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Clean Combustion— Perspectives from Chemistry and Diagnostics



Katharina Kohse-Höinghaus addresses high-temperature reactive systems in her research, where she combines expertise and methods from chemistry, physics, and engineering. Her core topics include spectroscopy and kinetics to understand combustion processes. Her recent contributions, often in collaboration across disciplines with partners worldwide, focus on alternative transportation fuels, and formation of hazardous combustion emissions such as gaseous air pollutants and soot. Combining advanced experimental techniques while relying on instrumentation from the laboratory scale to multi-user facilities such as synchrotrons, her group has participated over more than 20 years in pioneering research to detect reactive combustion intermediates.



Andreas Brockhinke uses sophisticated laser techniques to characterize important properties of systems in a broad interdisciplinary range of fields, reaching from physics and engineering to biomedical applications. His most recent work is devoted to aspects in energy conversion. Respective topics include fundamental spectroscopy of luminescent molecules for photovoltaics, quantum cascade laser spectroscopy and chemiluminescence as sensors for combustion processes and their active control, and fundamental aspects of metal combustion for energy storage applications.



Michael Letzgus enables research on reactive systems by design and adaptation of advanced instrumentation for their interrogation, characterization, and control. His work includes hardware and software solutions for combining multi-component instruments into working one-of-a-kind diagnostic tools as a prerequisite for forefront applications.

Which chemical processes will lead to harmful soot emissions from combustion? Can we inspect the combustion process in an engine in real-time? Are biofuels a sustainable alternative to fossil ones? And how reliable are computer models for the development of combustion engines and gas turbines? These and other questions were at the focus of the International Discussion Meeting on 'Chemistry and Diagnostics for Clean Combustion' that was held June 21–23, 2017 at the Center for Interdisciplinary Research (ZiF) at Bielefeld University.** The ZiF workshop was co-organized by the German Bunsen

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** For further information on this meeting see the workshop report pp. 61–63.

Society for Physical Chemistry and the European COST Action SMARTCATs (Chemistry of Smart Energy Carriers and Technologies) and supported by the German Research Foundation (DFG). More than 100 researchers from three continents addressed acute and ‘burning’ topics, such as the potential for efficiency increase and for the reduction of greenhouse gases and emissions from combustion processes, in keynote and discussion talks, breakout and panel discussions, and poster contributions. The article presents a short summary and perspective from this Discussion Meeting.

1. Introduction

More than 80% of the global primary energy for transportation and power generation currently still relies on the combustion of fossil fuels, with a slowly increasing contribution of biomass-derived fuels. Fossil fuel combustion releases carbon dioxide (CO₂) as a potent greenhouse gas into the atmosphere and leads to undesired pollutant emissions of substances such as nitrogen oxides (NO_x) and soot particles. The effects of such emissions for climate change, their deleterious influence on air quality, and the associated environmental and health risks have received increasing global attention. Because of the sheer magnitude of the energy needed which is still exacerbated—in spite of potential savings—by global population growth and increasing demands in emerging economies, a short-to-midterm transition from combustion to renewable techniques is highly demanding. With the high energy density presented by liquid energy carriers such as the conventional hydrocarbon fuels, combustion technology will also remain a valuable building block in energy storage concepts. Making combustion more efficient and cleaner while introducing regenerative energy sources is thus urgently desired. Higher combustion efficiency will contribute to a lower carbon footprint, potentially by relying on alternative fuels and different process variables. The reduction of harmful combustion emissions requires better knowledge of the fuel dependence and of the pertinent chemical reaction sequences of their formation, information that can then serve as a basis for abatement strategies or for the introduction of appropriate emission standards.

Current international combustion research emphasizes a variety of thematic foci that are also influenced by geopolitical dependences because of locally available resources such as coal, petroleum, natural gas, or biomass. Important fundamental questions and urgent problems must, however, include the international perspective, the more so since emission standards and regulations as well as the introduction of alternative fuels cannot be done purely from a national side. A particularly interesting example is China with its large population and its industrial transition that depends massively on coal as primary energy source. China is reported to have witnessed a more than two-fold increase in the usage of primary energy within about the last decade^[1]. The replacement of coal by other energy carriers is only slowly picking up momentum. Within the same decade, the transportation fleet has more than tripled from about 40 to 130 vehicles per thousand inhabitants, including an increased share of passenger cars^[2]. Compared to 600–800 vehicles per thousand inhabitants in the EU and USA^[3], similar transportation habits seem unfeasible for China, especially if relying on fossil transportation fuels or fossil energy (for electric powertrains). It is quite clear that the scale of the transformation process towards renewables is colossal, also acknowledging an on average moderate emission standard of the technology currently in use^[4].

Against this background, for which the previous paragraph provided only one illustrative example, the Discussion Meeting intended to bring together results from top institutions and different international perspectives, to foster the exchange of ideas, to discuss perspectives for the future, and to identify nuclei for collaborative research. Convenors MARCUS ALDÉN (Lund), MARA DE JOANNON (Naples), CHRISTOF SCHULZ (Duisburg), and KATHARINA KOHSE-HÖINGHAUS (Bielefeld) therefore

relied on the interdisciplinary setting and discursive tradition at the ZiF for the identification and definition of common goals, especially since decisions in the near future will entail long-term effects. The Meeting focused on the presentation and discussion of fundamental aspects, four representative ones of which will be briefly addressed in the following.

2. Understanding soot nanoparticle formation and their properties

Soot particles, and especially very small nanometer-sized ones, are counted among the most dangerous emissions from combustion. Soot (and other particulates) may be formed from various combustion processes including open burning such as from land clearing or agricultural burning. They may result from land, sea, and air transportation, from industrial burners and processes such as used in ceramic kilns or in blast furnaces for iron production, as well as from residential heating and cooking. The broad spectrum of fuels, from coal and biomass (*e.g.*, wood, grassland, peat, organic waste) *via* conventional petroleum-based (*e.g.*, Diesel, gasoline, kerosene) and biomass-derived (*e.g.*, ethanol, biodiesel) transportation fuels to natural gas is matched by a similarly broad variety of combustion processes including open fires, traditional and modern cooking stoves and heating devices, combustors for power generation and industrial production, as well as gas turbines and internal combustion engines for transportation. The combination of fuel and combustion system is of sensitive influence on the nature and amount of soot formed, and the decisive properties of soot particles emerging from such a plethora of combustion conditions—including size, absorption characteristics, reactivity, and toxicity—cannot be predicted on the basis of today’s scientific knowledge. On the one hand, soot-particle-laden aerosols can cause a variety of respiratory and cardiovascular diseases^[5] and are suspected to cause a significant burden of severe health conditions and deaths^[6]. On the other hand, the climate effects from soot emissions have been underestimated and are only recently acknowledged as the potentially second-largest influence on climate change from anthropogenic processes^[7,8]. Soot particles may contribute to climate forcing by direct absorption or scattering of sun light, they may support nucleation of clouds, and soot deposits on surfaces such as snow may change the albedo and accelerate melting. The influence of soot emitted into the upper atmosphere can thus have far-reaching consequences. Figure 1 illustrates that the major air traffic routes can be traced by estimating aircraft black carbon emissions^[9]. To construct this image, engine, ground emission, and cruise altitude data was interpreted using models that include terms for soot formation and oxidation with a limited consideration of physico-chemical soot properties and reaction kinetics. The prediction of such effects still carries large uncertainties, however, because of the complexity of the influence of soot.

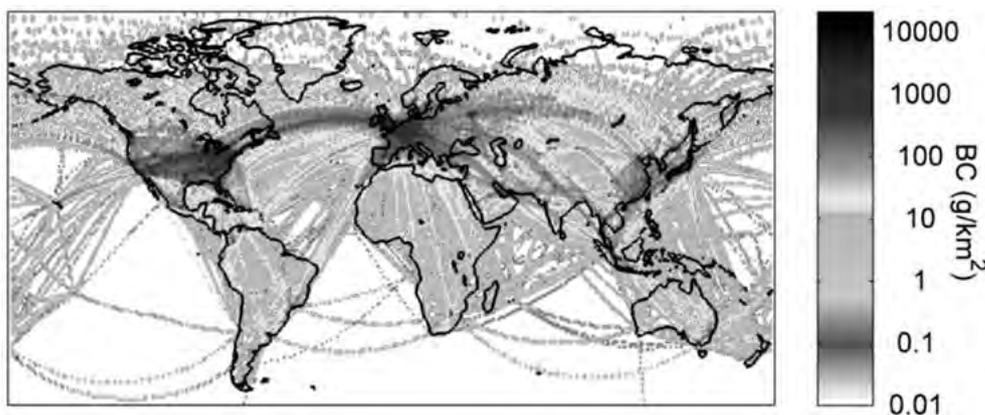
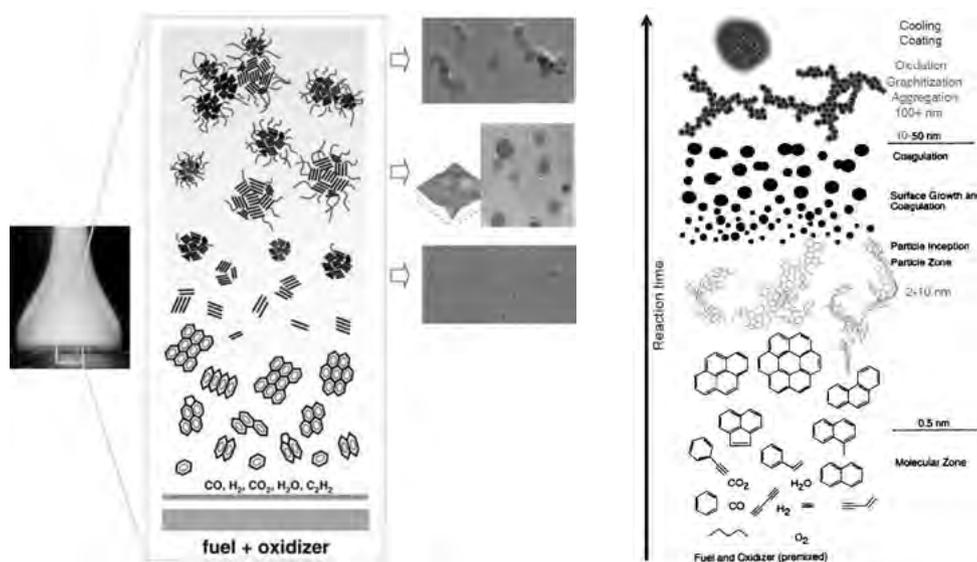


Figure 1: Global map of black carbon (BC) emissions from air traffic estimated from available data with the aid of models; grey shades represent BC density in g/km² on a logarithmic scale. For details see the original publication. Adapted from STETTLER *et al.*^[9] with permission. Copyright (2013) American Chemical Society.

It comes therefore as no surprise that a large part of the workshop, through invited presentations, posters, and breakout discussions, addressed the current status of the understanding of the soot formation process that would enable predictive modeling (see also Section 4) of the soot emissions and their properties. Why is it so complicated to predict soot properties? The formation process of particles from rather small fuel molecules and *via* large aggregates is a challenge for both experimentalists and modelers. Figure 2 illustrates major stages for the formation of soot by means of a conceptual model from 2011^[10] shown on the left side, which highlights the development, with increasing reaction time, from the molecular precursor phase near the burner exit *via* aromatic ring structures to nanometer-sized particles that emit blackbody radiation and cause the yellow luminosity of the flame.

Figure 2: Conceptual model of soot formation. *Left:* Reproduced from WANG^[10] with permission of The Combustion Institute/Elsevier. *Right:* With permission from H. A. MICHELSEN, Sandia National Laboratories, Livermore, USA, private communication, 2017.



This model and different similar variants by other groups are still quite sketchy, however, regarding the physico-chemical processes that lead from the largest multi-ring planar structures to the smallest soot nanoparticles. An updated diagram from 2017 is shown on the right side in Figure 2; it provides more detail in the particle precursor zone and is based on work of a large number of research contributions that are summarized in a recent review by MICHELSEN^[11]. Although the progress in this active research field is rapid, obtaining more insight is not easy. One of the major reasons for this lack of detailed information is the absence of experimental techniques (see also Section 3) that would permit following the reaction process *in situ*. A major part of the discussions at the Meeting addressed therefore some recent advances in pushing beyond the current experimental limits from both, the molecular and the particle ends. Several major obstacles must be overcome. First, more information is needed on nascent particles ‘in the making’, *i.e.* on the dynamic molecular growth and nucleation process in the flame itself. While this is already difficult for idealized laboratory situations, such direct inspection seems overly challenging at present for practical combustion conditions. Second, important properties of soot nanoparticles including their morphology, surface functions, optical behavior (important for radiative forcing), and chemical reactivity, as well as their toxicity are mostly determined from soot samples extracted from flames. With more details becoming available from advanced microscopy and laser techniques^[12,13], it appears that the collection and analysis procedures may change the particle’s nature, casting some doubt on some of the established measurement protocols. Third, most of what is known today on soot particle characteristics is derived from analyzing particle ensembles, not individual particles and their property distribution, a potential

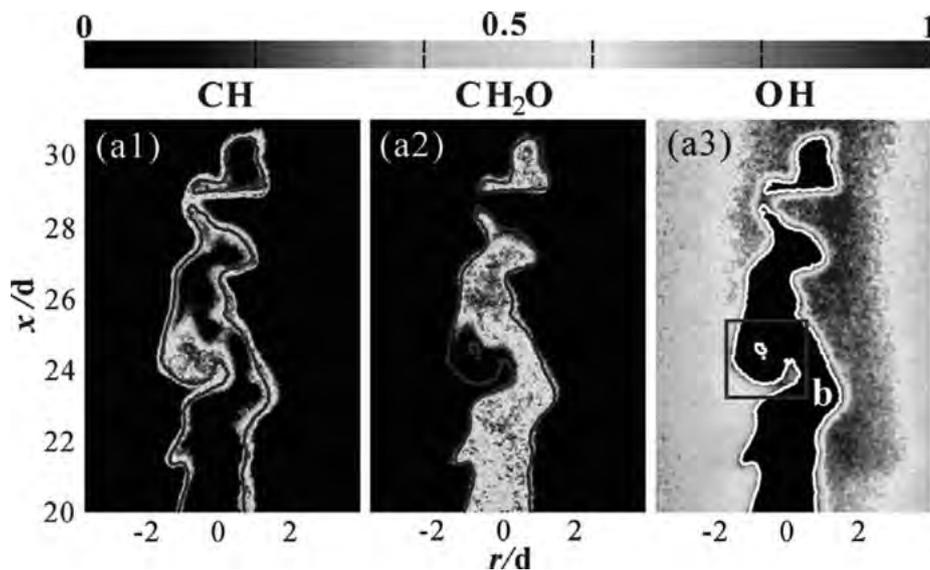
shortcoming for concepts about the interaction of particles with the environment or with living cells. Only a deeper understanding of the formation process and the relationships between fuel and combustion system on the one side and particle concentrations and properties on the other, can form a physico-chemically well founded basis for phenomenological models that can then assist in the design and optimization of low-emission strategies.

3. Examining combustion behavior with advanced diagnostics

For the longest part of a century of technology development, the processes in practical combustion systems have been inaccessible to direct inspection. Combustion diagnostics has meanwhile developed as a field of its own to overcome such limitations and to measure relevant quantities accurately in internal combustion engines or gas turbine combustors. Since it is the chemical energy stored in the fuel that is harvested by such combustion devices, the efficiency and the emissions of the particular engine or combustor depend sensitively on the respective chemical reactions. These complex fuel-specific reaction sequences proceed from the fuel and oxidizer (mostly oxygen from the surrounding air) via many reactive intermediate species to the final products, mainly carbon dioxide and water. Undesired byproducts include regulated emissions (such as carbon monoxide, CO, and NO_x) and other chemicals (such as various hydrocarbon and oxygenated compounds). The reactions typically proceed under rather harsh conditions that are characterized by turbulent flow to ensure fast mixing, phase transitions between liquid fuels and gaseous combustion reactions, as well as high and rapidly changing temperature and pressure. Techniques that can provide insight into such technical combustion processes in real-time are highly specialized, costly, and only available in a few laboratories worldwide. Experts from such centers shared their recent results at the Discussion Meeting, mostly focusing on laser and mass spectrometric techniques.

Using combinations of laser techniques, the four-dimensional evolution of the combustion process in space and time is now becoming accessible even in near-production engines and other practical combustors^[14–16]. Nevertheless, progress regarding the fundamental understanding of the flow physics, the reaction chemistry, and interactions between these, is being made mainly in dedicated laboratory experiments that allow for good diagnostic access and ensure high reproducibility. Conditions of such benchmark experiments are designed so that a certain range of relevant quantities can be addressed sensitively, especially as a test of model hypotheses. A large number of variables should be detected in real-time, including pressure, temperature, flow field, and important reactive chemical species as markers for the reaction progress. It is currently discussed whether the structure of the chemical reaction zone can be so much thickened and distorted by the turbulent motion of the flow that current models might no longer describe their behavior. Most recently, ZHOU *et al.*^[17] presented experimental evidence for such broadened reaction zones, with an example from their study shown in Figure 3. Here, the interaction of a vortex in a turbulent methane-air jet flame is captured with three simultaneous, independent snapshots obtained from laser-induced fluorescence (LIF) of CH, CH₂O (formaldehyde), and OH using three laser systems in a highly involved experimental set-up. Each species characterizes a different part of the reaction sequence: CH₂O is a marker for the early fuel consumption reactions in the inner preheat zone, the CH radical represents the immediate reaction zone at molecular contact of fuel and oxidizer, and the OH radical marks the outer oxidation and post-flame zone. A significantly widened CH area is seen near the vortex, compatible with the assumption that fast turbulent mixing occurs during the relevant chemical reaction time and thickens the flame front.

Figure 3: Simultaneous snapshots taken with laser-induced fluorescence of CH, CH₂O, and OH in a turbulent methane-air flame. The focus is on the interaction of the chemical species with the vortex structure marked with the square and labeled by the letter b in the image on the right. Adapted from Zhou *et al.* [17] with permission of The Combustion Institute/Elsevier.



Further diagnostic challenges are presented, for example, by the need to study the interaction of enclosed flames in a combustor with the surrounding walls [18], or by ignition and spray formation, especially at high pressures [19]. As one of the results of the discussions at the Meeting, well-defined, open-access-to-all test beds with ‘standard’ conditions and equipped with the enabling diagnostics to study turbulent systems at high pressure were suggested, including flames as well as generic engine and gas turbine combustors that could be established and maintained by dedicated host centers.

While the example showed instantaneous fluorescence images of a few reactive species, including CH and OH radicals that are only very short-lived in flames, not all chemically relevant species can be detected with laser methods, not to mention in a practical surrounding. To understand the fuel-specific ignition process and formation of emissions, early decomposition products of the fuel molecule and their reaction pathways are of eminent importance, the more so since alternative fuels and an associated variety of chemicals have been introduced (see also Section 5). Detection of large numbers of reactive species *in situ* again demands highly specialized techniques, often at large-scale user facilities such as synchrotrons. Photoionization molecular-beam mass spectrometry (PI-MBMS) relying on synchrotron-generated vacuum-ultraviolet photons as a universal, structure-selective analysis technique [20] has become one of the most frequently employed methods to generate comprehensive species data sets from flames as a basis for combustion model development and validation.

One of the currently discussed concepts for high-efficiency low-emission engines involves low-temperature combustion [21]. In this regime, previously unidentified classes of highly oxygenated species (*i.e.* hydroperoxides, keto-hydroperoxides, *etc.*) can be formed in the early reactions of fuel decomposition products with oxygen [22,23]. Competing reactions of these low-temperature species and the radicals (such as OH) representative of high-temperature oxidation are of decisive influence on ignition processes. Because of their unstable nature, the detection of these oxygenated intermediates turned out to be extremely demanding [23,24]. New experimental observations are being examined to improve concepts of the respective reaction sequences, with combustion models for this regime just emerging (see also Section 4). Figure 4 shows one very recent example from the oxidation of dimethyl ether, a potential alternative fuel [24]. Here, experimental results for three of the smallest doubly-oxygenated species, *i.e.* hydrogen peroxide (H₂O₂), formic acid (CH₂O₂), and methyl formate (CH₃OCHO), obtained under the idealized conditions in a jet-stirred reactor using PI-MBMS at the synchrotron in Berkeley, USA, are compared to three different recent reaction models.

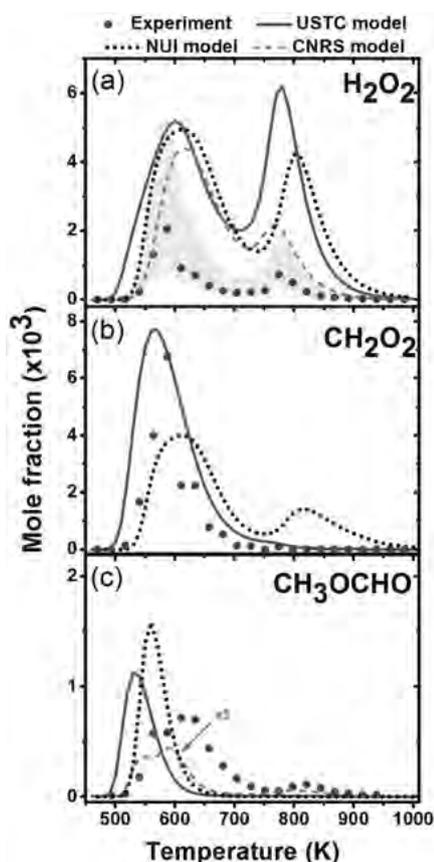


Figure 4: Mole fractions of hydrogen peroxide (H_2O_2), formic acid (CH_2O_2), and methyl formate (CH_3OCHO) as a function of temperature in the oxidation of dimethyl ether; experimental results (*symbols*) from a jet-stirred reactor are compared to simulations with three different recent chemical-kinetic models (*lines*). Reproduced from MOSHAMMER *et al.* [24], with permission. Copyright (2016) American Chemical Society.

Several aspects are worth noting in this comparison. First, larger fuel molecules than dimethyl ether (CH_3OCH_3) such as the linear or branched alkanes representative of current petroleum-based fuels are subject to similar low-temperature oxidation mechanisms. However, they give rise to a much larger structural variety of immediate fuel decomposition products and resulting highly oxidized intermediates [25]. Second, only smaller oxygenated intermediates such as those shown in Figure 4 can at present be reliably identified and detected quantitatively, because necessary quantities needed for the evaluation (*e.g.*, ionization potentials and photoionization cross sections) are yet unavailable. Third, it is obvious that the three models used in Figure 4 yield different results, and that they do not even predict the temperature behavior correctly. Such experimental data will thus improve the knowledge on reaction pathways that are essential for a reliable prediction of the fuel-specific ignition processes. It should be mentioned that the interaction of experimentalists, theoreticians, and modelers has just started to provide fruitful results in this area.

Similar techniques employing mass spectrometry and synchrotron radiation have been successfully used for further chemically complex combustion problems, such as in the detection of high-molecular-weight soot precursors [26]. Since reaction mechanism development and combustion model validation depend sensitively on the quality of the data reported from such experiments, it is highly desirable to assess the associated uncertainties realistically [27]. Again, cross-examination of generic flame or oxidation reactor conditions by several groups, or interrogation of the process in question with several methods is highly advisable, but—as highlighted at the Discussion Meeting—not always common practice.

The numerous diagnostic techniques developed to probe combustion processes while they occur, have also been transferred to different areas, including energy-related catalysis, for example [28,29]. BLOMBERG *et al.* [28] have used the LIF technique mentioned above in the infrared spectral range to

detect the oxidation of carbon monoxide in real-time over a catalyst surface. Such processes can be important in aftertreatment of combustion emissions. Also, the PI-MBMS technique has been used to investigate the catalytic conversion of synthesis gas to light olefins^[29]. By unambiguous identification of intermediate species, plausible steps in the reaction mechanism could be determined, and it could be established that the reaction towards methanol is of minor importance, while C-C coupling towards alkanes was successful. Among other uses, such processes would be useful for synthetic fuel production (see also Section 5).

The value of highly specialized and complex diagnostics for unraveling chemical reactions *in situ* has been demonstrated in the above examples. However, demands for industrial process control are usually different, aiming at robust, low-cost, easy-to-operate, reliable sensors. The discussions at the Meeting addressed the high potential of such sensors for on-board combustion control, for example for autonomous driving, or for emission and air quality monitoring. Mass-market lasers such as in telecommunication or chemiluminescence sensors might offer realistic development chances, if not for passenger cars, then for larger combustion systems for which cost may not be a similarly stringent consideration.

4. Predicting system behavior with combustion modeling

Combustion models are complex. Such models must track a vast number of fuel-specific chemical reactions, embedded in a turbulent flow field, in their space-time behavior in a practical environment. They should provide realistic approximations of fuel delivery, mixing, ignition, the immediate combustion process (*e.g.*, inside the engine), heat release, interactions with the surroundings, formation and aftertreatment of emissions, and other important details. Frequently, sub-models addressing different aspects of the process are developed independently and are combined afterwards. Despite the increase in computer power and the development of fast algorithms, it is not yet possible to follow the development of a large number of chemical reactions in a turbulent flow field and to trace the flow field-chemistry interactions in space and time. The level of detail that can be implemented into a combustion model must be adapted to the particular needs, and the model can be reduced for this purpose. For example, the number of chemical reactions to be considered can be smaller for information on combustion efficiency or CO₂ level than for the prediction of combustion emissions such as soot (see also Section 2). The discussions at the Meeting distinguished between the purposes of ‘engineering models’ *versus* ‘scientific models’: Workable models, if only with limited predictive power, can be used to optimize engineering aspects, whereas consideration of details from first principles may foster deeper understanding, thus enabling next-generation engineering models. The discussion here will be limited to the aspect of chemical complexity only. Realistic descriptions of the fuel decomposition and oxidation chemistry can lead to reaction mechanisms with hundreds of chemical species and thousands of elementary reactions^[30]. They can focus on specific aspects, such as low-temperature chemistry in novel combustion systems^[21,22,31] (see also Section 3). They can address reactions of small and chemically excited radicals that lead to observable chemiluminescence as a potential combustion sensor^[32,33], or concentrate on the soot formation process^[34] (see also Section 2). They can also focus on reaction classes and sequences for certain fuel categories such as alkanes^[35], alcohols^[36], esters representative of biodiesel^[37,38], or alternative fuels derived from cellulosic biomass^[39] (see also Section 5). The example in Figure 5 from the work of ZHANG *et al.*^[40] shows a section of a reaction pathway diagram, provided on the basis of a chemical-kinetic reaction model for the combustion of the alkane family. For longer-chain alkanes such as *n*-heptane (*n*-C₇H₁₆) and *n*-decane (*n*-C₁₀H₂₂) that may be components of petroleum-based Diesel-type transportation

domains, the necessary chemical knowledge must be generated in sufficient detail to allow at least for useful engineering-type modeling under the specific conditions. The examination of models can then rely on benchmark laboratory and near-practical systems experiments to provide the necessary validation data. Deeper understanding of radical reactions and fuel-structure-related chemical pathways from both theory and experiment will assist in making such engineering models more reliable by bringing in the necessary fundamental foundation. Similarly to the advances in chemistry, all further aspects of the combustion system, regarding turbulent flow, flame-wall interactions, phase transitions, *etc.* are receiving similar attention in the combustion science community, so that with such coupled knowledge, increased computer power, and enhanced simulation techniques, a step-wise progress towards model-based design of cleaner processes becomes feasible.

5. Extending the fuel spectrum

Much of the current knowledge on the combustion behavior of liquid transportation fuels (including Diesel, gasoline, and kerosene) has been gained from investigations of the properties of hydrocarbons. These chemical compounds, typically including alkanes, alkenes, their cyclic variants, and some aromatic components, form the substance spectrum in conventional petroleum-based fuels for combustion engines and gas turbines. With the introduction of biomass-derived fuels, this pool has been extended mainly to include oxygenated molecules, *i.e.* fuel structures with functional groups containing oxygen, such as ethers, esters, alcohols, aldehydes and ketones^[36-39]. With these changes, not only physico-chemical properties such as viscosity, boiling point, heat of vaporization, and other important variables may vary, but reactivity as well as fuel decomposition and oxidation pathways may differ from those of hydrocarbons^[41,42], owed to changes of the overall molecular structure and the chemical bond strengths. Mainly ethanol and biodiesel are currently deployed, particularly in fuel blends of conventional fuels with these additives. Oxygenated fuels may lead to a different emission spectrum from that of hydrocarbons, *e.g.*, regarding the formation of hazardous aldehydes, for which the use of ethanol in Brazil has provided extensive experience^[43]. Biomass-based fuels can reduce soot emissions: Using a mixture with bio-kerosene from hydrotreated esters and fatty acids has proven valuable in this respect regarding aircraft emissions into the higher atmosphere^[44] (compare also Figure 1).

Advantages and limitations of biofuels include the promise to reduce the carbon footprint *versus* the potential competition of land use with food production, the impact of energy plants on biodiversity or on water and soil management. Further considerations concern toxicity, required infrastructure, economic aspects, and the scale of biomass needed for conversion to fuels. Assuming that biomass-derived fuels, especially those from non-edible cellulosic biomass^[45-47], can contribute to alleviate the carbon burden, it would be useful to consider chemical and engineering aspects for their production and their use in propulsion as part of a fuel design process^[47-49]. Figure 6 provides an overview of options for such tailored biofuels^[49]: From the polymer structure of cellulose and hemicellulose in 'woody' plant material, a large number of intermediate structures can be obtained and upgraded to potential biofuels. Their molecular structure should meet certain desirable criteria for use in spark-ignition (Otto) and compression-ignition (Diesel) combustion engines, regarding their knock resistance, auto-ignition, mixture formation, and regulated emission levels. With the current state of knowledge on fuel properties and reaction models (see also Section 4), screening of novel fuels for advanced engines^[47,50] and computer-aided biofuel design including their production^[47-49] seems almost within reach and may be expected to contribute to avenues towards more highly efficient, cleaner combustion.

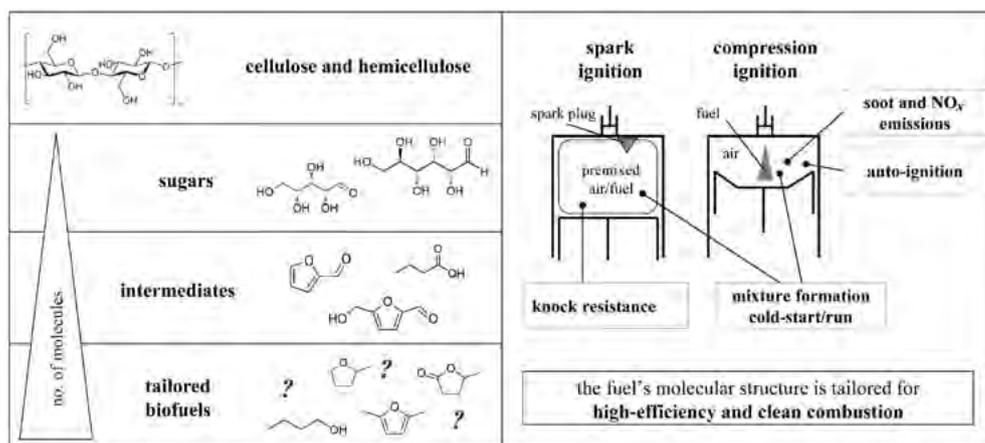


Figure 6: Fuel design challenge: Which molecular structures can be made from lignocellulosic biomass? Which of these structures exhibit physico-chemical properties necessary for high-efficiency and clean combustion in either spark-ignition or compression-ignition engines? Reproduced from DAHMEN *et al.* [49] with permission. Copyright (2016) American Chemical Society.

Numerous biomass conversion strategies are pursued towards biofuel production for ground and air transportation [45,46,51,52]. A newly discussed option is the use of ammonia as a fuel and energy carrier [53,54]. Ammonia, NH₃, a potential fuel without a carbon atom in its structure, could be a building block in a carbon-free power system [54]. Ammonia is discussed as advantageous over hydrogen because of its lower flammability and thus better handling and distribution, its higher energy density per volume, and estimated lower costs [54]. It could also be used as alternative transportation fuel, and prognoses are discussed that changes towards ammonia in the power and propulsion system could contribute to significant greenhouse gas reductions [53], awaiting a full lifecycle assessment, however. While such new options always entail demands for more detailed and quantitative information on the combustion process, existing technologies can be used to handle the expected increased production of NO_x from ammonia combustion. It is not evident which fuels (also as part of hybrid electric propulsion) will be used in the future, and choices may be regionally quite different. However, specific knowledge on their 'green' production, their handling, and—most important in the present context—combustion properties will be needed for any novel fuels or fuel mixtures, demanding systematic and fast experimental and modeling assessment strategies.

6. Future combustion research

The perspectives from the discussions at the Meeting were manifold. First, global energy and transportation systems will include a combustion component in the foreseeable future. Even adaptation of present infrastructure to different fuels or different combustion technology—from household burners to power plants worldwide—will take more than a decade. Second, many liquid fuels, because of their energy density, may not only be 'just burnt' but are interesting energy carriers and offer attractive combinations with renewable power generation. Furthermore, conversion of material (such as, *e.g.*, biomass or waste) to fuels is an active area and merits closer interaction of combustion with related fields. Using flames to make materials such as nanoparticles for different applications is another promising research area [53]. Combustion science is highly interdisciplinary and has much to offer in interaction with other fields. Last but not least, addressing the 'dirty' connotation of combustion in the public—who should make combustion cleaner, especially on such scales and in appreciable time, if not the combustion community? The Discussion Meeting has provided a forum and a nucleus for such joint investigations in the future.

Acknowledgements

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