

Special issue and perspective on the chemistry and physics of carbonaceous particle formation

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Abstract

Carbonaceous particles formed during the partial oxidation of a fuel constitute a primary pollutant (i.e., soot) impacting human health and the environment. The competing soot formation and oxidation pathways associated with fossil fuels and carbon-containing renewable fuels must be understood to support the development of energy-conversion devices that limit health and environmental impacts. Such knowledge is also helpful in optimizing the properties of carbon black and other carbonaceous materials used in major industrial manufacturing processes, such as graphene, nanotubes, and (functional) carbon-coated nanoparticles. The current Special Issue comprises 16 articles that highlight progress relevant to carbonaceous particles.

Soot particles are carbonaceous particulates formed during incomplete combustion or pyrolysis of carbon-containing fuels. Soot emitted into the atmosphere has well-known detrimental effects on human health, agriculture, air quality, and global and regional climate. Soot has been linked to increased risks for cancer and pulmonary, cardiovascular, and neurological illnesses, such as Alzheimer's disease and Parkinson's disease [1, 2]. Sawyer [3] noted that, as early as 1775, Percivall Pott identified the role of high soot exposure levels as a cause of cancer in adolescent chimney sweeps in London, and current health-related work seeks to delineate the impact of particle size and toxicity on bio-reactivity. Both size and toxicity have been shown to be linked to the parent fuel and particle formation conditions. While a

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complete understanding of how exposure to particulate matter promotes cancer formation is lacking, significant progress is being made in understanding how particles $\leq \text{PM}_{2.5}$ promote lung cancer [4] by acting on cells that harbour pre-existing oncogenic mutations. The complexities associated with the bio-reactivity of different types of carbonaceous materials has been further highlighted by Smyth et al. [2] who showed that the impact of Diesel exhaust and carbon black is qualitatively different in terms of increased cardiovascular risk. Furthermore, indications are that rapeseed-methyl-ester (RME), a bio-derived Diesel replacement, can activate airway sensory nerves in a manner similar to conventional Diesel [5]. Additionally, the fuel-dependent distribution of combustion-related species deposited on soot particles will likely impact their toxicity. As an example, the amount of benzo[a]pyrene stored on soot particles is up to five times higher than in the gas-phase [6]. Benzo[a]pyrene is a Group 1 carcinogen known to cause skin tumors and is a potential cause of the carcinoma of the scrotum identified by Percivall Pott [3], and contact with soot particles could greatly enhance exposure to this carcinogen. Such adsorption of co-emitted combustion byproducts onto soot surfaces also increases the particle chemical reactivity [7, 8, 9, 10].

Soot is the second largest contributor to climate change via its large positive direct radiative forcing and through indirect effects, such as contributions to reductions in snow and ice albedo following deposition [11]. Soot plays a significant (though not well understood) role in the Earth’s hydrological cycle through high-altitude cloud formation via aviation contrails and lofted ground-based emissions and low-altitude cloud dissipation through ground-based sources [12, 13]; such indirect effects make it a leading source of uncertainty in climate models [14]. As understanding of the environmental and health effects of soot improves, government regulations are being tightened on soot emissions from combustion systems for power generation and ground and air transportation, with increasing emphasis on soot number densities [15] and even potentially particular sizes in the future.

Radiative heat transfer from soot facilitates fire propagation in building and wildland fires and is a problem of growing concern as wildfires increase in frequency and magnitude in the wake of climate change [16, 17, 18]. On the other hand, soot plays a critical role in the operation of high-temperature devices, such as furnaces and kilns, via radiative heat transfer. In fact, a major challenge in the conversion of these applications to zero-carbon fuels, such as hydrogen, is the reduced heat transfer efficiency without soot, requiring a redesign of large facilities to address decarbonization [19]. In some cases,

the loss of radiative heat transfer from soot is compensated by the increased radiative heat transfer from the additional production of water [20], and the use of carbon-capture and storage technologies is also possible [19, 21].

Carbon black and other synthesized carbon particles are extremely important for a range of commercial applications, perhaps most notably as a filler and reinforcement material for rubber and plastic products [22, 23]. Even the use of these synthesized particles, however, requires additional research and development to address concerns related to particle emissions, such as from tire wear [24] for which the rate of wear and associated particle emissions are linked to the properties of the carbon blacks used.

Fully addressing and mitigating the negative impacts of soot emissions and capitalizing on its positive uses requires an understanding of the fundamental mechanisms of soot inception, growth, and destruction, its interactions with gas-phase chemistry and molecular transport, and its additional interactions with turbulent transport. Probing its formation and physiochemical evolution enables the development of predictive computational models, but also necessitates further innovations in experimental capabilities. Advances in experimental techniques and theoretical models over the last several years have significantly increased our understanding and predictive capability, but these developments have also initiated new questions and new challenges.

Advances in temporally and spatially resolved laser diagnostics have ushered in unprecedented understanding of the interactions between gas-phase chemistry, soot, and turbulence. Non-invasive measurements of volume fractions of mature soot in laminar and turbulent flames using laser-induced incandescence (LII) or elastic light scattering (ELS) have become commonplace, though quantitative measurements tend to have substantial uncertainties largely because of uncertainties in the optical properties of soot [25, 26]. Conversely, non-invasive measurements of incipient particles have thus far proven to be elusive or, at best, inconclusive [27]. Incipient particles link the formation of gas-phase precursors to condensed-phase particles via the process of soot inception, and their measurements are thus crucial to the understanding of soot inception, which is a priority area of inquiry identified by the ISF Workshop for the Measurement and Computation of Reacting Flows with Carbon Nanoparticles (hereafter ISF). Capabilities have also been developed for non-invasive measurements of mean primary-particle and aggregate sizes of mature soot, primary-particle core-shell structures, soot and gas-phase temperatures, flow velocities, and mass fractions of some small

species [26, 28, 29, 30, 31, 32, 33, 34]. *In situ* techniques have been developed for measuring molar particle C/H ratios, which are an indication of particle maturity and can be inferred from *in situ* measurements of optical properties, such as the dispersion exponent or optical band gap [34, 35, 36]. Inferring C/H ratios from such optical measurements, however, relies on the correlations between them, and very few measurements of such correlations have been reported in the literature. Some *in situ* techniques can even be implemented simultaneously or with a single laser shot, i.e., without extended averaging; both simultaneous and single-shot measurements are desirable for turbulent flames. These capabilities have provided valuable insights into mature-soot volume fractions and the parameters that influence them.

Ex situ measurements, on the other hand, have provided much of our current understanding of soot elemental and fine-structure evolution and chemical mechanisms involved in soot inception, growth, and oxidation [37]. Measurements of C/H ratios have been made primarily using elemental and FTIR spectroscopic analysis of extracted particles [35, 38, 39]. The C/H ratio is a measure of soot maturity and increases from a value close to two at inception to values of close to 10 at full maturity [27, 36]. As particles grow and mature at high temperatures, they lose hydrogen, and many of their chemical and physical properties change: their density increases and specific heat decreases [36]; their chemical reactivity decreases [40, 41, 42, 43, 44]; their hygroscopicity decreases, reducing their ability to adsorb water and act as cloud-condensation nuclei [44, 45]; and their absorption efficiency increases and becomes much broader with much stronger absorption in the visible and near IR spectral regions, such that the dispersion exponent and optical band gap decrease [27, 35, 36]. Incipient particles have disordered fine structure and appear to be waxy or liquid-like [34, 27, 46]. As these particles mature, they acquire a core-shell structure in which the core is disordered, and the outer shell is composed of turbostratic graphite crystallites aligned preferentially parallel to the primary-particle surface. These crystallites grow in size as the particles mature. These property changes can have substantial effects on not only climate and air quality but also on after-treatment (i.e., filtration) approaches.

Scanning mobility particle sizing (SMPS) is a common technique for measuring an effective particle-size distribution associated with the electric-mobility diameter [47]. Details about the evolution of aggregate morphology and primary-particle size in flames have been derived from an extensive history of particle imaging, including scanning electron microscopy (SEM),

transmission electron microscopy (TEM), atomic force microscopy (AFM), and helium ion microscopy (HeIM) [47], whereas information about particle fine structure, from amorphous incipient particles to the polycrystalline turbostratic graphitic structure of mature-soot particles, has largely been provided by high-resolution transmission electron microscopy (HRTEM), selected area electron diffraction (SAED), and X-ray diffraction (XRD) [48, 49, 50, 51].

Experimental evidence for chemical mechanisms has been derived predominantly by mass spectrometric analysis of particles and gas-phase species extracted from flames and pyrolysis systems. Molecular beam mass spectrometry (MBMS) and gas chromatography (GC) coupled with mass spectrometry (MS) have provided the foundation for the understanding of gas-phase chemistry leading to precursor formation [52, 53, 54]. Clues about particle inception and growth and the precursors involved have primarily come from mass spectrometry of vaporized particles extracted from flames and pyrolysis systems; these studies have suggested the active involvement of molecular species with radical character, five-membered rings, odd numbers of carbon atoms, and aliphatic sidechains and bridges between aromatic adducts [54, 55, 56, 57, 58, 59, 60]. Recent molecular images from high-resolution atomic force microscopy have supported these results [61, 62].

In general, these developments have provided invaluable information about soot inception, growth, chemical evolution, and oxidation, but more work needs to be done to develop an understanding of the chemical mechanisms involved in these processes. There is a particularly strong need for experimental capabilities that can elucidate the chemical mechanisms leading to soot inception and growth. As a measure of soot maturity, the C/H ratio is particularly useful for validating chemical models of soot formation and evolution, and the ISF community has targeted *in situ* measurements of C/H ratios using non-invasive approaches as a priority. Accordingly, there continues to be a need for the development of *in situ* measurement capabilities that yield additional information about particle characteristics.

In the current Special Issue, the paper by Kelesidis et al. [63] relates mature-soot angular ELS distributions to aggregate mobility diameters, facilitating connections between *in situ* laser diagnostics and *ex situ* electric-mobility-diameter measurements. The paper by Bauer et al. [64] demonstrates an experimental approach to making two-dimensional measurements of the optical band gap and dispersion exponent using hyperspectral absorption tomography. Because these optical parameters are associated with par-

ticle maturity, this elegant approach enables assessment of the soot maturity throughout a sample, such as a flame. In fact, these measurements could be used to infer C/H ratios of particles simultaneously in two dimensions. Such measurements would be exceptionally useful in the context of determining a range of particle characteristics tied to soot maturity. Particle density and specific heat could be directly estimated from the C/H ratio [36], but other properties, such as chemical reactivity and hygroscopicity, will require more detailed investigations to explore any quantitative correlations.

With respect to chemistry, both Zhou et al. [65] and Zheng et al. [66] used LII calibrated with extinction to measure soot volume fractions and spectroscopic techniques to measure temperature in counterflow diffusion flames. Both papers focus on the effects of increasing oxygen near the flame front by increasing oxygen either in the oxidizer stream [66] or in the fuel stream by premixing [65]. Both studies show that increasing oxygen increases temperature, which increases soot volume fractions. Zheng et al. [66] demonstrate that increasing oxygen increases both soot maturity and particle sizes, and Zhou et al. [65] show that increasing the oxygen concentration does not change the influence of the rate of strain on the rate of soot formation. Zheng et al. [66] used their results to test the influence of dimensionality in counterflow flames (one-dimensional versus two-dimensional), concluding that thermophoretic and radial diffusion effects need to be taken into account in one-dimensional modeling of the flames studied. These studies also highlight the need to further delineate the influence of the chemical (oxidative) and thermal (temperature) environments experienced by soot particles.

Multiple papers in this Special Issue address the need for investigations targeting the chemistry leading to soot inception. The paper by Rundel et al. [67] presents aerosol mass spectra of particles produced during pyrolysis of propyne and propene; the results indicate that incipient-particle precursors include species with significant aliphatic content, such as aliphatic-linked aromatics and aliphatic side chains. The results demonstrate that particles lose hydrogen, becoming less saturated, with increasing temperature, but never reach the C/H ratios characteristic of pericondensed polycyclic aromatic hydrocarbons (PAHs). Particle precursors also include resonance-stabilized radicals (RSRs), a significant fraction of which are associated with aromatic species with odd numbers of carbon atoms and five-membered rings. These results demonstrate that the enhanced formation of RSRs leads to facile particle formation through hydrocarbon clustering, possibly via a mechanism known as the clustering of hydrocarbons by radical chain reactions

(CHRCR) [58]. Propyne is a direct precursor to the RSR propargyl, and propene is a direct precursor to the RSR allyl. Propyne generates particles at lower temperatures than does propene, and both fuels form particles at lower temperatures than observed for ethylene [68, 67]. If ethylene is seeded with a small amount of an RSR precursor, such as indene, which forms the RSR indenyl, its temperature for particle formation onset is lowered to a value between those of propyne and propene. These results shed light on previous studies that demonstrated that propene formed sub-10-nm size particles much more readily than did ethylene in laminar [69] and turbulent [70] flames. This work strongly suggests the need to augment the common use of ethylene in fundamental sooting flame studies by the inclusion of unsaturated C_3 and other fuels. Di Liddo et al. [71] used a dataset from Xu et al. [72] combined with stochastic molecular dynamics (MD) and computational fluid dynamics (CFD) simulations as training data for machine learning for inception rates. Their results are consistent with those of Rundel et al. [67] and show that precursors with five-membered rings, radical character, and aliphatic side chains best reproduce the experimental results, providing further evidence that such species are likely important in soot inception.

Liu et al. [73] investigated the effects of the CO_2/CH_4 ratio on selected gas-phase species production and soot formation in an inverse diffusion flame operated under conditions relevant for auto-thermal reforming (ATR) of methane. They found that soot formation decreases with increasing CO_2/CH_4 ratio, but this effect saturates at high pressures. A non-sooting flame is achievable at high pressures for high CO_2/CH_4 ratios and relatively low syngas yield. Their measurements demonstrate that the soot volume fraction reaches a plateau as a function of height above the burner (HAB) while the PAH concentration continues to increase, a result that cannot be reproduced by their soot-inception model, which is based on physical nucleation by PAHs. They conclude that soot inception is likely initiated by radical species and suggest that inverse diffusion flames are a good choice for studying soot-inception mechanisms.

Hagen et al. [74] investigated soot formation in a counterflow diffusion flame using a range of *in situ* and *ex situ* measurement techniques, including LII for soot volume fraction, primary-particle size, and ratios of absorption probabilities at different wavelengths; GC for gas composition; SMPS for aggregate and non-aggregated primary-particle size; and HRTEM for particle fine structure. Their results show soot formation on the fuel side of the stagnation plane with bimodal distributions in particle size with max-

ima at 5 nm and 20 nm. Soot volume fractions appear to peak very close to the stagnation plane. Increases in soot volume fraction are accompanied by increases in volume fractions of small aromatics (benzene, naphthalene, and acenaphthylene) assumed to be soot precursors. Soot volume fraction is also correlated with long-range order of the fine structure and absorption at longer wavelengths, both of which are indicative of increasing soot maturity. Their chemical kinetic model simulations provide reasonable agreement with the experimental results. Langer et al. [75] developed a new gas-phase chemical kinetic model, starting from C_3H_4 isomers (e.g., propyne) and accounting for molecular weight growth up to acenaphthylene; they validated this model extensively by comparisons with published experimental results. They concluded that the most abundant isomers of $C_{12}H_8$ are 1-ethynylnaphthalene, 2-ethynylnaphthalene, and acenaphthylene, the latter of which was also observed by Hagen et al. [74] in the gas phase. Rundel et al. [67] also concluded that the isomers observed in the aerosol mass spectra during pyrolysis of propyne and propene are consistent with acenaphthylene and 1-ethynylnaphthalene.² The ability to reproduce the PAH distribution through detailed chemical kinetic models opens an opportunity to understand the fuel dependency of the chemical pathways leading to the formation of particularly harmful compounds (e.g., Class 1 carcinogens). Such models are also a prerequisite for investigating soot inception and for deriving simplified models that target specific conditions.

The development of these *in situ* and *ex situ* measurement techniques, combined with our understanding and modeling of soot chemistry, is also useful for developing a better understanding of other carbon-based particles produced under high-temperature conditions. López-Cámara et al. [76] used LII, TEM, and Raman spectroscopy to investigate the formation of soot-like particles and particles composed of several layers of graphene generated by plasma synthesis. A chemical kinetic model, originally developed for studying soot formation, was used to simulate particle formation and graphene growth. It was concluded that the ratio of amorphous to graphene particles formed depends predominantly on the concentration of acetylene in the post-plasma region, which in turn is determined by the oxygen content of the reactant

²Rundel et al. [67] mistakenly wrote “1-ethylnaphthalene” instead of “1-ethynylnaphthalene” in the description of $C_{12}H_8$ isomers, and Langer et al. [75] mistakenly wrote “acenaphthene” instead of “acenaphthylene” or “acenaphthalene” in the abstract.

and the reactant concentration. More generally, such synthesis methods can lead to the efficient production of materials that require careful control of process parameters [77].

In turbulent reacting flows, there is a key need for simultaneous high-resolution (spatially and temporally) measurements of flow velocity, gas-phase composition, temperature, and mixture fraction with soot volume fraction and soot particle characteristics. In the current Special Issue, the paper by Stöhr et al. [78] demonstrates the state-of-the-art in simultaneous planar measurements of the turbulent flow field using Particle Image Velocimetry (PIV), from which qualitative soot volume fractions were also derived using the Rayleigh scattering signal, and OH using Planar Laser-Induced Fluorescence (PLIF). From these measurements, the soot fluxes and source terms were determined experimentally for the first time. Applied to a turbulent swirl flame, the measurements revealed the formation of soot within the recirculation zone where it is then transported toward the flame base and oxidized. These results indicate the ability of modern laser diagnostics techniques to not only provide data for model validation but also provide mechanistic understanding in their own right. As discussed above, new *in situ* laser diagnostics capability is required to measure not only soot volume fraction but also soot composition including the C/H ratio, simultaneously with gas-phase quantities, to understand how soot maturity evolves in turbulent flames and how this process may differ from laminar flames; such development remains a priority for the ISF community.

Computationally, advancements in gas-phase and soot modeling, combined with large-scale computing, have allowed the insight gained from experimental measurements to be augmented by Direct Numerical Simulation (DNS) [79, 80]. Taken together, these insights have enabled the development of sophisticated models for unresolved soot, turbulence, and gas-phase interactions for coarse-grained simulations including both Reynolds-Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES) [81, 82]. Owing to the complexity of the problem, a diversity of coarse-grained modeling approaches have been pursued that allocate model fidelity (and thus computational resources) differently. While real advancements and predictive capability have been made, these various modeling approaches all suffer from some weaknesses including, for example, the presumption of particular flame structures (e.g., mixture fraction-based models for asymptotically non-premixed combustion), decoupling of the fast heat release and slow soot and radiation time scales in manifold-based combustion models, and differential diffusion

between soot and gas-phase species and unresolved turbulent mixing processes in transported and presumed (subfilter) probability density function (PDF) approaches. Research activity on improving these models for unresolved soot, chemistry, and turbulence phenomena remains intense, ongoing, and a priority of the ISF community.

In this Special Issue, Maldonado Colmán et al. [83] developed a new presumed soot subfilter PDF model for LES to include the unresolved transport of soot with respect to the flame. The soot subfilter PDF model is an important modeling quantity since it provides closure for the filtered source term in LES (or analogously the averaged source term in RANS). Compared to previous work where soot oxidation was presumed to be either strictly kinetically controlled or strictly mixing controlled to derive a soot subfilter PDF model, their new soot subfilter PDF model accounts for finite-rate oxidation relative to the transport of soot with respect to the flame. In a turbulent non-premixed piloted jet flame, their model was shown to reproduce both the soot inception regions and the final soot oxidation regions more accurately than prior models. Perhaps more important, consistent with the experimental measurements and previous computational studies of Tian et al. [84] using a transported PDF method, the new soot subfilter PDF model was shown to predict minor soot leakage from fuel-rich regions into fuel-lean regions.

Additionally, the need to model the influence of, and interactions with, additional multi-physics phenomena including radiation and liquid fuel sprays presents a key challenge. Contributions addressing such phenomena form part of the current Special Issue. For radiation, many computational modeling approaches leverage a simple grey, optically thin approach because they are validated against relatively small laboratory-scale flames that are (nearly) optically thin. However, many practical systems at higher pressure and higher soot loading are not optically thin³. Liu et al. [85] reviewed (1) non-grey soot models and their importance in even laminar flames and (2) turbulence-radiation interaction models and their influence on not only flame temperature but also soot volume fraction, where predictions with and without consideration of turbulence-radiation interactions can differ by a factor of a few to several. For liquid fuel sprays, the dynamics of fuel vaporization

³In fact, the broader issue of modeling not just soot but the production of carbonaceous materials when the volume fraction is not small but very large has been identified as a priority area of the ISF community.

play a critical role in forming fuel-rich regions where PAH can form and ultimately lead to soot. Gallen et al. [86] combined Lagrangian spray and soot models to provide new insights into the influence of liquid fuel sprays on soot evolution using LES. One marked feature of liquid fuel spray combustion is the presence of multi-modal combustion, even in a nominally non-premixed system [87], further emphasising challenges associated with oversimplified presumed flame structure models. Gallen et al. [86] show that soot inception occurs preferentially in regions of premixed combustion while soot oxidation occurs preferentially in regions of non-premixed combustion. These results highlight the important, though sometimes unexpected, interactions that can lead to increased physiochemical complexity in multiphysics turbulent reacting flows.

The progress outlined above has enabled predictive modeling capabilities to be deployed for real fuels and real combustion systems. While more fundamental soot research tends to feature ethylene flames because of the nominally better knowledge of soot precursor chemistry, soot models are being used for the simulation of combustion processes with practical fossil-derived and sustainable alternative hydrocarbon fuels. In this Special Issue, Gallen et al. [86] simulated a jet fuel by leveraging Analytically Reduced Chemistry (ARC) leading to 29 transported species, including PAHs, to make the computations affordable. From a systems standpoint, with advancements in CFD technology for complex geometries, soot models are now being used to make predictions in real geometries at real operating conditions, with aviation combustors continuing to be a major driver whose importance will not diminish in any foreseeable future. In the paper of Grader et al. [88], a model aviation engine combustor was simulated at multiple operating points. Modal analysis was used to understand the intricate coupling between soot evolution, fuel-air mixing, and a complex turbulent flow field including recirculation and secondary air injection.

Interest is also intensely ramping up to understand the behavior of soot in blends of hydrocarbon and zero-carbon fuels. Tian and Lindstedt [89] analysed the influence of ammonia addition on soot formation in ethylene flames. They showed that the experimentally observed suppression of small soot particles with the addition of ammonia could be predicted quantitatively using detailed PAH chemistry when coupled with a mass and number density preserving sectional model. The analysis highlighted the influence of changes in the H radical concentration leading to the reduced soot surface growth with ammonia addition. The experimentally observed diminished impact

of ammonia addition in turbulent flames compared to laminar flames was also predicted, emphasising the importance of the flow field in determining soot concentrations. The latter computations were performed using a fully coupled transported PDF method featuring an 84-dimensional joint-scalar space. Taken together, modeling capabilities for soot have reached a point where reliable predictions are starting to be feasible in real systems with real fuels, but the uncertainties are still considerable. For example, particulate formation has been shown to be sensitive to fuel composition [90, 91, 92], but it is not yet known whether such sensitivities can be generally predicted with current modeling capabilities.

Despite significant advances in predicting the soot evolution in turbulent reacting flows, numerous challenges still remain, two of which are highlighted here. First, little is known about the evolution of the soot particle size distribution in turbulent flames. At this point in time, only probe measurements are possible in turbulent flames, and these are very few [93, 94, 95, 70] with limited associated modeling studies [96]. Sectional models have been coupled to both RANS and LES, but remain computationally expensive with typically 60–70 sections required to discretize soot particle size distributions. Despite this cost, some limited investigations into how soot, turbulence, chemistry interactions depend on soot particle size have been undertaken including in this Special Issue [86, 88, 89]. New, more efficient statistical models for the soot size distribution that could be used with DNS would provide tremendous insights and could also be used to lower the cost of RANS and LES. Second, while detailed radiation models have been coupled to soot models in RANS and LES (as reviewed by Liu et al. [85]), many uncertainties for soot, turbulence, radiation interactions remain. DNS could be a useful tool, but is computationally challenged by the large system sizes required for a non-optically thin system combined with the relatively long time scales associated with soot formation and complex hydrocarbon chemistry. Therefore, new experimental configurations and diagnostics specifically designed to probe soot, turbulence, radiation interactions could be helpful [97]. Taken together, predicting the soot size distribution and soot, turbulence, radiation interactions would be most helpful in predicting “smoking” combustion, which is still not completely understood and remains an elusive modeling challenge.

The work outlined above highlights the progress made towards understanding the processes leading from a parent fuel to soot inception via gas-phase precursors and the subsequent evolution of particle size distributions. Such understanding is essential for supporting the development of efficient

energy conversion devices and providing a framework for improved industrial processes relating to products as diverse as carbon black and cement, understanding the formation of soot in, and radiative heat transfer effects from, (natural) fires and, perhaps, in the future leading towards a choice of carbon-containing fuels that minimize the prevalence of key carcinogens, such as benzo[a]pyrene. This work also highlights applications of this progress in understanding towards the production of other carbon-based nanoparticles.

This Special Issue cannot include all work related to carbonaceous particles. Rather it presents a snapshot of the current state-of-the-art in terms of our understanding of the relevant physics and chemistry, complementary diagnostic methods, modeling approaches, and their application. The articles are accordingly diverse and include five articles on fundamental soot physiochemical phenomena and chemistry, four articles on soot evolution in laminar flames, four articles on soot evolution in turbulent flames, two articles on soot evolution in aviation combustors, and one article on particle synthesis. The contributions include not only new understanding of soot phenomena but also advancements in experimental measurement capabilities and predictive modeling capabilities.

Acknowledgements We are grateful to the authors for their diligent efforts in preparing the manuscripts for this Special Issue and to the reviewers who provided detailed feedback that improved each of the articles. RPL was supported by the European Union under the HORIZON 2020 framework through the SOPRANO project under Award No. 690724. HAM and MEM were supported by the U. S. National Science Foundation, Division of Chemical, Bioengineering, Environmental, and Transport Systems; HAM, under Grant No. 2328647, and MEM, under Grant No. 2028318. MEM was also supported by the National Aeronautics and Space Administration under Grant No. NNX16AP90A.

References

- [1] H. J. Heusinkveld, T. Wahle, A. Campbell, R. H. Westerink, L. Tran, H. Johnston, V. Stone, F. R. Cassee, R. P. Schins, Neurodegenerative and neurological disorders by small inhaled particles, *NeuroToxicology* 56 (2016) 94 – 106.
- [2] E. Smyth, A. Solomon, M. A. Birrell, M. J. Smallwood, P. G. Winyard, T. D. Tetley, M. Emerson, Influence of inflammation and nitric oxide

- upon platelet aggregation following deposition of diesel exhaust particles in the airways, *British Journal of Pharmacology* 174 (13) (2017) 2130–2139.
- [3] R. F. Sawyer, The formation and destruction of pollutants in combustion processes: Clearing the air on the role of combustion research, Invited Plenary Lecture, *Proc. Combust. Inst.* 18 (1981) 1–22.
 - [4] W. Hill, E. Lim, C. Weeden, et al., Lung adenocarcinoma promotion by air pollutants, *Nature* 616 (2023) 159–167.
 - [5] J. A. Bolaji, J. J. Adcock, T. Sandström, I. Mudway, A. Bloomberg, J. Bosson, T. D. Tetley, M. A. Birrell, M. G. Belvisi, Biodiesel: is it any safer to use?, *European Respiratory Journal* 52 (suppl 62) (2018).
 - [6] H. Shariatmadar, F. Hampp, R. P. Lindstedt, Quantification of PAH concentrations in premixed turbulent flames crossing the soot inception limit, *Proc. Combust. Inst.* 38 (1) (2021) 1163–1172.
 - [7] M. Antiñolo, M. D. Willis, S. Zhou, J. P. Abbatt, Connecting the oxidation of soot to its redox cycling abilities, *Nature Commun.* 6 (2015) 6812.
 - [8] E. C. Browne, J. P. Franklin, M. R. Canagaratna, P. Massoli, T. W. Kirchstetter, D. R. Worsnop, K. R. Wilson, J. H. Kroll, Changes to the chemical composition of soot from heterogeneous oxidation reactions, *J. Phys. Chem. A* 119 (2015) 1154–1163.
 - [9] W. Esteve, H. Budzinski, E. Villenand, Relative rate constants for the heterogeneous reactions of OH, NO₂ and NO radicals with polycyclic aromatic hydrocarbons adsorbed on carbonaceous particles. part 1: Pahs adsorbed on 1–2 µm calibrated graphite particles, *Atmos. Environ.* 38 (2004) 6063–6072.
 - [10] W. Esteve, H. Budzinski, E. Villenand, Relative rate constants for the heterogeneous reactions of NO₂ and OH radicals with polycyclic aromatic hydrocarbons adsorbed on carbonaceous particles. part 2: Pahs adsorbed on diesel particulate exhaust srm 1650a, *Atmos. Environ.* 40 (2006) 201–211.

- [11] T. C. Bond, S. J. Doherty, D. W. Fahey, P. M. Forster, T. Berntsen, B. J. DeAngelo, M. G. Flanner, S. Ghan, B. Kärcher, D. Koch, S. Kinne, Y. Kondo, P. K. Quinn, M. C. Sarofim, M. G. Schultz, M. Schulz, C. Venkataraman, H. Zhang, S. Zhang, N. Bellouin, S. K. Guttikunda, P. K. Hopke, M. Z. Jacobson, J. W. Kaiser, Z. Klimont, U. Lohmann, J. P. Schwarz, D. Shindell, T. Storelvmo, S. G. Warren, C. S. Zender, Bounding the role of black carbon in the climate system: A scientific assessment, *J. Geophys. Res. Atmos.* 118 (11) (2013) 5380–5552.
- [12] U. Lohmann, F. Friebel, Z. A. Kanji, F. Mahrt, A. A. Mensah, D. Neubauer, Future warming exacerbated by aged-soot effect on cloud formation, *Nature Geosci.* 13 (2020) 674–680.
- [13] U. Burkhardt, L. Bock, A. Bier, Mitigating the contrail cirrus climate impact by reducing aircraft soot number emissions, *NPJ Clim. Atmos. Sci.* 1 (2018) 37.
- [14] J. E. Penner, Soot, sulfate, dust and the climate – three ways through the fog, *Nature* 570 (2019) 158–159.
- [15] Commission Regulation (EU) No 459/2012 of 29 May 2012 amending Regulation (EC) No 715/2007 of the European Parliament and of the Council and Commission Regulation (EC) No 692/2008 as regards emissions from light passenger and commercial vehicles (Euro 6) (2012).
URL <http://data.europa.eu/eli/reg/2012/459/oj>
- [16] J. G. Pausas, J. E. Keeley, Wildfires and global change, *Front. Ecol. Environ.* 19 (2021) 387–395.
- [17] M. Flannigan, B. Stocks, B. Wotton, Climate change and forest fires, *Sci. Total Environ.* 262 (2000) 221–229.
- [18] S. Mansoor, I. Farooq, M. M. Kachroo, A. E. D. Mahmoud, M. Fawzy, S. M. Popescu, M. Alyemeni, C. Sonne, J. Rinklebe, P. Ahmad, Elevation in wildfire frequencies with respect to the climate change, *J. Environ. Manage.* 301 (2022) 113769.
- [19] M. Pisciotta, H. Pilorgé, J. Feldmann, R. Jacobson, J. Davids, S. Swett, Z. Sasso, J. Wilcox, Current state of industrial heating and opportunities for decarbonization, *Prog. Energy Combust. Sci.* 91 (2022) 100982.

- [20] H. Yang, X. Lin, H. Pan, S. Geng, Z. Chen, Y. Liu, Energy saving analysis and thermal performance evaluation of a hydrogen-enriched natural gas-fired condensing boiler, *Int. J. Hydrogen Energy* 48 (2023) 19279–19296.
- [21] F. Schiro, A. Stoppato, A. Benato, Modelling and analyzing the impact of hydrogen enriched natural gas on domestic gas boilers in a decarbonization perspective, *Carbon Resources Conversion* 3 (2020) 122–129.
- [22] J.-B. Donnet, R. C. Bansal, M.-J. Wang, *Carbon Black: Science and Technology*. 2nd ed., Marcel Dekker, Inc.: New York, NY, 1993.
- [23] C.-S. Wu, T.-W. Chang, H. Teng, Y.-L. Lee, High performance carbon black counter electrodes for dye-sensitized solar cells, *Energy* 115 (2016) 513–518.
- [24] S. Wagner, T. Hüffer, P. Klöckner, M. Wehrhahn, T. Hofmann, T. Reemtsma, Tire wear particles in the aquatic environment - a review on generation, analysis, occurrence, fate and effects, *Water Research* 139 (2018) 83–100.
- [25] Z. Zhang, L. Zhou, X. He, Can laser-induced incandescence calibrated by laser extinction method be used for quantitative determination of soot volume fraction in laminar flames?, *Appl. Energy Combust. Sci.* 13 (2023) 100103.
- [26] H. A. Michelsen, C. Schulz, G. J. Smallwood, S. Will, Laser-induced incandescence: Particulate diagnostics for combustion, atmospheric, and industrial applications, *Prog. Energy Combust. Sci.* 15 (2015) 2–48.
- [27] H. A. Michelsen, Probing soot formation, chemical and physical evolution, and oxidation: A review of in situ diagnostic techniques and needs, *Proc. Combust. Inst.* 36 (2017) 717–735.
- [28] R. S. Barlow, Laser diagnostics and their interplay with computations to understand turbulent combustion, *Proc. Combust. Inst.* 31 (2007) 49–75.
- [29] R. K. Hanson, Applications of quantitative laser sensors to kinetics, propulsion and practical energy systems, *Proc. Combust. Inst.* 33 (2011) 1–40.

- [30] V. Sick, High speed imaging in fundamental and applied combustion research, *Proc. Combust. Inst.* 34 (2013) 3509–3530.
- [31] A. Dreizler, B. Böhm, Advanced laser diagnostics for an improved understanding of premixed flame-wall interactions, *Proc. Combust. Inst.* 35 (2015) 37–64.
- [32] C. Abram, B. Fond, F. Beyrau, Temperature measurement techniques for gas and liquid flows using thermographic phosphor tracer particles, *Prog. Energy Combust. Sci.* 64 (2018) 93–156.
- [33] M. Aldén, Spatially and temporally resolved laser/optical diagnostics of combustion processes: From fundamentals to practical applications, *Proc. Combust. Inst.* 39 (2023) 1185–1228.
- [34] H. A. Michelsen, M. F. Campbell, K. O. Johansson, I. C. Tran, P. E. Schrader, R. P. Bambha, E. Cenker, J. A. Hammons, C. Zhu, E. Schaible, A. van Buuren, Soot-particle core-shell and fractal structures from small-angle X-ray scattering measurements in a flame, *Carbon* 196 (2022) 440–456.
- [35] A. D’Alessio, F. Beretta, C. Venitozzi, Optical investigations on soot forming methane-oxygen flames, *Combust. Sci. Technol* 5 (1972) 263–272.
- [36] H. A. Michelsen, Effects of maturity and temperature on soot density and specific heat, *Proc. Combust. Inst.* 38 (2021) 1197–1205.
- [37] A. D’Anna, Combustion-formed nanoparticles, *Proc. Combust. Inst.* 32 (2009) 593–613.
- [38] A. Ciajolo, R. Barbella, A. Tregrossi, L. Bonfanti, Spectroscopic and compositional signatures of pah-loaded mixtures in the soot inception region of a premixed ethylene flame, *Proc. Combust. Inst.* 27 (1998) 1481–1487.
- [39] C. Russo, A. Tregrossi, A. Ciajolo, Dehydrogenation and growth of soot in premixed flames, *Proc. Combust. Inst.* 35 (2015) 1803–1809.
- [40] P. Liu, H. Ahmad, X. Jiang, H. Chen, Y. Lin, B. Mei, Y. Li, Evolution of structure and oxidation reactivity from early-stage soot to mature soot

- sampled from a laminar coflow diffusion flame of ethylene, *Combust. Flame* 228 (2021) 202–209.
- [41] K. Alexandrino, J. Salinas, Ángela Millera, R. Bilbao, M. U. Alzueta, Sooting propensity of dimethyl carbonate, soot reactivity and characterization, *Fuel* 183 (2016) 64–72.
 - [42] C. Russo, A. Ciajolo, S. C. aand V. La Matta, A. L. Rocca, B. Apicella, Reactivity of soot emitted from different hydrocarbon fuels: Effect of nanostructure on oxidation kinetics, *Fuel Process. Technol.* 236 (2022) 107401.
 - [43] J. Camacho, Y. Tao, H. Wang, Kinetics of nascent soot oxidation by molecular oxygen in a flow reactor, *Proc. Combust. Inst.* 35 (2015) 1887–1894.
 - [44] J. Wu, A. Faccinnetto, S. Grimonprez, S. Batut, J. Yon, P. Desgroux, D. Petitprez, Influence of the dry aerosol particle size distribution and morphology on the cloud condensation nuclei activation. an experimental and theoretical investigation, *Atmos. Chem. Phys.* 20 (2020) 4209–4225.
 - [45] S. Grimonprez, A. Faccinnetto, S. Batut, J. Wu, P. Desgroux, D. Petitprez, Cloud condensation nuclei from the activation with ozone of soot particles sampled from a kerosene diffusion flame, *Aerosol Sci. Technol.* 52 (2018) 814–827.
 - [46] H. A. Michelsen, M. B. Colket, P.-E. Bengtsson, A. D’Anna, P. Desgroux, B. S. Haynes, J. H. Miller, G. J. Nathan, H. Pitsch, H. Wang, A review of terminology used to describe soot formation and evolution under combustion and pyrolytic conditions, *ACS Nano* 14 (2020) 12470–12490.
 - [47] T. A. Sipkens, A. Boies, J. C. Corbin, R. K. Chakrabarty, J. Olfert, S. N. Rogak, Overview of methods to characterize the mass, size, and morphology of soot, *J. Aerosol Sci.* 173 (2023) 01211.
 - [48] R. L. Vander Wal, A TEM methodology for the study of soot particle structure, *Combust. Sci. Technol.* 126 (1997) 333–351.

- [49] R. L. Vander Wal, Soot precursor carbonization: Visualization using LIF and LII and comparison using bright and dark field TEM, *Combust. Flame* 12 (1998) 607–616.
- [50] H. Chen, R. Dobbins, Crystallogenesi s of particles formed in hydrocarbon combustion, *Combust. Sci. Technol.* 151 (2000) 109–128.
- [51] M. Lapuerta, J. Rodríguez-Fernández, J. Sánchez-Valdepeñas, Soot reactivity analysis and implications on diesel filter regeneration, *Prog. Energy Combust. Sci.* 78 (2020) 100833.
- [52] N. Hansen, T. A. Cool, P. R. Westmoreland, K. Kohse-Höinghaus, Recent contributions of flame-sampling molecular-beam mass spectrometry to a fundamental understanding of combustion chemistry, *Prog. Energy Combust. Sci.* 35 (2009) 168–191.
- [53] F. Egolfopoulos, N. Hansen, Y. Ju, K. Kohse-Höinghaus, C. Law, F. Qi, Advances and challenges in laminar flame experiments and implications for combustion chemistry, *Prog. Energy Combust. Sci.* 43 (2014) 36–67.
- [54] Y. Wang, S. H. Chung, Soot formation in laminar counterflow flames, *Prog. Energy Combust. Sci.* 74 (2019) 152–238.
- [55] R. A. Dobbins, R. A. Fletcher, H.-C. Chang, The evolution of soot precursor particles in a diffusion flame, *Combust. Flame* 115 (1998) 285–298.
- [56] L. G. Blevins, R. A. Fletcher, J. Bruce A. Benner, E. B. Steel, G. W. Mulholland, The existence of young soot in the exhaust of inverse diffusion flames, *Proc. Combust. Inst.* 29 (2002) 2325–2333.
- [57] B. Öktem, M. P. Tolocka, B. Zhao, H. Wang, M. V. Johnston, Chemical species associated with the early stage of soot growth in a laminar premixed ethylene–oxygen–argon flame, *Combust. Flame* 142 (2005) 364–373.
- [58] K. O. Johansson, M. P. Head-Gordon, P. E. Schrader, K. R. Wilson, H. A. Michelsen, Resonance-stabilized hydrocarbon radical chain reactions may explain soot inception and growth, *Science* 361 (2018) 997–1000.

- [59] B. D. Adamson, S. A. Skeen, M. Ahmed, N. Hansen, Detection of aliphatically bridged multi-core polycyclic aromatic hydrocarbons in sooting flames with atmospheric-sampling high- resolution tandem mass spectrometry, *J. Phys. Chem. A* 122 (2018) 9338–9349.
- [60] J. A. Rundel, C. Martí, J. Zádor, P. E. Schrader, K. O. Johansson, R. P. Bambha, G. T. Buckingham, J. P. Porterfield, O. Kostko, H. A. Michelsen, The identity and chemistry of c7h7 radicals observed during soot formation, *J. Phys. Chem. A* 127 (2023) 3000–3019.
- [61] M. Commodo, K. Kaiser, G. D. Falco, P. Minutolo, F. Schulz, A. D’Anna, L. Gross, On the early stages of soot formation: Molecular structure elucidation by high-resolution atomic force microscopy, *Combust. Flame* 205 (2019) 154–164.
- [62] F. Schulz, M. Commodo, K. Kaiser, G. D. Falco, P. Minutolo, G. Meyer, A. D’Anna, L. Gross, Insights into incipient soot formation by atomic force microscopy, *Proc. Combust. Inst.* 37 (2019) 885–892.
- [63] G. A. Kelesidis, P. Crepaldi, M. Allemann, A. Duric, S. E. Pratsinis, The mobility diameter of soot determines its angular light scattering distribution, *Combust. Flame* (2022) in press-
doi:<https://doi.org/10.1016/j.combustflame.2023.112476>.
- [64] F. J. Bauer, P. A. Braeuer, M. W. Wilke, S. Will, 2D in situ determination of soot optical band gaps in flames using hyperspectral absorption tomography, *Combust. Flame* (2022) in press-
doi:<https://doi.org/10.1016/j.combustflame.2023.112730>.
- [65] M. Zhou, L. Xu, S. H. Chung, Y. Wang, Effects of oxygen partial premixing on soot formation in ethylene counterflow flames with oscillating strain rates, *Combust. Flame* (2022) in press-
doi:<https://doi.org/10.1016/j.combustflame.2022.112442>.
- [66] D. Zheng, A. Nobili, A. Cuoci, M. Pelucchi, X. Hui, T. Faravelli, Soot formation from n-heptane counterflow diffusion flames: Two-dimensional and oxygen effects, *Combust. Flame* (2022) in press-
doi:<https://doi.org/10.1016/j.combustflame.2022.112441>.

- [67] J. A. Rundel, K. O. Johansson, P. E. Schrader, R. P. Bambha, K. R. Wilson, J. Zador, G. B. Ellison, H. A. Michelsen, Production of aliphatic-linked polycyclic hydrocarbons during radical-driven particle formation from propyne and propene pyrolysis, *Combust. Flame* (2022) in press-doi:<https://doi.org/10.1016/j.combustflame.2022.112457>.
- [68] J. A. Rundel, C. M. Thomas, P. E. Schrader, K. R. Wilson, K. O. Johansson, R. P. Bambha, H. A. Michelsen, Promotion of particle formation by resonance-stabilized radicals during hydrocarbon pyrolysis, *Combust. Flame* 243 (2022) 11942.
- [69] H. Lin, C. Gu, J. Camacho, B. Lin, C. Shao, R. Li, H. Gu, B. Guan, H. Wang, Z. Huang, Mobility size distributions of soot in premixed propene flames, *Combust. Flame* 172 (2016) 365–373.
- [70] H. Shariatmadar, R. P. Lindstedt, Soot particle size distributions in turbulent opposed jet flames with premixed propene–air reactants, *Proc. Combust. Inst.* 39 (1) (2023) 1089–1097.
- [71] L. Di Liddo, J. C. Saldinger, M. Jadidi, P. Elvati, A. Violi, S. B. Dworkin, Exploring soot inception rate with stochastic modelling and machine learning, *Combust. Flame* (2023) in press-doi:<https://doi.org/10.1016/j.combustflame.2022.112375>.
- [72] F. Xu, P. B. Sunderland, G. M. Faeth, Soot formation in laminar premixed ethylene/air flames at atmospheric pressure, *Combust. Flame* 108 (1997) 471–493.
- [73] P. Liu, J. Guo, H. G. Im, W. L. Roberts, The effects of co_2/ch_4 ratio on soot formation for autothermal reforming of methane at elevated pressure, *Combust. Flame* (2022) in press-doi:<https://doi.org/10.1016/j.combustflame.2022.112375>.
- [74] F. P. Hagen, P. Vlavakis, H. Bockhorn, R. Suntz, D. Trimis, From molecular to sub-mm scale: The interplay of precursor concentrations, primary particle size, and carbon nanostructure during soot formation in counter-flow diffusion flames, *Combust. Flame* (2023) in press-doi:<https://doi.org/10.1016/j.combustflame.2023.112729>.
- [75] R. Langer, Q. Mao, H. Pitsch, A detailed kinetic model for aromatics formation from small hydrocarbon and gasoline

- surrogate fuel combustion, *Combust. Flame* (2022) in press-
doi:<https://doi.org/10.1016/j.combustflame.2023.112574>.
- [76] C.-F. López-Cámara, P. Fortugno, M. Asif, S. Musikhin, C. Prindler, H. Wiggers, T. Endres, N. Eaves, K. J. Daun, C. Schulz, Evolution of particle size and morphology in plasma synthesis of few-layer graphene and soot, *Combust. Flame* (2022) in press-
doi:<https://doi.org/10.1016/j.combustflame.2023.112713>.
 - [77] M. Underberg, M. M. Prenting, M. Sieber, S. Schimek, C. O. Paschereit, T. Hülser, T. Endres, C. Schulz, H. Wiggers, S. M. Schnurre, A hydrogen-based burner concept for pilot-scale spray-flame synthesis of nanoparticles: Investigation of flames and iron oxide product materials, *Applications in Energy and Combustion Science* 15 (2023) 100165.
 - [78] M. Stöhr, I. Boxx, K. P. Geigle, Flux-based measurement of local scalar source terms in turbulent reacting flows: Theory and application to soot formation in an aero-engine model combustor, *Combust. Flame* (2022) in press-
doi:<https://doi.org/10.1016/j.combustflame.2022.112456>.
 - [79] D. O. Lignell, J. H. Chen, P. J. Smith, Three-dimensional direct numerical simulation of soot formation and transport in a temporally evolving nonpremixed ethylene jet flame, *Combust. Flame* 155 (2008) 316–333.
 - [80] A. Attili, F. Bisetti, M. E. Mueller, H. Pitsch, Formation, growth, and transport of soot in a three-dimensional turbulent non-premixed jet flame, *Combust. Flame* 161 (2014) 1849–1865.
 - [81] V. Raman, R. O. Fox, Modeling of fine-particle formation in turbulent flames, *Ann. Rev. Fluid Mech.* 48 (2016) 159–190.
 - [82] S. Rigopoulos, Modelling of soot aerosol dynamics in turbulent flow, *Flow Turb. Combust.* 103 (2019) 565–604.
 - [83] H. Maldonado Colmán, A. Attili, M. E. Mueller, Large eddy simulation of turbulent nonpremixed sooting flames: Presumed subfilter pdf model for finite-rate oxidation of soot, *Combust. Flame* (2022) in press-
doi:<https://doi.org/10.1016/j.combustflame.2022.112602>.

- [84] L. Tian, M. A. Schiener, R. P. Lindstedt, Fully coupled sectional modelling of soot particle dynamics in a turbulent diffusion flame, *Proc. Combust. Inst.* 38 (1) (2021) 1365–1373.
- [85] F. Liu, J.-L. Consalvi, F. Nmira, The importance of accurately modelling soot and radiation coupling in laminar and laboratory-scale turbulent diffusion flames, *Combust. Flame* (2022) in press-doi:<https://doi.org/10.1016/j.combustflame.2022.112573>.
- [86] L. Gallen, E. Riber, B. Cuenot, Investigation of soot formation in turbulent spray flame burning real fuel, *Combust. Flame* (2022) in press-doi:<https://doi.org/10.1016/j.combustflame.2022.112621>.
- [87] A. R. Masri, Challenges for turbulent combustion, *Proc. Combust. Inst.* 38 (2021) 121–155.
- [88] M. Grader, P. Gerlinger, Influence of operating conditions on flow field dynamics and soot formation in an aero-engine model combustor, *Combust. Flame* (2022) in press-doi:<https://doi.org/10.1016/j.combustflame.2023.112712>.
- [89] L. Tian, R. P. Lindstedt, The impact of ammonia addition on soot formation in ethylene flames, *Combust. Flame* (2022) in press-doi:<https://doi.org/10.1016/j.combustflame.2023.112724>.
- [90] E. Corporan, J. T. Edwards, S. Stouffer, M. DeWitt, Z. West, C. Klingshirn, C. Bruening, Impacts of Fuel Properties on Combustor Performance, Operability and Emissions Characteristics, 2017. doi:<https://doi.org/10.2514/6.2017-0380>.
URL <https://arc.aiaa.org/doi/abs/10.2514/6.2017-0380>
- [91] L. Zheng, C. Ling, E. A. Ubogu, J. Cronly, I. Ahmed, Y. Zhang, B. Khandelwal, Effects of alternative fuel properties on particulate matter produced in a gas turbine, *Energy Fuels* 32 (2018) 9883–9897. doi:10.1021/acs.energyfuels.8b01442.
- [92] A. E. Karataş, Ömer L. Gülder, Soot formation in high pressure laminar diffusion flames, *Prog Energy Combust. Sci.* 38 (2012) 818–845. doi:10.1016/j.pecs.2012.04.003.

- [93] W. Boyette, S. Chowdhury, W. Roberts, Soot particle size distribution functions in a turbulent non-premixed ethylene-nitrogen flame, *Flow. Turb. Combust.* 98 (2017) 1173–1186.
- [94] S. Chowdhury, W. R. Boyette, W. L. Roberts, Time-averaged probability density functions of soot nanoparticles along the centerline of a piloted turbulent diffusion flame using a scanning mobility particle sizer, *J. Aerosol Sci.* 106 (2017) 56–67.
- [95] S. Shariatmadar, P. Aleiferis, R. P. Lindstedt, Particle size distributions in turbulent premixed ethylene flames crossing the soot inception limit, *Combust. Flame* 243 (2022) 1–20.
- [96] M. A. Schiener, R. P. Lindstedt, Transported probability density function based modelling of soot particle size distributions in non-premixed turbulent jet flames, *Proc. Combust. Inst.* 37 (1) (2019) 1049–1056.
- [97] G. J. Nathan, P. A. M. Kalt, Z. T. Alwahabi, B. B. Dally, P. R. Medwell, Q. N. Chan, Recent advances in the measurement of strongly radiating, turbulent reacting flows, *Prog. Energy Combust. Sci.* 38 (2012) 41–61.