frontiers | Frontiers in Energy Research

TYPE Editorial
PUBLISHED 06 September 2022
DOI 10.3389/fenrg.2022.974691

OPEN ACCESS

EDITED BY
Chungen Yin,
Aalborg University, Denmark

REVIEWED BY
Qingyan Fang,
Huazhong University of Science and Technology, China

*CORRESPONDENCE
Mario Commodo,
mario.commodo@stems.cnr.it

SPECIALTY SECTION
This article was submitted to Advanced Clean Fuel Technologies,
a section of the journal
Frontiers in Energy Research

RECEIVED 21 June 2022
ACCEPTED 20 July 2022
PUBLISHED 06 September 2022

CITATION
Pelucchi M, Abian M and Commodo M (2022), Editorial: Experimental and modelling approaches for clean combustion technologies.
Front. Energy Res. 10:974691.
doi: 10.3389/fenrg.2022.974691

Editorial: Experimental and modelling approaches for clean combustion technologies

Matteo Pelucchi[1], Maria Abian[2] and Mario Commodo[3]*

[1]Department of Chemistry, Materials and Chemical Engineering "G. Natta", Politecnico di Milano, Milano, Italy, [2]Department of Chemical and Environmental Engineering, Aragón Institute of Engineering Research (I3A), University of Zaragoza, Zaragoza, Spain, [3]Institute of Sciences and Technologies for Sustainable Energy and Mobility (STEMS), National Research Council-CNR, Naples, Italy

KEYWORDS

combustion, flames, advanced diagnostics, numerical modelling, chemical kinetics, pollutants and greenhouse gases

Editorial on the Research Topic
Experimental and modelling approaches for clean combustion technologies

Despite the rapid growth in alternative energy source utilization, combustion technologies will still play a major role in the years to come. Indeed, the energy mix of the next decades will see a coexistence of wind and solar sources and of combustion of e-fuels or synthetic fuels derived from renewable energies or produced from electricity excess, biofuels produced from non-edible biomass conversion (Dryer 2015; Elishav et al., 2020; Kohse-Höinghaus 2022), or unconventional sour fuels (Gupta et al., 2016). Combustion processes are almost ubiquitous in modern societies through power generation systems, transportation engines, and industrial and domestic heating applications. Nevertheless, combustion also represents the major source of atmospheric pollution, and thus new or improved low-emission/low-carbon technologies are continuously sought by scientists and industry players. To achieve this goal, considerable multidisciplinary experimental, theoretical, and modelling efforts are necessary to improve the understanding of the physics and chemistry of flame propagation, fuel ignition, and pollutant formation paving the way for carbon-neutral technologies and greenhouse gas and pollutant emission reduction.

The aim of this research topic was to present new results, findings, and developments in various disciplines associated with combustion science and pollutant formation and destruction.

Chen et al. investigated the recycling of exhaust heat in internal combustion engines to dissociate methanol, followed by its blending with methanol to produce engine fuel, as a promising technical solution for improving engine efficiency, and reducing emissions. Specifically, methanol was vaporized by the exhaust heat of the internal combustion engine through a methanol dissociation device and then dissociated using a catalyst to generate a mixture of hydrogen (H_2) and carbon monoxide (CO) with a ratio of 2:1. A kinetic model for the methanol–syngas fuel is proposed by reducing a detailed chemical kinetic model, making it applicable to large-scale simulations of real devices. Shock tube experiments were carried out to measure the ignition delay time of methanol blended with dissociated methanol gas. The effects of the equivalence ratio, pressure, and of the ratio of dissociation on ignition delay times were investigated through reaction path analysis and sensitivity analysis.

In the framework of using biomass-derived fuels to replace fossil-based fuels as a promising way to contribute to net-zero carbon dioxide emissions, Wang et al. investigated the ignition and combustion characteristics of fast pyrolysis bio-oil (FPBO) in a constant-volume combustion chamber. n-Butanol and 2-ethylhexyl nitrate (EHN) addition was found to largely improve the atomization and ignition properties of the fuel blends, respectively. An appropriate proportion of EHN additive into n-butanol is determined based on the balance between the ignition improvement and the amount of EHN addition. Then, the effects of FPBO content (up to 30%) on FPBO/n-butanol blends with the same EHN addition were investigated. The experimental results showed that a distinct two-stage ignition process can be observed for all cases. The increase in the EHN content until 8% advances both the low- and high-temperature reaction phases of n-butanol. Increasing amounts of FPBO in FPBO/n-butanol/EHN blends have little effect on the low-temperature reaction phase but delay the high-temperature reaction phase. The chamber wall temperature is found to have a significant influence on the ignition and combustion processes of the tested blends, and the occurrence of a negative temperature coefficient behavior is observed in a chamber wall temperature in the range of 535–565°C.

Advanced combustion technologies will play a dominant role as short-to-midterm solutions to the energy transition, and even in a much longer perspective for hard to electrify, or hard to decarbonize, sectors such as heavy duty, marine, or air transport. Under the typical operating conditions of such combustion devices, i.e., low temperatures and fuel lean combustion, complete fuel conversion can be achieved while avoiding soot and nitrogen oxide formation. In this context, Shaqiri et al. provided new experimental data for iso-octane, an important reference compound for both conventional and sustainable fuel surrogates. The oxidation of stoichiometric iso-octane/air mixtures is investigated in a flow reactor at pressures of 1, 10, and 20 bar and temperatures in the range of 473K–973 K. The experimental data are compared to simulations with recent reaction mechanisms from the literature.

The formation of particulate matter in fuel-rich combustion systems has been the object of numerous studies in consideration of its negative effects on the human health and on the environment. In this regard, soot oxidation is particularly relevant for mitigating the amount of carbon particulates released from a combustion process (Niessner, 2014). De Falco et al. have applied Raman spectroscopy to investigate structural modification of nascent soot particles subject to oxidation. In this work, three different soot samples were chosen as representatives of the early evolution of nascent soot in flames. These are characterized by a different size and a different percentage of the elemental carbon and the pyrolytic fraction of the organic carbon. Raman spectroscopy reveals that the thermal oxidation treatment performed on the sample of just-nucleated particles, with the highest organic carbon content, results in a reduction of the amorphous carbon component. Conversely, the sample of mature soot, with the highest elemental carbon content, shows an increase in the amorphous carbon phase after oxidation, which is attributed to fragmentation or the formation of point defects by O_2 oxidation.

In conclusion, the research topic provides an overview of some key aspects and existing challenges in the experimental and modelling efforts for clean combustion technologies. Research efforts in combustion science and engineering allow indeed to develop and optimize new, carbon-neutral fuels, to assess their impact on pollutant emissions and to evaluate their applicability in existing or advanced combustion devices providing tools to enable, smooth, and speed-up the energy transition.

Author contributions

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

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

References

Dryer, F. L. (2015). Chemical kinetic and combustion characteristics of transportation fuels. *Proc. Combust. Inst.* 35 (1), 117–144. doi:10.1016/j.proci.2014.09.008

Elishav, O., Lis, B. M., Miller, E. M., Arent, D. J., Valera-Medina, A., Dana, A. G., et al. (2020). Progress and prospective of nitrogen-based alternative fuels. *Chem. Rev.* 120 (12), 5352–5436. doi:10.1021/acs.chemrev.9b00538

Gupta, A. K., Ibrahim, S., and Al Shoaibi, A. (2016). Advances in sulfur chemistry for treatment of acid gases. *Prog. Energy Combust. Sci.* 54, 65–92. doi:10.1016/j.pecs.2015.11.001

Kohse-Höinghaus, K. (2021). Combustion in the future: The importance of chemistry. *Proc. Combust. Inst.* 38 (1), 1–56. doi:10.1016/j.proci.2020.06.375

Niessner, R. (2014). The many faces of soot: Characterization of soot nanoparticles produced by engines. *Angew. Chem. Int. Ed. Engl.* 53, 12366–12379. doi:10.1002/anie.201402812