 4-way Catalyzed Filtration Systems

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The next generation of emission control devices includes 4-way catalyzed filtration systems (4WCFS) that include both NOx and DPM removal technology. Toyota Motor Corporation introduced the first successful 4WCFS concept in the early 2000s that they referred to as a "diesel particulate – NOx reduction" system or DPNR [1]. In brief, this version of a 4WCFS consists of a bare DPF substrate that has been washcoated with a NOx storage catalyst. Thus, DPM and NOx are reduced simultaneously by a single control device. The bare DPF used in this study is made from an advanced ceramic material (ACM). The ACM manufacturing process is controlled so that the microstructure, total porosity, and pore size distribution are tailored to meet requirements for DPM emission control. Additionally, ACM is suitable for catalyzed applications. By increasing the porosity of the ACM filters, it was hypothesized that larger amounts of NOx storage catalyst could be loaded onto the filters. Previous studies have shown that ACM DPFs demonstrate high filtration efficiency, low-pressure drop, high-temperature handling capability, and excellent mechanical integrity at a porosity of 60% or higher [2, 3, 4, 5].

The focus of this work is twofold. The first objective was to develop a methodology to simultaneously evaluate the NOx and DPM control performance of mini 4WCFS that are challenged with diesel exhaust from a 2005 John Deere off-road diesel engine. The experimental mini filters evaluated were 1.9 x 1.9 x 7.5 cm square prisms. Thus, the method differs from traditional tests where full-sized aftertreatment exhaust systems are evaluated. It is a cost effective method to evaluate prototype filters rapidly and consistently with control of temperature, flow rate, and face velocity. The second objective was to evaluate the impact of catalyst loading and substrate porosity on (1) pressure drop, (2) catalytic performance, (3) the particle filtration performance of catalyst-coated standard (STD) and high porosity (HP) test filters as stand-alone 4-way catalyzed filtration systems. The catalyst coatings used in this study were basic research coatings and were used due to availability within the project timeframe to test the catalyst loading capacity of the STD and HP test filters and are not intended for production applications. Further work would be needed with commercial automotive catalyst companies to optimize for their commercial coatings.

Experimental measurements included simultaneous and time resolved total and solid particle filtration efficiency (FE), size resolved FE, pressure drop (ΔP), and NOx removal performance. Preliminary results indicated that the use of HP ACM 4WCFS results in 98% reductions in NOx and 95% reductions in solid and semi-volatile particulate matter averaged over 10 regeneration cycles. Similarly, STD ACM 4WCFS exhibited high filtration efficiencies but slightly reduced NOx control performance. The rich / lean cycling that is used to regenerate the filter has almost no impact on solid particle filtration efficiency, but impacts NOx removal efficiencies. Shorter lean times (more frequent regeneration) lead to higher removal efficiencies but more reductant is consumed. Overall, the new methodology for simultaneously evaluating the FE and NOx removal performance of small scale emission control devices has proven to be a valuable developmental tool. Future work includes optimization and evaluation of additional filters and catalysts and scaling up the system to evaluate larger prototypes.

References

[1] K Nakatani, S. Hirota, S. Takeshima, K. Itoh, *SAE Technical Paper* 2002-01-0957, 2002.

[2] A.J. Pyzik, C.G. Li. *Int. J. Appl. Ceram. Technol*. 2(6):440–451, 2005.

[3] A.J. Pyzik, C.S. Todd, C. Han. *J. European Ceramic Society* 28:383–391, 2008.

[4] C.G. Li, H. Koelman, R. Ramanathan, U. Baretzky, G. Forbriger, T. Meunier. *SAE Int. J. Fuels Lubr*. 1(1): 1307-1312, 2008.

[5] J. Swanson, M. Schumacher, W. Watts. D. Kittelson, R. Newman, R. Ziebarth. *29th AAAR Conference*, Portland, OR, October 25 – 29, 2010

The Centrifugal Particle Mass Analyser as a Fundamental Particle Mass Standard

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The CPMA classifies aerosol particles by their mass to charge ratio. A flow of pre-charged particles enters a classification region between two concentric cylinders. The cylinders are rotated, and a potential difference is applied between them, thus causing opposing electrical and centrifugal forces to act on the particles. Only particles of the correct mass to charge ratio will emerge from the classification region, others will be lost to the cylinder surfaces. A slight difference in the speeds of the cylinders allows the two forces to balance at all radii across the classification region, which improves the transmission efficiency.

We present here an evaluation of a new commercial version of the CPMA, including its performance when classifying test aerosols such as Polystyrene Latex standards. We show data using the CPMA to calculate the density and mass-mobility exponent for soot aerosols. We also present a new *suspended mass standard* as an application of the CPMA when combined with a charger and aerosol electrometer. The use of an aerosol electrometer (as opposed to a CPC) as a detector allows automatic compensation for multiply charged particles. This method allows other instruments to be calibrated for mass concentration.

Studies of Particulate Matter Emissions of Automotive Engines Using Biofuels

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The control of the PM emissions is expected to commence in European regulation which will require not only the monitoring of PM mass emissions, but also the PM number for all light-duty vehicles. One the other hand, the use of ethanol and other alternative fuels (including bio-fuels) is expected to increase. In this study, the characteristics of PM emissions in a direct injection spark ignition engine are examined with respect to fuel properties and injection strategies. It is shown that the ethanol fraction with dual-injection results in a unimodal mass distribution where the larger, accumulation mode particles are removed. Compared to blends in DI, the dual-injection strategy helps to lower the total PM emissions