Numerical Investigation of Fuel Injection Control on Aerosol Formation and Transport in Canyons and Open Areas

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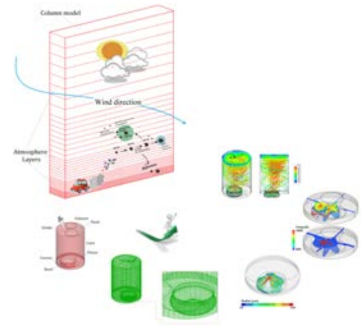
Combustion processes are a significant source of air pollutants, contributing to atmospheric aerosol formation and adversely affecting air quality [1]. Modelling the combustion chamber is essential for accurately predicting pollutant emissions, optimizing combustion efficiency, and minimizing the environmental impact of fuel combustion [2]. Moreover, modelling air quality is crucial for understanding the dispersion and transformation of pollutants, enabling the assessment of their impact on human health and the environment [4]. In this study, we present a comprehensive numerical modelling approach to predict pollutant emissions from a combustion chamber and their subsequent transport and transformation into aerosols within street canyons and open areas. The first phase of our work involved developing a detailed combustion chamber model to quantify the impact of fuel injection control on emissions of key pollutants, including particulate matter (PM), nitrogen oxides (NO_x), and volatile organic compounds (VOCs). It underscored two pivotal characteristics for injection pressure function: a continuous increase coupled with specific number of vibrations, forming an increasing oscillatory function. Not only did it enhance power efficiency and reduced VOC emissions, but it also yielded more irreversibility, opening opportunities for more waste heat recovery. The predicted emission profiles were then used as input for the second phase, which focuses on simulating the dispersion, chemical transformation, and secondary aerosol formation in both open areas and street canyon environments. Advanced computational fluid dynamics (CFD) techniques, coupled with atmospheric chemistry models, were employed to capture the complex interactions between emitted pollutants, meteorological conditions, and environmental geometries. The study aims to provide insights into the spatial and temporal evolution of aerosol concentrations, contributing to better air quality management and emission control strategies. Preliminary results highlight the influence of fuel injection strategy, canyon geometry, and atmospheric conditions on pollutant dispersion and aerosol formation. This research can aid policymakers in designing effective mitigation strategies to reduce human exposure to harmful airborne pollutants.



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Lithium-ion battery thermal runaway particle emissions

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In recent years, the use of lithium-ion (Li-ion) batteries has seen significant growth, driven by their widespread application in electric vehicles and the broader energy transition. However, this increased use has brought to the forefront safety concerns, particularly regarding their susceptibility to thermal runaway. Battery fires are known to pose significant risks as they release toxic gaseous and particulate emissions that can adversely affect human health and the environment. Moreover, the methods used to extinguish these fires can alter the composition and nature of these emissions, further complicating the risks. In this study, experiments were conduced with modules composed of li-ion cells that were triggered into thermal runaway by overcharging them. Experiments were conducted in a 20-ft container that was equipped with instrumentation to measure temperature, pressure and particulate emissions. Three experiments were conducted as a part of this study – one involving no fire suppression, and two tests during which fire suppressants were engaged. Among these two tests, water was used as the suppressant for one of the tests, and an aerosol-based suppressant was used for the other. Detailed characterization of emissions included collection of fine particulate matter (PM) on filter media, and real-time measurement of particle number concentration and size distribution. Near-real-time metal concentration was measured with a toxic metal aerosol analyzer (TARTA). Further analysis of PM filters to examine chemical composition of PM (via inductively coupled plasma mass spectrometry), morphology (via scanning electron microscopy), the presence of particle phase inorganic ions (ion chromatography) and polycyclic aromatic hydrocarbons (via gas chromatography) was conducted. Results from this program will provide critical insight into airborne emissions from battery fires, and the influence of suppressants on these emissions. Such information will be invaluable for first responders, and stakeholders focusing on the environmental impact.

Relating condensable reaction product formation with nanoparticle growth rates: Select monoterpene + NO_3 reactions under varying oxidizing conditions

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Secondary aerosol (SecA) formation is a leading cause of air quality issues, and a critical process in the formation of clouds droplets. Notwithstanding the importance, the first steps of secondary aerosol formation keep eluding the researchers. The single most important molecular property describing SecA formation potential is the compound vapor pressure. As most of fresh molecular clusters and small secondary nanoparticles are prone to evaporation and scavenging by larger particles and surfaces, the rate at which condensable products are provided determines their probability to survive. The smallest clusters requiring the lowest vapor pressure molecules to induce SecA growth.

The tendency to form new particles and the subsequent generation of SecA mass was studied in the CESAM atmospheric simulation chamber in Paris Creteil. Several monoterpene + NO_3 reactions were investigated including a- and g-terpinene, limonene and a-pinene. The nitrate radical was prepared either by N_2O_5 decomposition or by mixing NO_2 + O_3 in the chamber. Significant differences were observed between the reaction systems likely due to O_3 involvement in the second case. The oxidized gas-phase product distributions were quantified by NO_3^- and Br^- chemical ionization mass spectrometry (CIMS) and the dynamics of the nanoparticle formation were monitored by a combination of a particle-size magnifier (PSM) and a scanning mobility particle sizer (SMPS). The resulting aerosol chemical composition was determined by an aerosol chemical speciation monitor (ACSM). By combining information on the rate of direct aerosol precursor formation (*e.g.*, highly oxygenated organic molecules, HOMs) and the rate of nanoparticle growth (*i.e.*, formation and growth rates of ca. 2 to 10 nm particles), allows to assess the efficiency of SecA mass generation at a molecular level. The studied monoterpenes contained distinct functional features (*e.g.*, different number and type of double bonds) and offer insights into molecular reactivity and closely related affinity for oxidative molecular growth.

Real-time analysis of trace metals in air by microwave induced plasma time-of-flight mass spectrometry (mipTOF)

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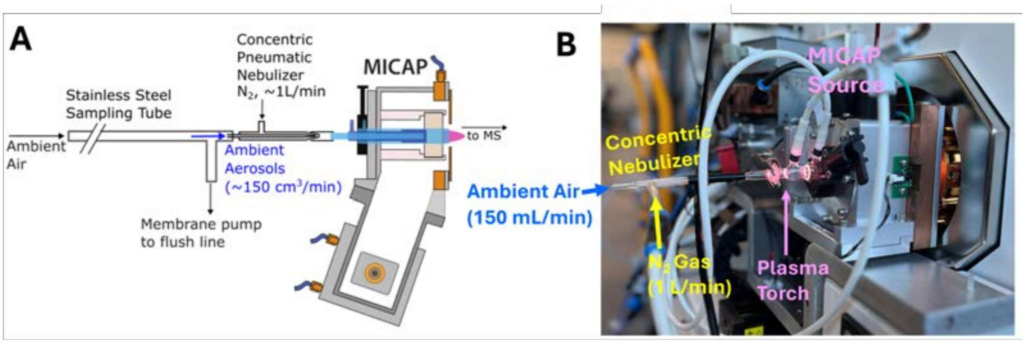
Determination of the elemental composition of airborne nanoparticles and micro-particles is essential to understand the source(s) of these particles and also to predict potential health effects. [1] The most common approach to measure the metal content of air is to collect samples on filters and then analyze digests by ICP-MS; [2] however, this strategy offers poor time resolution (e.g. days) and only provides bulk element composition information. To understand the spatiotemporal characteristics of the emission of metal-containing aerosols, which is key to assessing exposure, real-time analysis strategies are essential. Here, we report the development of a microwave induced plasma time-of-flight mass spectrometer (mipTOF) that can be used for the direct analysis of metal-containing airborne particles.



A) Schematic of venturi sampling setup. B) Image of plasma source with direct introduction of ambient air.

The mipTOF is a field-deployable trace-element mass spectrometer. It uses a nitrogen-sustained high-power plasma (MICAP, Radom Instruments) [3, 4] to vaporize, atomize, and ionize aerosols with sizes from the ultrafine to PM10. Ambient air is sampled into the plasma via a concentric pneumatic nebulizer set up as a Venturi pump (see figure). Atomic ions generated in the plasma are extracted into the mass spectrometer, where they are sorted according to mass-to-charge ratio (m/Q) and recorded. With the mipTOF, concentration LODs range from 10 ng/m^3 (potassium) to 0.05 ng/m^3 (lead) in a 10 second measurement. The high-sensitivity, high-speed metal-aerosol measurements possible with mipTOF enable new research into real-time spatiotemporal analysis of metals in air. We will report on the use of the mipTOF in long-term air monitoring and mobile lab measurements.

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Performance and Uncertainty of Portable Emissions Measurement Systems (PEMS) in Laboratory and On-Road Tests for Improved Quantification of Vehicle Exhaust Particles

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Ultrafine particles (UFP) and gaseous pollutants emitted from vehicle exhausts are major contributors to air pollution in urban areas. In the EU, the number of solid exhaust particles larger than 23 nm is regulated for type approval of vehicles by testing real driving emissions (RDE) using portable emissions measurement systems (PEMS). However, PEMS have larger measurement uncertainty than reference instruments used in dynamometer test setting and their metrological validation is currently lacking. Thus, it is critical to determine this uncertainty to underpin the current and future conformity factors.

In this study, the performance of four PEMS devices were evaluated by performing dynamometer and RDE tests. The PEMS devices were evaluated with four Euro 6 passenger cars and in Finland and Denmark. Over the course of three years during this study, three commercial PEMS devices were evaluated as well as a 'GoldenPEMS' which was validated metrologically by three National Metrology Institutes (NMIs). The PEMS devices used condensation particle counting (CPC) and diffusion charging (DC) technologies for particle number concentration (PN) measurement.

The results showed that a significant day-to-day variation exists in RDE tests performed with the same vehicle, test route, and driver. Day-to-day variations are mostly larger than device-to-device variation. Measured PN can vary by more than 50% depending on the PN measurement system. In addition, the RDE results recorded with DC-based PEMS correlated better with laboratory results for tests producing lower PN emissions (diesel engines), while the CPC-based PEMS performed better for tests producing higher PN emissions (gasoline engines). The results suggest that the two PN PEMS devices may have to be tuned for different emission matrixes.

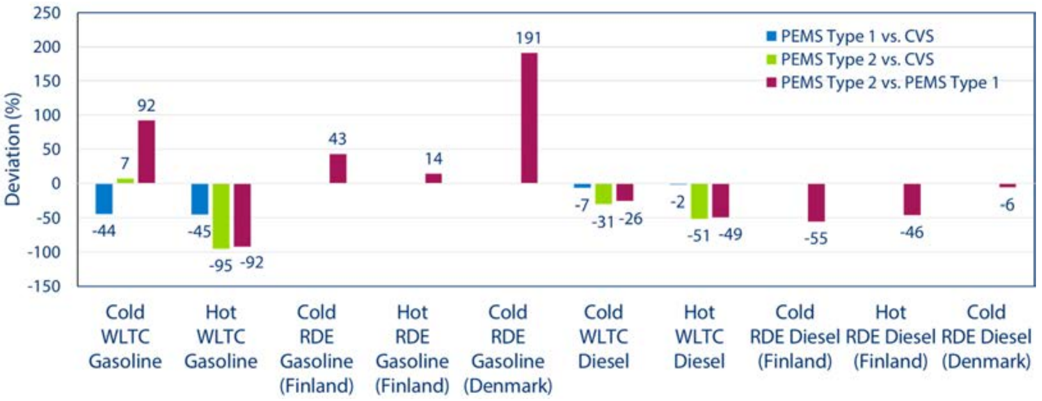

Figure 1. Comparison of measurements by different PN-PEMS devices under laboratory (WLTC) and on-road (RDE) testing conditions

On-road PN and BC emission measurements of L-category vehicles

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This study aims at quantifying the in-use particulate emission levels of L-category vehicles, by performing on-road PN and BC measurements on actual vehicles. The use of PEMS devices, commonly used in cars and trucks for RDE-ISC testing, was rejected due to limited space for equipment installation and safety concerns. Instead, a commercially available miniaturized DC particle counter was used for PN emission measurement, and a novel optoacoustic BC sensor for BC emissions measurement.

The emission measurements were conducted in the metropolitan area of Thessaloniki. Different types of vehicles were selected to be tested, of varying age, representative of the current EU L-category vehicle fleet, including L1eB, L2e, L3eA1, L3eA2 and L3eA3. The devices installed on each bike were the particle measurement devices either BC sensor or DC counter, a GPS receiver, OBD data recorder, a SEMS device measuring CO, CO2 and NO and an EFM pitot tube wherever possible.

Considerable amounts of particle emissions were found for specific subgroups of vehicles, especially under high load operation, but less particle emissions in others. The experimental campaign demonstrated that on-road emissions testing of L-category vehicles is difficult yet feasible with devices such as SEMS, BC sensors and miniaturized PN DC counters.

Acknowledgments

This research has been co-financed by the European Union’s Horizon Europe research and innovation programme under grant agreement No 101056777 (LENS).