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Editorial: Particulate Matter Emissions From Conventional and Reformulated Fuel Combustion: Advances in Experiments and Simulations

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Editorial on the Research Topic

Particulate Matter Emissions From Conventional and Reformulated Fuel Combustion: Advances in Experiments and Simulations

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Particulate matter (PM or soot) emissions generated by combustion of conventional and reformulated fuels adversely impact the environment and human health (Bond et al., 2013; Landrigan et al., 2018; World Health Organization (WHO), 2016), generating public awareness and motivating efforts towards the mitigation of their harmful effects.

Soot formation is one of the most complex phenomena in combustion, involving interactions between combustion chemistry, fluid mechanics, mass/heat transport, and particle dynamics, spanning different spatial and temporal scales. A fundamental understanding of soot formation process is thus necessary to achieve a strong reduction of PM emissions and design cleaner and more efficient combustion systems. This has motivated a longstanding and ongoing research activity aimed at improving our understanding of the physical and chemical processes involved in soot formation, well reviewed in these recent works (Wang and Chung, 2019; Michelsen et al., 2020; Martin et al., 2022).

Despite the wide interest, the transition from gas-phase molecules to incipient soot particles is still elusive and the successive particle growth and oxidation processes are far from being fully understood, especially in conditions relevant to real-world applications. Recent advances in combustion PM emission diagnostic and computational capabilities helped in improving the predictability of fundamental chemical and aerosol models for practical applications, thus tackling some of the above-mentioned challenges.

The aim of this research topic is to display the ongoing research efforts in addressing the existing gaps on particulate formation from various fuel sources and in conditions typical of practical combustion applications (e.g. flames, engines, pool fires), through both experimental and numerical approaches.

The contributions of this research topic can be grouped in two topical areas.

The first one focuses on developing and applying advanced diagnostic techniques to study different stages of soot formation in conditions relevant to practical applications.

Zhou et al. measured soot volume fraction (SVF) with a new diagnostic method in counterflow diffusion flames, which are one of the most representative laminar diffusion flames with a configuration well suited for soot research. The authors showed that the planar light extinction method with a diffuse optical layout is effective and robust for SVF measurements, with superior spatial resolution compared to the previous pointwise laser extinction method. With a focus on real-world applications, Dasappa et al. investigated particulate matter formation in premixed flames at elevated temperatures and oxygen enriched conditions, which are characteristic of methane and natural gas combustion applications. The authors measured particle size distributions for several equivalence ratios and found that the volume fraction decreases with increasing flame temperature. Using a detailed kinetics, they modeled these flames and highlighted the main pathways towards soot formation under oxygen enriched conditions.

In their work, Cruz et al. characterized the production of soot in a surrogate pool fire, which is a common form of fire in industrial applications. The auto-compensating laser-induced incandescence technique was applied for the first time to measure the local SVF from an ethylene flame burning in still air, thus providing a valuable data set for validating soot production models in pool fire configurations.

A fundamental study on the effect of fuel film on premixed flame combustion and emissions characteristics was presented by Bai et al., through joint experimental and numerical techniques. The authors found that the wall film tended to promote emissions, producing more unburned hydrocarbons, soot precursors and aldehydes. These results can help optimize the design of diesel engine combustion systems, improve in-cylinder combustion processes, increase engine thermal efficiency, and reduce emissions.

The second topical area comprises works in which various numerical techniques are applied to have a better understanding of soot particle properties at the nanoscale, to study the influence of oxygenated fuels on soot formation when blended with conventional fuels and to study soot growth in engine relevant conditions.

In the work of Wang et al., the surface reactivity of carbonaceous nanoparticles, comprised of small polycyclic aromatic hydrocarbons (PAHs), is revealed through density functional theory (DFT) calculations. The authors explored the energy barriers of hydrogen abstraction reactions from a set of model systems of soot by H radicals, which are key representative reactions of the soot growth and oxidation processes. The authors found that the surface reactivity depends on the particle size and the most reactive sites always locate at the surface pockets. On the other hand, Xu et al. used DFT method to investigate the electronic properties of PAHs molecules, well-known soot precursors. The authors calculated the HOMO-LUMO gaps of several PAHs. Gap values of all PAH molecules were found to exhibit a size dependency to some extent. However, results showed that the substitution of ketone group and the five-member rings forming nonplanar PAHs have the greatest impact on the HOMO-LUMO gap of PAHs.

Schmitz et al. evaluated the effect on soot particle formation of blending oxygenated fuels with conventional fuels, which are promising synthetic fuel candidates deployable in self-ignition engines. The sooting propensity of ethylene blended with oxymethylene ether-3 (OME3) was numerically investigated on a series of premixed flames. A linear correlation was identified between the OME3 content in the fuel and the reduction in the soot volume fraction of larger aggregates, while smaller blending ratios led to an increased number of nanoparticles. Killingsworth et al. performed Computational Fluid Dynamics (CFD) simulations of n-dodecane soot formation process under engine relevant conditions. The simulations were setup to model pyrolysis experiments in a constant-volume chamber at high-pressure with several different literature PAH and soot models. All simulation results predict lower soot mass compared to the experiments, as well as later soot inception indicating that further work is needed to improve chemical mechanisms in tandem with soot models under pyrolysis conditions.

In conclusion, this research topic provides an overview of the large breadth of soot research and its importance for reducing soot emissions in a variety of real-world combustion applications. Numerical and experimental investigations herein are once again confirming the complexity of the soot nucleation and growth process and its dependency on multiple factors, such as operating conditions, fuel source, combustion systems. A better knowledge of the interplay of these factors on soot formation should be obtained to predict soot formation in large-scale combustion devices.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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