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Abstracts

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A chemical kinetic study of tetrahydropyran high-pressure oxidation in a jet-stirred reactor

Bakr Hoblos * [1,2], Zeynep Serinyel† [1,2], Guillaume Dayma [1,2], Philippe Dagaut [1]

[1] Institut de Combustion, Aérothermique, Réactivité et Environnement – Centre National de la Recherche Scientifique - CNRS – France
[2] Université d'Orléans – Ville d'Orléans – France

Tetrahydropyran (THP) is an important cyclic ether abundantly formed as an intermediate during the low-temperature oxidation of many hydrocarbons, especially normal alkanes. It is also considered as an interesting and promising oxygenated molecule in the context of next-generation biofuels development. This is essentially due to its substantial existence in the structural core of glucose and many other sugars, which play a crucial role in the oxidation and pyrolysis chemistry of lignocellulosic biomass. In the present work, the oxidation of THP was studied in a jet-stirred reactor (JSR). Fuel-lean ($\phi = 0.5$), stoichiometric ($\phi = 1$) and fuel-rich ($\phi = 2$ and 4) mixtures were oxidized at an initial fuel mole fraction of 1000 ppm, a pressure of 10 atm, a residence time of 700 ms, and for temperatures ranging from 480 to 1260 K. Gas chromatography and Fourier transform infrared spectroscopy were used to determine the mole fraction profiles of the different reactant, product and intermediate species. Based on these profiles, a detailed kinetic mechanism for the oxidation of THP was developed in this work. THP exhibits a low-temperature reactivity which becomes less pronounced with the increase of equivalence ratio and completely disappears at $\phi = 4$. Reaction pathway analyses were performed with the present model. As expected, the hydrogen-atom abstraction reactions from the fuel were found to be the most favorable at the carbon adjacent to the ether group. As a result, the overall reactivity is primarily driven by the chemistry of the corresponding fuel radical formed. The proposed mechanism shows a good performance for representing the present experimental data. However, more data (including atmospheric pressure speciation, ignition delay times and laminar flame speeds) are required for further validation of the present mechanism and in order to have a better understanding of the kinetic behavior of THP.

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*Speaker

†Corresponding author: zeynep.serinyel@cnrs-orleans.fr

An initial step in the experimental characterization of ultra-lean hydrogen/air turbulent spherical flames for internal combustion engine applications

Nicolas Villenave *† [1], Pierre Bréquigny [1], Fabrice Foucher [1]

[1] Laboratoire pluridisciplinaire de recherche en ingénierie des systèmes, mécanique et énergétique –
Université d'Orléans : EA4229, Institut National des Sciences Appliquées - Centre Val de Loire :
EA4229, Université d'Orléans, Institut National des Sciences Appliquées - Centre Val de Loire – France

Kick-starting the decarbonization of the heavy-duty transport sector is vital to slowdown global warming. The use of green e-fuel such as hydrogen for spark ignition engine applications is currently a promising solution. In order to mitigate pollutant emissions, these engines are designed to operate with low volumetric hydrogen content. However, under these conditions, the flame propagation is subject to intrinsic instabilities. Very few studies characterize ultra-lean premixed turbulent flame propagation, especially due to a lack of unambiguous definitions of hydrogen combustion fundamental properties such as laminar flame thickness and speed. To the best of the authors' knowledge, the first turbulent flame speed measurements are presented for ultra-lean hydrogen/air mixtures, under spark ignition engine conditions. Literature correlations considering important turbulent combustion parameters were appraised at engine-like conditions (high pressure and temperature). The results shows that turbulent flame speed increases with increasing volumic hydrogen content, pressure and turbulence intensity. A correlation taking into account preferential diffusion effect, dimensionless Karlovitz and Damkohler numbers was validated on present¨ experiments and literature datasets. As a matter of fact, including the interaction of the multi-scale turbulent vortex with the flame front is important in order to characterize the propagation of such thermo-diffusionally unstable turbulent flames. The conclusions of this work are relevant to the modeling of ultra-lean turbulent premixed hydrogen/air flames and thus of practical necessity.

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[*] Speaker

[†] Corresponding author: nicolas.villenave@univ-orleans.fr

Biomass Pellet degradation under a controlled heat flux

Alexis Coppalle* [1], Pahola Acevedo [2], Carole Gobin [2], Corine Lacour † [2], Vincent Morel [2]

[1] Complexe de recherche interprofessionnel en aérothermochimie – Université de Rouen Normandie, Institut national des sciences appliquées Rouen Normandie, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR6614 – France
[2] Complexe de recherche interprofessionnel en aérothermochimie – Université de Rouen Normandie, Institut national des sciences appliquées Rouen Normandie, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR6614 – France

At the domestic scale, pellet stoves or boilers are now widely used but it still requires fundamental knowledge to overcome efficiency, pollutant emissions, and ash-related issues. Among the different types of solid biomass that are used, lignocellulosic biomass is the most suitable for the combustion process.
Studies have been carried out on small particles injected in flames (1-2), for applications on pulverized combustion. Other works (3-4) have dealt with the combustion of a single pellet or large particle in a small furnace at a controlled temperature. This latter method is often referred to as macro-thermogravimetric analysis (macro-TGA), in reference to conventional TGA, for which the mass of sample is very small. In the present study, the degradation of the pellets of different origins have been used, wood, agro-fuels (miscanthus) or co-products of traditional crops (barley straw).

The degradation process of pellets is studied with samples installed in the centre of an electrical heating cone, which plays the role of a radiative source. The electrical power of the heater has been tuned to a set point so that the heat flux on the axis is 34 kW.m-2, and the pellets ignite

The sample is carried by a thermocouple, which holder is installed on a weighting scale for the mass degradation measurement. So mass and temperature measurements are monitored every 500 ms.

Results that will be presented and discussed*:*

The main stages of a pellet combustion

The sequential steps of the mass degradation for wood pellets are observed as a function of the temperature and can be detailed as below: 1- Drying of the sample (6.2% mass loss) 2- Heating and start of devolatilisation, 3- Devolatilisation and gas phase combustion resulting in a rapid mass loss and more intense heating due to the additional heat flux provided by the flame, 4- Devolatilisation, gas phase combustion and start of char oxidation evidenced by an increase of the heating speed (dTc/dt) for Tc about 450∘C (just after 100 s) corresponding to the char combustion initiation, 5-Char oxidation alone

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*Corresponding author: alexis.coppalle@coria.fr

†Speaker

Mass loss and central temperature of wood pellets under 34 kW.m2

Mass loss and central temperature of wood, miscanthus

and barley straw pellets under 34 kW.m2

Wood, miscanthus and barley straw pellets degradations.

The figure above shows that the main stages of combustion occurs at different times for wood, miscanthus and barley straw. This will be discussed as a function of their main characteristics provided by the proximate analysis (using TGA analysis).

(1) Weng W., Feuk H., Li S., Richter M., Aldén M.,, Li Z., Temporal temperature measurement on burning biomass pellets using phosphor thermometry and two-line atomic fluorescence, Proceedings of the Combustion Institute 38 3929–3938 (2021)

(2) Tian Lia T., , Niub Y., , Wang L., Shaddix C., Løvåsa T. High temperature gasification of high heating-rate chars using a flat-flame reactor. Applied Energy, 227, 100-107 (2018)

(3) Guo G. et al Comparative investigation on thermal decomposition of powdered and pelletized biomasses: Thermal conversion characteristics and apparent kinetics Bioresource Technology 301, 1-9 (2020)
(4) Corbetta M. et al. Pyrolysis of Centimeter-Scale Woody Biomass Particles: Kinetic Modeling and Experimental Validation, Energy & Fuels 28, 3884–3898 (2014)

COMPARISON OF KINETIC MECHANISM PREDICTIONS OF IGNITION DELAY TIME AT HIGH PRESSURE FOR PARTIALLY-CRACKED AMMONIA

Florian Hurault * [1], Pierre Bréquigny [1], Fabrice Foucher [1], Christine MounaÏm-Rousselle [1]

[1] Laboratoire pluridisciplinaire de recherche en ingénierie des systèmes, mécanique et énergétique – Université d'Orléans : EA4229, Institut National des Sciences Appliquées - Centre Val de Loire : EA4229, Université d'Orléans, Institut National des Sciences Appliquées - Centre Val de Loire – France

INTRODUCTION

Today, the urge to replace fossil fuel is more important than ever before. Ammonia is a good candidate as not only a hydrogen carrier but also as a carbon free fuel itself since it is already largely synthesised, easily transportable and storable. However, ammonia can be blended with Hydrogen (H_2) or partially cracked (NH_3 3/2 H_2+ 1/2 N_2) to enhance ammonia combustion's properties but unfortunately favouring the knock phenomena. To predict this phenomena, Ignition Delay Times (IDTs) have to be well simulated at high pressure (40-70 bars) and medium temperature (950 to 1050 K). From literature, IDTs are available at this initial pressure range between 40 and 70 bars but not with 2.5 to 5% of cracked ammonia. During this study, a Rapid Compression Machine was used to expand this database with this pressure range and medium temperature for ammonia blended with hydrogen in order to determine which kinetics mechanism can agree accurately.

SETUPS AND METHODOLOGY

Experiments were performed on a Rapid Compression Machine (RCM), which compresses a gas in less than 33 ms. This RCM is pneumatically driven and equipped with a stroke of 300 mm while the bore is 50 mm diameter. Dead volumes can also be adapted by means of some additional spacers to obtain the desired compression ratio of 11.75. The piston is braked, close to the top dead centre, in an oil chamber. The RCM is equipped with a Kistler 6054BRU59-3-1 pressure sensor with a 0-300 bars range and a linearity of 0.2%. To provide consistent experimental data and perform simulations, a first experimental campaign was done with non-reactive blends, i.e., by replacing oxygen (O_2) by nitrogen (N_2) to unable the oxidation reaction but to keep an equivalent global heat capacity and thus measuring thermal losses and pressure evolution inside the combustion since non-reactive experiments are strictly identical in terms of temperature, pressure and composition to reactive experiments. Then the second experimental campaign was performed with reactive blends i.e. with ammonia (NH_3), hydrogen (H_2) and nitrogen (N_2) at various percentage, oxygen (O_2) and argon (Ar), to replace nitrogen content in the air, for the reactive blend. Ar is used in this study to easily reach high temperature since its heat capacity is twice lower than nitrogen's. As soon as the tank is filled as desired with the

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*Speaker

various gases, vacuum is made inside the combustion chamber. Then, the piston is set to its initial position before the combustion chamber is fuelled in with mixed gases. Once the initial pressure is reached, the intake valve is closed and the piston is released to compress gases The oxidation occurs in the second campaign tests which produce a brutal pressure rising. From this, an IDT can be measured between the end of the compression and the maximum pressure gradient.

Simulations are performed by using ChemKin Pro ANSYS software. Reactive initial conditions, pressure evolutions obtained with non reactive compositions and the kinetic mechanism tested are implemented inside the Closed Homogeneous Batch Reactor software's module to obtain the simulated IDT. The closest this simulated IDT is to experiments and the better the mechanism is. One way to rank the different kinetic mechanisms is to use Kawka's method, but, this method can only be used for non-null Standard Deviation. However, simulations or experiments can lead to no ignition, in this case, IDT value is arbitrary set to 1 second, Standard Deviation is therefore null. A new quantification method was then developed based on Kawka's one. The aim is to compute the relative error between experimental and simulated IDTs for each set and then to average it for each temperature at a given pressure and equivalence ratio ($E\Phi$,P,T). Then, average the previous result for each pressure at a given equivalence ratio ($E\Phi$,P). Finally, it is possible to average all $E\Phi$,P to obtain a relative error for each equivalence ratio ($E\Phi$).

RESULTS AND CONCLUSION

Almost all mechanisms predictions are better for cracked ammonia than pure ammonia. However, reaching 5 % of cracked ammonia does not necessarily mean that mechanism do better predictions. For some of them, predictions are better with 2.5% cracked than 5% cracked. However, when partially cracked ammonia is added, many mechanisms predict IDTs with less than 100% relative error.

Can chemiluminescence be used as preferential diffusion indicator in partially cracked ammonia flames on a Bunsen burner?

Alka Karan *† [1], Guillaume Dayma [2], Christian Chauveau [3], Fabien Halter [2]

[1] Institut de Combustion, Aérothermique, Réactivité et Environnement – Université d'Orléans : UPR3021, Université d'Orléans – France
[2] Institut de Combustion, Aérothermique, Réactivité et Environnement – Université d'Orléans, Centre National de la Recherche Scientifique, Institut des Sciences de l'Ingénierie et des Systèmes - CNRS Ingénierie – France
[3] Institut de Combustion, Aérothermique, Réactivité et Environnement – Centre National de la Recherche Scientifique, Institut des Sciences de l'Ingénierie et des Systèmes - CNRS Ingénierie – France

Ammonia as a fuel has become a topic of wide interest in recent years, aligning with initiatives on mitigating carbon-based emissions. Despite its potential as a fuel for spark-ignition engines due to certain beneficial properties, the laminar flame speeds of ammonia-air mixtures are notably low. It is often combined with hydrogen to overcome some unwanted properties of both fuels when employed independently. Since every mole of ammonia contains 3 moles of H atom, it is often considered as hydrogen carrier. Researchers have come up with a solution to use the best of both fuels by partially cracking ammonia to have mixtures of ammonia/hydrogen/nitrogen. As the cracking percentage changes, the blended fuel properties differ. There are multiple methods to crack ammonia, including thermal, thermo-chemical, and catalytic cracking, all of which can yield hydrogen. There is a wealth of literature available on measuring various parameters such as flame speed, flame stretch, NOx emissions, and chemiluminescence for ammonia/hydrogen flames. The presence of hydrogen in the initial mixture significantly modifies the diffusive transfers. Coulon et al. (1) show the preferential diffusion of H2 and H especially in highly curved flames via DNS. Another DNS study (2) highlighted the effect of the preferential diffusion of H atoms on NO production.

The main objective is to identify markers that would indicate the presence of preferential diffusion. Additional goals encompass the qualitative use of chemiluminescence to assess NOx levels and to investigate the chemistry of NOx formation as the radical pool alters when the composition of the fresh gas mixture changes. Spectroscopic measurements are recorded to compare NO* quantities and to establish correlations with other excited species and NOx (from simulations) NH2* has been identified as an indicator of preferential diffusion for pure ammonia-air flames. It has been noted that ammonia decomposes into hydrogen which diffuses faster than the fresh gas mixture leading to a local enhanced reactivity. It was also found that for those flames whose Le $>$ 1, negative curvature tends to promote hydrogen production leading to increased local reactivity and vice versa. For cracked premixed ammonia-air flames, both NH2* and OH* have been selected as potential tracers. Zhu et al.(3) suggest OH* as a substitute for NO in very lean to stoichiometric ammonia-hydrogen-air flames. The experiments were performed at $\phi = 1.1$ for a cracking percentage of 0-40% leading to χH2 in fuel (ammonia + hydrogen) of 0-0.5 on a Bun-

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*Speaker

†Corresponding author: alka.karan@cnrs-orleans.fr

sen burner at atmospheric conditions. The mixtures were diluted with an excess of nitrogen to stabilize these flames once it was established that the addition of nitrogen didn't affect the point of preferential diffusion. Upon diluting the mixtures, the intensity and thickness of the excited species changed as the flame temperature decreased. Identical patterns were observed in both NH2* and OH* inverse Abel-transformed 2D images. A shift in the local intensity along the flame contour was observed at the same point for both species, with this transition point being dependent on the fresh gas mixture. Finally, a 1D profile of both species was extracted for the different cases and compared with a 1D simulation using Ansys Chemkin. Both the simulation and experimental profiles of the species showed an increase in intensity and narrower profiles (low FWHM) when the fresh gas had a higher hydrogen content. The intensity of both NH2* and OH* decreased with an increase in thickness as the content of H2 dropped. As the flame temperature rises (with higher hydrogen content in fresh gases), the probability of collisions also increases, leading to an increase in the quantities of both species. Simulations also revealed that the non-excited state of both species increases with the rise in hydrogen content. This high concentration also explains the trend observed in the case of the excited species. Emission spectroscopy was also performed for the UV-VIS range and it was observed that the emission spectra of NO* increased as the emission of both OH* and NH2* increased. On probing into NO, N2O, and NO2 concentrations as provided by the simulations, it was seen that as the mole fraction of H2 increases, the concentration of these species also increases.

In summary, as the hydrogen content in the fresh gas increased, the excited species (NH2* and OH*, NO*) , non-excited species (NH2, OH, NO, N2O, and NO2) all increased, as observed in both the experiment and simulation.

References:

(1) Coulon V, Gaucherand J, Xing V, Laera D, Lapeyre C, Poinsot T. Direct numerical simulations of methane, ammonia-hydrogen and hydrogen turbulent premixed flames. Combust Flame 2023;256:112933. https://doi.org/10.1016/j.combustflame.2023.112933.

(2) Mukundakumar N, Bastiaans R. DNS Study of Spherically Expanding Premixed Turbulent Ammonia-Hydrogen Flame Kernels, Effect of Equivalence Ratio and Hydrogen Content. Energies 2022;15:4749. https://doi.org/10.3390/en15134749.

(3) Zhu X, Khateeb AA, Guiberti TF, Roberts WL. NO and OH* emission characteristics of very-lean to stoichiometric ammonia–hydrogen–air swirl flames. Proc Combust Inst 2021;38:5155–62. https://doi.org/10.1016/j.proci.2020.06.275.

Combustion of NH3/CH4 Mixtures in a Swirl Burner: Study of Non-Premixed Flames with Fuel Radial Injection

Antoine Morel *† [1], Toufik Boushaki‡ [1]

[1] Institut de Combustion, Aérothermique, Réactivité et Environnement – Université d'Orléans : UPR3021, Centre National de la Recherche Scientifique : UPR3021, Université d'Orléans, Centre National de la Recherche Scientifique – France

The transition to renewable energy sources is crucial to fight climate change. While the use of natural gas is an important step in this transition, it leads to carbon dioxide (CO2) emissions, contributing to the climate problem. As a response to this challenge, ammonia (NH3) combustion is being considered as a promising alternative. However, the burning of ammonia presents technical and scientific challenges, including its low flame speed, limited calorific value, stabilization difficulties, and high NOx emissions. In this study, the effect of ammonia addition to methane and swirl number are investigated, focusing on pollutant emissions (NOx, CO), exhaust temperature, and flame stability. Experiments are conducted on non-premixed flames with a swirl burner and radial injection of fuel in a 1m high combustion chamber. The burner comprises two concentric tubes, with the inner tube delivering the fuel flow and the outer one delivering the air flow. The fuel is injected radially through eight radial holes. The NH3 fraction varies from 0 to 100% and the swirl number from 0.8 to 1.4. The flame power is fixed at 10kW for all cases. NO, CO, CH4 and CO2 emissions are measured on dry gases using a multi-gas analyzer. The flame structure is investigated throughout OH*, NH* and NH2* chemiluminescence. The results indicate that NO emissions firstly increase, the decrease continually with NH3. CO emissions have a variable evolution with NH3 fraction and flame behavior, in particular with the stabilization zone. Until 50% of NH3, the flame seems very stable, then it becomes fluctuating in stabilization point when ammonia increases. Changing the swirl number has an effect on emissions and flame stabilization. The temperatures taken inside the combustion chamber decrease with the rise of NH3 fraction as expected.

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[*] Speaker

[†] Corresponding author: antoine.morel@cnrs-orleans.fr

[‡] Corresponding author: toufik.boushaki@cnrs-orleans.fr

Comparative study on the effect of premixed equivalence ratio on engine characteristics of ammonia fuelled engine under CI vs SI combustion mode

Caneon Kurien * [1], Pierre Bréquigny [1], Bruno Moreau [1], Christine MounaÏm-Rousselle† [1]

[1] Laboratoire pluridisciplinaire de recherche en ingénierie des systèmes, mécanique et énergétique – Université d'Orléans – France

The adoption of zero-carbon fuels will play a key role in the achievement of carbon neutrality targets and there is an increased focus on the effective utilization of carbon-free fuels like ammonia and hydrogen in internal combustion engines and other power generation applications. Ammonia has emerged as a superior alternative fuel owing to its competitive energy density with lower energy storage costs, and better commercial viability with established infrastructure for production, storage, and transportation as compared to hydrogen. Higher auto-ignition temperature of ammonia limits the operation of pure ammonia in CI engines, hence dual fuel operation with other conventional fuels is preferred since it would otherwise require extremely high compression ratios ($>$ 35:1) to auto-ignite ammonia. Spark ignition mode of combustion is reported to be more suitable for ammonia fuel owing to its higher knock resistance but slow combustion of ammonia due to its lower laminar flame speed will result in poor combustion in current SI engine configuration with lower compression ratio. Hence, for neat ammonia operation, it is favorable to convert the CI engine to SI engine mode to take advantage of a higher compression ratio. This work reports a comparative study on the effect of premixed equivalence ratio (varied from 0.8 to 1.25) on combustion and emission characteristics of ammonia fuelled engine operating initially under (a) compression ignition mode (ignited by dodecane pilot injection), and then converted to (b) spark ignition mode (by replacing fuel injector with spark plug). The experiments were performed in a single-cylinder engine with re-entrant bowl-type piston geometry at a compression ratio of 16.4:1 and the test data was recorded by operating the engine at a constant speed of 1000 rpm with the intake manifold pressure of 1 bar. The ammonia energy fraction was maintained at 95% during the compression ignition mode of operation with dodecane direct injection, and 100% ammonia combustion was achieved in the spark ignition mode. Fourier Transform Infra-Red (FTIR) spectrometer was used for measuring the exhaust emissions, which included unburned NH3, nitrogen oxide, nitrous oxide, carbon monoxide, and carbon dioxide. The results of this study indicated that neat ammonia operation could be achieved satisfactorily by converting the existing CI engine configuration to operate in spark ignition mode, and the stable engine operation with lower COVIMEP (less than 3%)was observed to be possible at near-stoichiometric to rich conditions. The carbon monoxide, carbon dioxide, and hydrocarbon emissions were reduced significantly in the SI mode of operation, however, the unburned ammonia emissions were observed to be higher in SI mode as compared to CI mode, especially in rich conditions. The power output and indicated thermal efficiency reduced in the SI mode and it was observed to be higher in the CI mode of operation owing to the occurrence of multi-point

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*Speaker

†Corresponding author: christine.rousselle@univ-orleans.fr

auto-ignition combustion. The results of this study provide a unique database for comparative analysis of performance, combustion, and emission characteristics of ammonia-fueled engines operating under CI and SI modes.

EXPERIMENTAL AND NUMERICAL COMPARISON OF HYDROXYL RADICAL DISTRIBUTIONS IN LEAN PREMIXED HYDROGEN-AIR FLAMES

Matthieu Durand * [1], Francesco Schiavone [2], Davide Laera [2], Schuller Thierry [3]

[1] Institut de mécanique des fluides de Toulouse – Institut National Polytechnique [Toulouse], Institut National Polytechnique (Toulouse) – France
[2] Polytechnic University of Bari / Politecnico di Bari – Italy
[3] Institut de mécanique des fluides de Toulouse – Université Toulouse III - Paul Sabatier, Institut Universitaire de France (IUF) – France

For the references and figures we refer the reader to the PDF version of this abstract. With growing interest in hydrogen as a low-emissions fuel, aspects of its combustion are being closely examined due to the differences with hydrocarbons. One of these is the chemistry of the excited state hydroxyl radical (OH*) whose production pathways are modified by the absence of carbon atoms in the reactions (1). In this study, lean premixed laminar and steady hydrogen-air flames burning at ambient temperature and pressure are used to compare experimentally measured chemiluminescence to the numerically predicted distributions of the OH* species.

The experimental set-up consists of a bluff-body burner with an annular nozzle outlet with an outer diameter of 12 mm and an inner diameter of 6 mm. A series of M-shaped flames at different laminar burning velocities are selected for investigation. Line-of-Sight (LoS) images of the OH* species are captured with an Intensified Charge-Coupled Device (ICCD) camera. The ground state hydroxyl radical (OH) is also examined as it has an important role in the chemistry of the excited molecule. Its distribution is inferred from Planar Laser-Induced Fluorescence of the OH radical (PLIF). Lastly, Particle Image Velocimetry (PIV) data are also recorded to validate the numerical set-up.

The numerical aspect of this study makes use of the high-fidelity flow solver AVBP (www.cerfacs.fr/avbp7x) to perform Direct Numerical Simulation (DNS) of the M-shaped flames studied in the experiments. These simulations are conducted with the San Diego C0 mechanism (2) to model the hydrogen-air combustion and the Kathrotia sub-mechanism (3) is adapted for the prediction of the light-emitting species. Comparisons between simulations and experiments are made in the axial plane of the burner for the velocity field, the OH, and the OH* distributions.

Figure 1 and Figure 2 compare the spatial distributions of OH* and OH, respectively, of a premixed hydrogen-air M-shaped flame with a global equivalence ratio of _g=0.5 and an injection velocity U_b=8.3 m sˆ(-1). The overall structure and shape of the distributions are similar between the experimental and numerical results. However, their height and thickness differ. Identifying the causes of these differences will provide insight for the improvement of the current chemiluminescence models. Further comparisons are going to be performed for addi-

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*Speaker

tional operating points, higher pressures, pre-heated fresh gases, more complex flows, and with quantitative measurements.

EXPERIMENTAL INVESTIGATION ON FLUIDIZED BED COMBUSTION OF SMASHED CORN COB AT 650-700 ◦C TEMPERATURES

Rolandas Paulauskas *† [1], Ignas Ambrazevičius [1], Kestutis Zakarauskas [1], Marius Praspaliauskas [2], Justas Eimontas [1], Nerijus Striūgas [1]

[1] Laboratory of Combustion Processes, Lithuanian Energy Institute Breslaujos st. 3, LT-44403 Kaunas – Lithuania
[2] Laboratory of Heat-equipment Research and Testing, Lithuanian Energy Institute Breslaujos st. 3, LT-44403 Kaunas – Lithuania

Due to high demand and high prices of good quality woody biomass for electricity and heat production prompt to search for alternatives. Agro biomass is the most common renewable energy source, but due to high alkali, chlorine content and low ash melting temperature (800-900 ◦C), the use of such fuel in convenient biomass furnaces leads to ash agglomeration, slagging, fouling of heating surfaces and corrosion problems. During the combustion of agricultural biomass, the presence of potassium (K), sodium (Na), sulphur (S), and chlorine (Cl) leads to the formation of chemical compounds regarding to the temperature. Over 700◦C, evaporation of gaseous potassium becomes intense and starts to form gaseous potassium chlorides (KCl), which adhere to the surfaces of the furnace and boiler and worsen the heat transfer process. Also these compounds leads to corrosion of these components. Elements like silicon (Si), phosphorus (P), and potassium (K) in agro-biomass form complex compounds as well, which in most cases leads to agglomeration or slagging on the surfaces. In the past decades, extensive studies have been carried out on the influence of biomass fuel properties on ash deposition, but the technologies developed to date still face these problems. In order to reduce the concentrations of alkali metal aerosols, the fuel must be burned at extremely low bed temperatures, reaching up to 600 - 700C.

For these reasons, corn cob combustion was investigated in a 500 kW fluidized bed combustor (FBC), which was designed for work under low bed temperatures (650-700 ◦C). During the experiments, the formed compounds from agro biomass combustion were measured by sampling particulate matter at three FBC locations and mineral compositions were determined. Also the temperature profile of the FBC was established.

It was determined that the emissions of K and Na elements from the FBC reaches up to 9% and 3%, and up to 11% and 4%, respectively at the bed temperature of 650 and 700 ◦C. The introduction of the dolomite as an inhibitor (3% of dry fuel) strongly reduced the emissions of S and Cl from the FCB. When increasing the bed temperature from 650 ◦C to 700 ◦C, the amount of sulfur and chlorine was reduced from 2.37 to 4 times and from 7.68 to 9.47 times, respectively, compared to combustion without the inhibitor addition. Also, after the introduction of dolomite, a slight decrease in the amount of potassium was found at a layer temperature of 650 ◦C and 700 ◦C. Comparing the combustion without and with the inhibitor, potassium content decreased by about 2% and 5%. At both temperature, the NOx and CO emissions were

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[*] Speaker

[†] Corresponding author: Rolandas.Paulauskas@lei.lt

at the limit, respectively 600-700 mg/m3 and 300-400 mg/m3. Moreover, no agglomeration of the fluidized bed was observed throughout extended experiments lasting 8 hours. Hence, the developed FBC and its operational parameters prove suitable for enabling the efficient combustion of agro biomass.

Early flame development characterization of ultra-lean hydrogen-air flames in an optical spark-ignition engine

Caio Ramalho Leite *[1], Pierre Bréquigny [1], Jacques Borée [2], Fabrice Foucher [1]

[1] Laboratoire PRISME – Univ. Orléans, INSA-CVL, PRISME, EA 4229, F45072, Orléans, France – France
[2] École Nationale Supérieure de Mécanique et d'Aérotechnique [Poitiers] – Intitut Pprime – France

Hydrogen-fueled internal combustion engines (H2ICEs) represent a promising technology for decarbonizing the transport sector. In pursuit of this goal, research is needed on lean hydrogen-air combustion under engine conditions aiming to mitigate NOx emissions. However, there is a limited amount of experimental data focusing on flame development at high pressure and temperature, especially in ultra-lean mixtures, which are recently considered to play an important role for future H2ICEs. This study investigates the behavior of very-lean to ultra-lean hydrogen-air flames (0.20 < < 0.55) in an optical spark-ignition engine, focusing on the early flame development phase. Fuel-air equivalence ratio and engine speed (900 < N < 1500 rpm) effects on hydrogen combustion are addressed with pressure-based heat release analysis and chemiluminescence flame imaging techniques. The findings revealed an intrinsic association between these two approaches. Hydrogen flames development measured before 2% of Mass Fraction Burned (MFB) strongly correlates with pressure-based quantities up to 50% MFB, underscoring the critical role of understanding the early flame phase for predicting total combustion duration and in-cylinder pressure traces. A model for hydrogen turbulent flames in the initial combustion stages is formulated based on the Zimont equation and the experimental data. An equation for 0D/1D combustion duration prediction up to 10% MFB is proposed, demonstrating its validity from the wrinkled flame to the well-stirred reactor premixed combustion regimes. Additionally, flame chemiluminescence images for each zone within the Peters-Borghi diagram are presented, offering valuable insights into the diverse characteristics of these flames.

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*Speaker

Early-stage flame acceleration in stratified hydrogen-air mixtures: theory and simulation

Sébastien Missey * [1], Omar Dounia [2], Laurent Selle [3]

[1] Institut de mécanique des fluides de Toulouse – Institut National Polytechnique [Toulouse], Institut National Polytechnique (Toulouse) – France
[2] Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique – Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique - CERFACS – France
[3] Institut de mécanique des fluides de Toulouse – Centre National de la Recherche Scientifique, Institut National Polytechnique (Toulouse) – France

The use of hydrogen as an energy vector calls for an in-depth analysis of the associated risks and the development of mitigation strategies. In the case of liquid hydrogen storage, there are virtually no norms for uses concerning the general public and there is little background on safety measures for an industrial use –with the notable exception of rocket propulsion, which is a very specific domain. The present works addresses the accidental release of liquid hydrogen, resulting in a pool that would create a flammable cloud because of its fast evaporation. This cloud is characterized by strong temperature and composition gradients that are likely to strongly affect the propagation of a flame kernel, in the event of an accidental ignition. The present work is dedicated to the prediction of the initial acceleration of the flame front in a canonical case : a tube with an axial stratification typical of what can be found in liquid-hydrogen spill. Numerical simulations and analytical developments are performed and compared in order to unravel the driving mechanisms and identify the risks of various scenarios : ignition at rich mixture but low temperature, ignition at stoichiometric with propagation of the flame front into the rich region and the lean region, or, ignition at lean mixture with higher temperature. It is shown that ignitions in lean regions may be particularly hazardous because of flame-front instabilities as well as composition gradients favoring acceleration.

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Effect of geometrical parameters on the mixing and stabilization of hydrogen flames in a swirled jet-in-cross-flow burner

Nicolas Vaysse * [1,2], Daniel Durox [2], Ronan Vicquelin [2], Sébastien Candel [2], Antoine Renaud [2]

[1] Laboratoire d'Énergétique Moléculaire et Macroscopique, Combustion – CentraleSupélec, Université Paris-Saclay, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UPR288 – France

[2] Laboratoire d'Énergétique Moléculaire et Macroscopique, Combustion – CentraleSupélec, Université Paris-Saclay, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UPR288 – France

Pure hydrogen combustion is currently being considered to enable the decarbonization of power generation and aircraft propulsion systems. However, hydrogen flames raise two main issues: first, their high burning velocity promotes flashback, and secondly, NOx emissions are favored by the high adiabatic temperatures of these flames. One then has to conceive an injector that will at the same time operate under lean conditions, enhance mixing to avoid hotspots, and produce a flame that can be stabilized at a distance from solid boundaries. This can be achieved using swirling flows. This article reports data from systematic experiments carried out in a single injector cylindrical combustor operating at atmospheric pressure. In the injector, the air flow passes through a radial swirler and mixes with gaseous transverse hydrogen jets. Different conical injectors are tested, featuring different angles and injection holes diameter. The swirl number and the recess of the injection unit with respect to the chamber backplane are also varied because they influence the level of mixing in the system. Laser measurements including tomography are used to determine the equivalence ratio distributions at the injector outlet in cold flow conditions, depending on these geometrical parameters. Resulting flame structures are visualized through OH* chemiluminescence and visible light emission images. They are used to classify the various types of flames and distinguish domains where stabilization takes place at a distance from the injector outlet. The flame behavior is examined for different values of power and global equivalence ratio. It is found that lifted flames are established when the system operates in the high-power range while at low power the flames remain attached to the injector. Velocity measurements in hot and cold conditions complement the analysis of the lifted flames stabilization. These systematic experiments help define operating conditions and design parameter ranges of interest.

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[*] Speaker

Effect of hydrogen dilution in a laminar diffusion ethylene flame: focus on soot formation

Geoffrey Guy *† 1, Christopher Betrancourt‡ 1, Jérôme Bonnety§ 1,
Benedetta Franzelli¶ 1

1 Laboratoire EM2C, CNRS, – CentraleSupélec, Université Paris-Saclay, 3 rue Joliot Curie, 91190
Gif-sur-Yvette, France – France

Soot particles are major air pollutants produced during the combustion of carbonaceous fuels. The detrimental effect of soot particles on health and the environment calls for reducing their emission levels. One possible way to reduce soot emission without drastic changes of the combustion systems may be to partially replace the traditional fuels -composed of hydrocarbons- with hydrogen (1).
At the same time, the thermal power and characteristics of the flame should not change much when replacing hydrocarbons with hydrogen-hydrocarbon fuel blends to avoid major modifications of the combustion systems.

Unfortunately, the effects of such fuel blends on soot production are difficult to predict. Indeed, studies have shown that soot production can be lowered (2) or enhanced (3) depending on the operating conditions.

In this work, we experimentally and numerically study two laminar co-flow flames generated by the Yale diffusion burner (4). The first is the reference laminar diffusion 60%C2H4+40%N2/air flame from the International Sooting Flame Workshop. In the second flame, N2 and a fraction of the C2H4 have been substituted by H2, keeping the thermal power and total volumetric flow rate constant. The flames have a similar structure and size, but the second flame has a lower carbon flow rate.

Experimental measurements based on the laser-induced incandescence (LII) principle (5) -a widely used experimental technique for soot study- are performed to provide the spatial distributions of complementary information on soot. The soot absorption function and gas temperature are obtained by separated-pulse LII (6), the soot volume fraction by auto-compensated LII (7), and the soot primary particle diameter by 2D gated imaging of the LII signal (8).

Results show a downstream shifted absorption function distribution and different soot volume fraction distribution, with a higher maximum soot volume fraction with the hydrogen blend flame than the reference flame, even if the carbon flow rate has been reduced.

In parallel, numerical simulations are performed for the two flames using the detailed kinetic

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[*] Speaker

[†] Corresponding author: geoffrey.guy@centralesupelec.fr

[‡] Corresponding author: christopher.betrancourt@centralesupelec.fr

[§] Corresponding author: jerome.bonnety@centralesupelec.fr

[¶] Corresponding author: benedetta.franzelli@centralesupelec.fr model CRECK (9). The experimental trends are recovered by the simulations, confirming the qualitatively good behaviour of the retained numerical strategy. Numerical results are then used to understand the effect of H2 dilution on soot formation.

References

(1) H. Alrazen *et al.* Renewable and Sustainable Energy Reviews, vol. 54, pp. 785–796 (2016).

(2) Y. Wang *et al.* International Journal of Hydrogen Energy. vol. 46, n. 61, pp. 31400-31427 (2021).

(3) S. Steinmetz *et al.* Fuel. vol. 307, pp. 121914 (2022).

(4) C. McEnally *et al.* Symposium (International) on Combustion. vol. 27, n. 1, pp. 1497-1505 (1998).

(5) R. Vander Wal *et al.* Applied Physics B. vol. 59, n. 4, pp. 445–452 (1994).

(6) G. Guy *et al.* Applied Physics B. vol. 129, n. 8, pp. 127 (2023).

(7) D. Snelling *et al.* Applied Optics. vol. 44, n. 31, pp. 6773 (2005).

(8) R. Hadef *et al.* Applied Physics B. vol. 112, n. 3, pp. 395-408 (2013).

(9) A. Nobili *et al.* Combustion and Flame B. vol. 243, n. 3, pp. 112073 (2022).

Efficiency of catalytic and non-catalytic ceramic foam for the filtration of particle emitted from a domestic wood stove

Valérie Tschamber * [1], Gontrand Leyssens [2], Gwenaelle Trouve [3], Guillaume Moser [3], Bruno Cartoixa [4]

[1] Laboratoire Gestion des Risques et Environnement - LGRE - UR2334 – Université de Haute-Alsace (UHA) Mulhouse - Colmar : UR2334, Université de Haute-Alsace (UHA) Mulhouse - Colmar – France
[2] Laboratoire Gestion des Risques et Environnement – Université de Haute Alsace - Mulhouse – France
[3] Laboratoire Gestion des Risques et Environnement – Université de Haute Alsace - Mulhouse – France
[4] ALSYS CTI – ALSYS CTI – France

The impact of wood combustion in domestic log stoves on the air quality and health is now well known from decades. To decrease particle and hydrocarbons (THC) emissions, the introduction of a specific post treatment system is needed. Such a technology has to be efficient but also needs to respect some requirements: easy to use, maintenance intervals in accordance with a domestic device, no combustion disturbance, no electric connection and acceptable extra cost. The objective of the present work is to test a solution for the treatment of particulate (TSP) and THC, via the implementation of a catalyzed ceramic filter.

Two iron cast log stoves (7 kW) were used. One was equipped with a double wall and a single control of air intake (primary, secondary and post-combustion). The second, less performing but more representative of the market, was equipped with a single wall and without insulating element in the combustion chamber.

Filtering medias tested were ceramic foams with variable thickness and porosity. The efficiency of catalyzed prototypes for TSP filtration and THC oxidation were investigated. A total of five catalytic formulations were tested.

Combustion tests were firstly performed at the laboratory scale, by bypassing a part of the flue gas through a sample of the filter media (Ø60 mm). Further experiments were tested with the filter media installed in the combustion chamber (292 x 288 mm) defined as pilot scale. The combustion tests were carried out according to a protocol representative of a real heating day at home, in natural draft.

The influence of the temperature of the non-catalyzed ceramic filter, their thickness and their porosity, investigated through tests performed by bypassing a part of the flue gas to a sample of the filter media, showed that the particle filtration efficiency increases with temperature up to 450○C. At this temperature, an efficiency of about 20% was obtained and it was shown that the particles trapped are strongly oxidized. A self-regeneration of the filter takes place. However, microscopic analysis reveals that particle oxidation was not complete. Aggregates of particles with close to 10 μm were observed. The porosity and the thickness of the filtering media did not significantly influence the TSP filtration efficiency. On the other hand, the non-catalyzed filters did not have any efficiency towards the gaseous compounds.

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Tests carried out with the catalyzed filter foams show that, whatever the catalytic formulation, TSP filtration efficiency is higher than those obtained with the non-catalyzed filters, with a filtration efficiency close to 40%. Moreover, all the studied with catalyzed filters allow at 450◦C, a total oxidation of CO into CO2 and an oxidation of approximately 50% of the THC. An estimation of the condensed phase within the TSP was performed. It represents 50% of the mass of the particles in the fume upstream the catalyst filter and less than 40% downstream the catalyst.

Tests performed with filter media installed in the combustion chamber confirm that the non-catalyzed ceramic filter foams had not any positive effect on gaseous emissions. However, particle filtration efficiency from catalyzed and non catalyzed filters varies between 25% and 50% depending on the operating conditions, with a TSP content regularly measured below 5 mg/Nm3 referred to 13% of O2 in fume This work shows that the catalyzed filtration technique is compatible with a usual use for a wood log stove.

Elemental analysis of biomass pellets using LIBS

Alexis Coppalle [1], Pahola Acevedo [2], Carole Gobin [1], Corine Lacour [1], Vincent Morel * [1]

[1] Complexe de recherche interprofessionnel en aérothermochimie – Université de Rouen Normandie, Institut national des sciences appliquées Rouen Normandie, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR6614 – France
[2] CORIA-PLASMA – Complexe de recherche interprofessionnel en aérothermochimie – France

At domestic scale, pellet combustion is now widely used in stoves and boilers, because it offers a number of advantages. It uses biomass resources, it can help to reduce the carbon emissions associated with the production of energy by combustion. Compared with the use of logs, feeding the fireplace with these small particles is more flexible. But it still requires more knowledges to solve the problems associated with efficiency, pollutant emissions and ash production.

Incomplete combustion can result in the emission of particles such as organic condensable matter (tar) and unburnt carbon (soot). However, even with complete combustion, particulate matter is still produced due to the behaviour of minor elements (K, Na, Ca, Si,...) in the virgin matter during the combustion process.

Along the combustion process, inorganic minerals are released mainly as salts (1), resulting in ash formation. Minor elements promote formation of fly ash during combustion in flame, and coarse ash that remains in the combustion system. The mechanism involves chemical reactions, particle coalescense, vaporization, and nucleation. The evolution of one mechanism or another depends on fuel material and combustion conditions, which will favor fly ashes in the exhaust or coarse ashes remaining in the system.

So the quantification of the minor elements in the virgin matter is important to be able to predict and optimise combustion systems using solid biomass for energy production.

There exist analytical methods, for instance, Induced Coupled Plasma-Optical Emission Spectrometry (ICP-OES). However they require reference materials or calibration curves by element, which are not easy to make.

Laser-Induced Breakdown Spectroscopy (LIBS) is an optical technique used to determine the composition of a given sample.

The process starts when the laser beam is focused on the sample and ablates the matter, as shown in fig. 1. The ablation causes the solid matter to vaporize, atomize, and ionize, creating the plasma. When the laser beam no longer interacts with the matter, the excited species release energy as photons, returning to their ground state. Quantitative analysis can be made from the spectrum observation based on the spectral signature properties of the elements. The following advantages of applying the LIBS technique are:-1 No special sample preparation required -2 Applicable to all phases of matter -3 In-situ application -3 Multi-elemental analysis, even for

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the major elements (C,O,H).

Calibration Free Laser Induced Breakdown Spectroscopy (CF-LIBS) is a way to apply the LIBS technique for element quantification that does not require a calibration sample (2). It consists to compare experimental spectrum to ab-initio calculations of,the line intensity, knowing the spectroscopic parameters of the element (level energies, line shapes and strengths). These theoretical results are given with the Multi-Elemental Radiative equiLibrIum emissioN (MERLIN) model developed at CORIA laboratory (3).
The composition calculation by CF-LIBS required plasma characterization; this means identifying electron temperature (T

Emissions Analyses of Humidified 20% (vol.) Cracked Ammonia Swirling Flows

Jordan Davies * [1], Syed Mashruk [1], Daisuke Sato [1], Luca Mazzotta [2],
Daniel Pugh [1], Agustin Valera Medina [1]

[1] Cardiff University – United Kingdom
[2] Dipartimento di Ingegneria Meccanica e Aerospaziale [Roma La Sapienza] – Italy

Using renewably produced ammonia as a zero-carbon fuel is gaining momentum due to its ease of transportation and storage as a hydrogen vector. This is particularly true for partially cracking ammonia immediately prior to use, injecting a blend of NH3, H2 and N2. Challenges with this fuel relate to the emissions of NOx and unburned NH3, as well as understanding flame stability. In this study, a 20%(vol.) cracked ammonia blend was investigated using a fully premixed swirl burner, operating at a thermal power of 10kW with steam injection of 30%(vol.) of the fuel and preheating inlet temperatures of up to 390K, for a range of equivalence ratios from lean to rich. Emissions of NO, NO2, N2O, NH3, O2 and H2O were recorded, along with OH*, NH* and NH2* chemiluminescence. Additionally, a numerical investigation was conducted using CHEMKIN-PRO to elucidate the main reactions responsible for reducing emissions by providing an ROP analysis. The 20%(vol.) cracked ammonia blend was found to reduce NO, NO2 and N2O significantly, with an increase in NH3 emissions at rich conditions and instabilities at both lean and rich extremes, compared to the widely investigated 70/30(vol%) ammonia/hydrogen blend. Humidification reduced NO and NO2 emissions due to a reduction in HNO production via OH and NH but caused an increase in N2O by reducing the flame temperature and unburned NH3 emissions at rich conditions due to combustion instabilities.

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*Speaker

Experimental and Modeling Study of the Oxidation of Methane in a Jet-Stirred Reactor with CO2 and H2O dilution

Le Minh Dinh * [1], Olivier Herbinet [1], Frédérique Battin-Leclerc [1]

[1] Laboratoire Réactions et Génie des Procédés – Université de Lorraine, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR7274 / UPR3349 – France

Recent research in oxy-fuel combustion technology has studied different combustion characteristics, which are crucial for optimizing and achieving higher efficiency and lower emissions compared to traditional air-fuel combustion (1–3). Among them, methane oxy-combustion is fundamental to many industrial processes as it is a highly exothermic reaction and minimizes nitrogen species emissions (4). In this work, the oxidation of methane (CH4) has been investigated in a jet-stirred reactor (JSR), usually used in chemical gas phase kinetics because of its efficient mixing. The operating conditions covered a wide range of inlet temperatures (from 850K to 1225K), from fuel-lean to fuel-rich mixtures, with pressure and residence time at 800 torr and 2s, respectively. Besides, CH4 mole fraction was fixed at xCH4 = 0.02, while CO2 was used as a diluting gas. The mole fraction profile of outlet products was obtained using gas chromatography equipment with two different detectors for quantification of the species in the gas phase (4). The influence of water on methane oxidation was also analyzed through experiments with the addition of H2O at 10% in the diluent. Different detailed kinetic models were introduced and simulations of the kinetic schemes were carried out by using CHEMKIN software. Preliminary results show that methane is not reactive at temperatures below about 950K. A benchmarking was reported to highlight the prediction capabilities of literature models under oxyfuel conditions. The study promises to contribute to the improvement of existing kinetic models for the oxidation of natural gas and biogas.

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*Speaker

Experimental and numerical study of the laminar burning velocity of benzaldehyde and benzylalcohol

Nicolas Delort * [1], Olivier Herbinet [1], Roda Bounaceur [1], Frédérique Battin-Leclerc† [1]

[1] LRGP-CNRS – Université de Lorraine -LRGP UMR 7274, CNRS : UMR7274 – France

Abstract

As part of the European goal to reach carbon neutrality in 2050, the EHCATHOL project (http://ehlcathol.eu/) aims to develop a new kind of Second Generation (2G) biofuels from Enzymatic Hydrolysis Lignin (EHL), a waste product of 2G bio-ethanol refinery. This biofuel is mainly composed of arenes and oxygenated aromatics (OA). The gas phase kinetics of the last ones were very little studied because of their low volatilities and high melting temperatures (1) (e.g., phenol melts at 314 K). Only works on anisole and methylanisole flames were reported in literature (1).

In this work, the Laminar Burning Velocity (LBV) of anisole, benzaldehyde, benzylalcohol, 2-phenylethanol, o-guaiacol, cresol isomers and phenol were measured using a flat flame burner with the heat flux method under atmospheric pressure for fresh gases at 398 K. Results are presented in Figure 1 where benzaldehyde and benzylalcohol have the highest LBV which is also significantly above that of alkylaromatics (2), surrogate compounds of petrol derived fuels.

A detailed kinetic model named COLIBRI (3,4) is developed in parallel to model the combustion of these compounds. It is mainly built as a merge of most precise existing models (5–11) for the compounds of interest and completed by new pathways and improvements based on theoretical calculations. It is validated against all experimental data available for oxygenated aromatics as well as for some small arenes. Benzylalcohol is mainly consumed by H-abstraction on the alcohol group, followed by a H-elimination forming benzaldehyde. Thus, the similar LBV of these two reactants is due to their linked decomposition pathways. Then, the high LBV of benzaldehyde and benzylalcohol is caused by their decomposition pathways leading quickly to phenyl which is involved in the accelerating branching reaction phenyl+O_2→phenoxy+O. Consequently, the LBV of benzaldehyde and benzylalcohol are very sensitive to reactions involving phenyl radicals. On the contrary, all other fuels decompose forming benzyl-like or phenoxy-like radicals which are resonantly stabilized radicals and slow the flame propagation.

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References

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*Speaker

†Corresponding author: frederique.battin-leclerc@univ-lorraine.fr

(1) F. Battin-Leclerc, N. Delort, I. Meziane, O. Herbinet, Y. Sang, Y. Li, Catalysis Today 408 (2023) 150–167.

(2) M. Mehl, O. Herbinet, P. Dirrenberger, R. Bounaceur, P.-A. Glaude, F. Battin-Leclerc, W.J. Pitz, Proceedings of the Combustion Institute 35 (2015) 341–348.

(3) I. Meziane, N. Delort, O. Herbinet, R. Bounaceur, F. Battin-Leclerc, Combustion and Flame 257 (2023) 113046.

(4) N. Delort, M. Ismahane, M. Framinet, R. Bounaceur, J. Bourgalais, F. Battin-Leclerc, O. Herbinet, Fuel 362 (2024) 130832.

(5) M. Nowakowska, O. Herbinet, A. Dufour, P.A. Glaude, J. Phys. Chem. A 122 (2018) 7894–7909.

(6) R.D. Büttgen, M. Tian, Y. Fenard, H. Minwegen, M.D. Boot, K.A. Heufer, Fuel 269 (2020) 117190.

(7) G. Kukkadapu, D. Kang, S.W. Wagnon, K. Zhang, M. Mehl, M. Monge-Palacios, H. Wang, S.S. Goldsborough, C.K. Westbrook, W.J. Pitz, Proceedings of the Combustion Institute 37 (2019) 521–529.

(8) W. Yuan, Y. Li, P. Dagaut, J. Yang, F. Qi, Combustion and Flame 162 (2015) 3–21.

(9) R. Fang, C.-J. Sung, Energies 14 (2021) 7708.

(10) L. Zhou, D. Yu, Z. Wang, L.-J. Cheng, Z.-H. Jin, J.-J. Weng, J.-Z. Yang, Z.-Y. Tian, Combustion and Flame 207 (2019) 10–19.

(11) J.-T. Chen, Z.-H. Jin, W. Li, K.-R. Jin, S.-B. Song, J.-Z. Yang, Z.-Y. Tian, Combustion and Flame 231 (2021) 111477.

Experimental flame-flow investigations on a dual-swirl coaxial injector

Maxime Leroy * [1,2], Clément Mirat [1], Antoine Renaud [1], Stefano Puggelli [2], Stéphan Zurbach [2], Ronan Vicquelin [1]

[1] Laboratoire EM2C – CentraleSupélec, Université Paris-Saclay, Centre National de la Recherche Scientifique : UPR288, Centre National de la Recherche Scientifique – France
[2] Safran Tech – Pôle Energetique et Propulsion – France

Decarbonization efforts are driving the development of various technologies to lower the environmental impact of various industrial activities. In this context, hydrogen is being evaluated as a possible alternative fuel for carbon-free combustion in aeronautics. As a result, different combustion technologies are being developed. Regarding the combustion chamber in aero-engines, stable and low-emission injection technologies are required due to the hydrogen's high reactivity and flame temperature, which can cause flashback and nitrogen oxide emissions. This study focuses on a specific hydrogen combustion technology derived from the conventional Rich-Quench-Lean (RQL) technology commonly used in aircraft engines. The technology involves injecting a rich air/H2 mixture followed by air injection to achieve globally lean conditions and complete combustion. This approach has the advantage of avoiding thermodiffusive instabilities that occur when hydrogen is burned in a lean regime, as the Markstein number of hydrogen goes from negative (the flame accelerates with stretch) in the lean domain to positive (the flame decelerates with stretch) in the rich domain. In addition, the high stretch resistance of hydrogen allows for a quick mixing of air to return to globally lean conditions using swirl. The study applies this combustion concept to a dual-swirl coaxial injector, with a central channel for hydrogen premixing and an annular channel for air. This configuration can achieve a variety of flame shapes and structures, including flames with two flame fronts (premixed and diffusion), which become more complex with the inclusion of swirl. The study aims to understand the potential interactions between multiple flame fronts in these intricate flame architectures, which are still poorly understood. To do this, several flames with different swirl and premixing equivalence ratio configurations are selected for experiments under atmospheric pressure. Each flame is analyzed by using various diagnostics, starting from cold flow stereoscopic particle-image velocimetry (S-PIV) using H2/N2 mixtures up to a study in reactive conditions synchronizing S-PIV with Laser-Induced Fluorescence on OH (OH-PLIF). These diagnostics help in understanding the impact of the different flames on the flow and the interactions between premixed and diffusive flame fronts. Finally, it gives elements to interpret in detail the NOx generation in this type of flame.

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*Speaker

Experimental investigations of OH and NO radicals in premixed hydrogen flames across a wide range of equivalence ratio

Tirthankar Mitra * [1], Yann Fenard [1], Nathalie Lamoureux [1], Pascale Desgroux† [1]

[1] Physicochimie des Processus de Combustion et de l'Atmosphère - UMR 8522 – Université de Lille : UMR8522, Centre National de la Recherche Scientifique : UMR8522, Université de Lille, Centre National de la Recherche Scientifique – France

Hydrogen combustion presents an alluring prospect for addressing the increasing energy demand while advancing the decarbonization of multiple sectors. However, its practical implementation raises concerns about the potential for significant NOx emissions that can adversely affect the climate and human health. The scientific community lacks a clear understanding of the NOx formation in hydrogen flames, particularly regarding the influence of fuel equivalence ratio on the underlying chemical pathways. Within the PEPR-H2 framework, the project ''MONTHY" (Understanding and MOdeling of NOx formation in Turbulent HYdrogen flames) aims at comprehensive understanding of NOx formation during hydrogen combustion. To this end, the OH and NO radicals have been studied in low-pressure premixed H2/O2/N2 flames using Laser Induced Fluorescence (LIF). The study encompasses a wide range of equivalence ratio (ϕ=0.35, 1.05, 1.3). The experimental results reveal two distinctive trends in OH formation in the lean flame. The NO mole fraction peaks under stochiometric flame conditions and decreases for both lean and rich flame conditions. The flame conditions were maintained in such a way that the maximum flame temperature is much lower than that (1800K) necessary for thermal NO formation. The experimental results suggest that the N2O and NNH pathways of NO formation are significant for lean and rich flame conditions respectively. Further studies are necessary to improve the N2O and NNH pathways. Furthermore, the role of the two trends of OH formation in NO formation dynamics should be explored.

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*Speaker

†Corresponding author: pascale.desgroux@univ-lille.fr

Experimental study of steam dilution effects on a lean premixed H/air flame

Erwann Bodin *† [1], Manuel Kuhni [1], Cédric Galizzi [1]

[1] Centre d'Energétique et de Thermique de Lyon – Université Claude Bernard Lyon 1, Institut National des Sciences Appliquées de Lyon – France

To achieve the goal of zero emission combustion (pollutants/greenhouse gases), the use of hydrogen (H) as fuel in an Internal Combustion Engine (ICE) seems to be an interesting way to explore, especially for trucks and buses. With ammonia, hydrogen is the only fuel that is potentially free of hydrocarbon, carbon monoxide and carbon dioxide emissions. Hydrogen has a very high combustion velocity and high adiabatic flame temperature (2480K) which contribute to high efficiency in ICE. But this last advantage leads to NO emissions. One solution to this problem is steam dilution to reduce the flame temperature. The presence of water will take a part of the energy released by the combustion due to its calorific capacity. However, comparing the reality the expected decrease in flame temperature is overestimated. Studies on H2/air/steam premixed flames have shown that steam does not act as an inert diluent but directly affects the chemistry of the combustion. The presence of water increases the reaction rate of , an exothermic chain termination reaction that contributes to a large part of the heat release of combustion of hydrogen. Even though this issue has been known for a long time, a lack experimental data on H2/air/steam premixed flames is reported in the literature. These data allow the validation of existing experimental data and the comparison with numerical studies are necessary for a better understanding of the impact of dilution on combustion. This study is carried out on an experimental bench allowing the stabilization of a premixed V-shaped flame. This is a wind tunnel allowing the quasi-homogeneous mixing of fresh gases with an outlet area of 115x115 mm^2. The H/air flame is stabilized on a 0.6 mm diameter platinum wire in which an electrical current is passed to facilitate the hydrogen flame stabilization in a lean or very lean configuration. The advantage of this academic configuration is that it allows a control of the boundary conditions facilitating the understanding of the phenomena involved. A study of the flame topology was carried out in the case of a laminar or turbulent premixed lean flame with and without the presence of steam. Turbulence grids with turbulent intensities of 4% and 8% were used. For the turbulent flame, interest was shown in flame brush thickness and the RMS (Root Mean Square) of the flame front position. The diagnostics used for this study are: tomography images, K-type thermocouples. Temperature measurements with K-type thermocouples were carried out in fresh and burnt gases. An additional study of the flame/wall interaction was carried out using a ceramic plate held close to one of the two flame fronts modelling the interaction between the flame and the wall of an engine. Tomographic images and thermocouple wall temperature measurements were taken to assess the interaction between the flame and the wall. The experiments are conducted for different equivalence ratio and dilution rate by steam to examine the influence of this parameter on the global characteristics of the lean premixed flame.

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[*] Speaker

[†] Corresponding author: erwann.bodin@insa-lyon.fr

Experimental study on the stabilization of premixed laminar flames of H2/CH4/air mixtures on a perforated plate

Adnane Soule * [1], Cédric Galizzi [1], Manuel Kuhni [1]

[1] Centre d'Energétique et de Thermique de Lyon – Université Claude Bernard Lyon 1, Institut National des Sciences Appliquées de Lyon, Centre National de la Recherche Scientifique – France

In a European context of energy transition aiming for carbon neutrality by 2050, hydrogen is an alternative to fossil fuels, particularly as a decarbonized fuel. Most of the burners used in boilers are premixed, fueled by natural gas and have a cylindrical geometry, with a multi-perforated structure for flame development and stabilization. However, the combustion characteristics of hydrogen are very different from those of conventional hydrocarbons: higher flame temperature and burning velocity, reduction in ignition energy, extension of the flammability range, reduction of the quenching distance, modification of the emission spectrum. This can lead to potentially harmful phenomena for the burner like the appearance of hot spots and an increased risk of flashback, hence the need to develop a burner adapted to hydrogen. At present, however, H2 burners are still at the prototype stage and are not on the market, while there are few experimental studies on hydrogen burners (1)(2). The global aim of this study is to develop a burner adapted to hydrogen and to determine the influence of the injection plate, in terms of size, shape and periodicity of the injection orifices, on the stabilization of premix flames. The experimental setup, specifically developed for this study, consists of a vein for laminarization of the flow, a mixer in which the premix is formed, and a flat injection plate with 1 mm diameter injection holes, acting as a burner head where the flames stabilize. The layout and size of the injection holes on the plate were chosen on the basis of literature and industrial patents. A single plate is used here, but others will be tested in order to assess the influence of the size and layout of the injection holes as the injection plate is the main parameter of the study. After a series of aerodynamic characterization tests on the system, it was established that for a flow rate of 20 NL/min, the corresponding jet velocities at the outlet of the injection holes were of the order of 1 m/s. Knowing that the burning velocity of hydrogen at standard conditions (1 atm, 298 K) is of the same order, it was decided to start flame stabilization tests with a fixed air flow rate of 20 NL/min in order to aim for a balance of velocities with the aim of stabilizing the flame without flashback or blowoff. Stabilization tests are carried out with H2-CH4/air mixtures: at a given equivalence ratio, starting with pure methane, the %vol.H2 is gradually increased to 100% H2 where possible, or to the point where stabilization is not achieved. A stabilization point, at a given equivalence ratio and %vol. H2, is reached and validated when the flame stabilizes on the plate for at least 15 minutes without flashback. A stabilization diagram has been drawn up, showing the stabilization points obtained as a function of equivalence ratio and %H2. K-type thermocouples are placed in the flame to record the flame temperature and under the plate to measure the fresh gas temperature. In parallel, numerical simulations using the GRI Mech 3.0 reaction mechanism were carried out to estimate burning velocity at a given configuration of equivalence ratio, %vol. H2 and fresh gas temperature. Analysis of all these data will improve our understanding of the stabilization of premixed hydrogen-air flames on this type of burner. From a practical point of view, this study will also provide elements to aid the design of multi-

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perforated burners to extend their range of use by integrating the increased risks of flashback associated with the use of hydrogen.
(1) A. Aniello et al., *Hydrogen substitution of natural-gas in premixed burners and implications for blow-off and flashback limits*, IJHE, 2022
(2) H. Pers et al., *Autoignition-induced flashback in hydrogen-enriched laminar premixed burners*, IJHE, 2023

Exploratory numerical study of potential ignition and combustion of leaked pressurized ammonia in auxiliaries to ammonia-fed gas turbines

Baopeng Xu [1], Jennifer X Wen * [1]

[1] University of Surrey – United Kingdom

Ammonia is considered as a potential fuel for both gas turbines and internal combustion engines. In such context, ammonia is normally stored and supplied as a pressurized gas. Incidental releases into the turbine/engine/ambient environment would incur safety concerns in addition to toxicity. Furthermore, to overcome the challenges associated with the challenges associated with difficulty to ignite and relatively low laminar flame speeds, blending it with highly active fuels like hydrogen, hydrocarbons, oxygenated hydrocarbons, etc., has been identified as an efficient way to improve the mixture's reactivity.

Exploratory numerical study has been conducted about the potential ignition and combustion of leaked pressurized ammonia in auxiliaries to ammonia-fed gas turbines. Simulations have been conducted for the dispersion, ignitibility, jet fire and explosions in situations with and without hydrogen blend. The source terms are calculated using a notional nozzle model. Three-dimensional multi-component compressible Reynolds-averaged Navier-Stokes equations are formulated for gas flow. The EDC model along with a detailed kinetic scheme is used to model the interaction of turbulence with chemical reactions. Results will be presented to shade light on potential safety issues for ammonia gas turbines.

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Exploring n-Propylbenzene Ignition in the Context of its Synthesis from Lignin: Experimental Investigation and Modeling Analysis of a Potential Sustainable Aviation Fuel

Mateus Paiva * [1,2], Yann Fenard [3], Robert Wojcieszak [2,4], Fabio Bellot Noronha [2,5], Guillaume Vanhove† [3]

[1] Physicochimie des Processus de Combustion et de l'Atmosphère - UMR 8522 – Univ. Lille, CNRS, F-59000 Lille – France
[2] Univ. Lille, CNRS, Centrale Lille, Univ. Artois, UMR 8181 – UCCS – Unité de Catalyse et Chimie du Solide – Univ. Lille, CNRS, F-59000 Lille – France
[3] Physicochimie des Processus de Combustion et de l'Atmosphère - UMR 8522 – Univ. Lille, CNRS, F-59000 Lille – France
[4] Universite de Lorraine and CNRS, L2CM UMR 7053 – Univ. Lorraine, CNRS, F-5400 Nancy – France
[5] National Institute of Technology, Catalysis, Biocatalysis and Chemical Processes Division – Brazil

The investigation of the combustion properties of short-chain alkyl aromatics, especially the C9H12 class, is of significant importance today, as it indicates a potential axis in lignin valorization processes (1,2). Lignin, a complex aromatic macromolecule abundant in lignocellulosic biomass, represents a significant challenge and opportunity in the pursuit of sustainable chemical products (3). Its catalytic reductive depolymerization generates oxygenated products that, upon undergoing a hydrodeoxygenation step, lead to the formation of an interesting range of alkylaromatics (2.4). Interest in alkylaromatics not only addresses current challenges in energy and environmental sustainability but also contributes to unlocking the full potential of biomass as a renewable resource for biofuel production (2). In the present study, the ignition behavior of n-propylbenzene was investigated through the measurement of ignition delay times in a rapid compression machine (5), as well as through the use of kinetic modeling of this same property, utilizing a n-propylbenzene sub-mechanism available in the literature (6). In a heated environment, to ensure complete fuel vaporization, samples were adequately prepared to respect the fuel/air equivalence ratios $\phi = 1.0$ and 0.5. They were then transferred through heated lines towards the combustion chamber to prevent any possibility of condensation. The geometry of the combustion chamber was kept constant at the top dead center, with the compression ratio adjusted to 12 and the initial temperature at 80$\circ$C. Various compositions of inert Ar/N2 gases were employed in different samples, covering a range of compressed gas pressure (10, 15, 20, and 25 bar) and compressed gas temperatures (650-970 K). Additionally, non-reactive mixtures were prepared for use in the variable volume ignition delay simulations. The experimental results obtained demonstrated that the ignition time varied in the range of 5-240 ms depending on the applied experimental conditions. Furthermore, it was observed that this property decreased exponentially with increasing system pressure, indicating a consistent trend of higher fuel reactivity with increasing pressure, with shorter ignition times measured at 25 bar. These results are typical of the pressure effect on ignition delay time for other hydrocarbons (7,8).

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*Speaker

†Corresponding author: guillaume.vanhove@univ-lille.fr

Finally, the simulations showed acceptable agreement between the measured experimental data and predicted ignition delay times. The findings are promising as they may aid in elucidating the kinetics of alkyl aromatic oxidation/combustion chemistry and thus better understand their role in lignin valorization processes and develop innovative strategies for biomass conversion and utilization, leading to advancements in biofuel optimization, in accordance with the fundamental science of combustion.

(1) Y.-X. Liu, Z.-Y. Tian, *Combust. Flame* **2019**, *205*, 165–179.

(2) S. Li, B. Liu, J. Truong, Z. Luo, P. C. Ford, M. M. Abu-Omar, *Green Chem.* **2020**, *22*, 7406–7416.

(3) F. Brienza, D. Cannella, D. Montesdeoca, I. Cybulska, D. P. Debecker, *RSC Sustain.* **2024**, *2*, 37–90.

(4) R. M. O'Dea, P. A. Pranda, Y. Luo, A. Amitrano, E. O. Ebikade, E. R. Gottlieb, O. Ajao, M. Benali, D. G. Vlachos, M. Ierapetritou, T. H. Epps, *Sci. Adv.* **2022**, *8*, DOI 10.1126/sciadv.abj7523.

(5) G. Vanhove, G. Petit, R. Minetti, *Combust. Flame* **2006**, *145*, 521–532.

(6) H. Nakamura, D. Darcy, M. Mehl, C. J. Tobin, W. K. Metcalfe, W. J. Pitz, C. K. Westbrook, H. J. Curran, *Combust. Flame* **2014**, *161*, 49–64.

(7) C. K. Westbrook, H. J. Curran, W. J. Pitz, J. F. Griffiths, C. Mohamed, S. K. Wo, *Symp. Combust.* **1998**, *27*, 371–378.

(8) A. Roubaud, R. Minetti, L. R. Sochet, *Combust. Flame* **2000**, *121*, 535–541.

Filtered tabulated chemistry for multi-regime hydrogen combustion

Samuel Dillon *† [1,2], Renaud Mercier [3], Benoît Fiorina [2]

[1] Safran Tech – Digital Sciences and Technologies Department, Rue des Jeunes Bois, Chateaufort, Magny-Les-Hameaux 78114, France – France
[2] Laboratoire d'Énergétique Moléculaire et Macroscopique, Combustion – CentraleSupélec, Université Paris-Saclay, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UPR288 – France
[3] Safran Tech – Safran Tech, Digital Sciences – France

Hydrogen represents a potential solution for the decarbonization of the aviation industry, however, new challenges arise due to transport and thermochemical properties which differ from conventional fuels. In practical applications, pure premixed injection is usually avoided to limit flashback propensity and both diffusion and partially-premixed flame structures, often stabilised by swirled injectors, are frequently observed in emerging burner designs. Multi-regime flamelet-type approaches for LES are popular due to their low cost, however, these approaches pose two key challenges: 1.) Correct distinction between combustion regimes and 2.) Coupling with the LES, where flame structures are unresolved at the mesh scale. The F-TACLES (Filtered tabulated chemistry for LES) model which couples tabulated chemistry with LES using the filtering approach, has been recently extended to account for multi-regime combustion by incorporating filtered 1-D partially-premixed flamelets. The distinction between combustion regimes is accounted for by the inclusion of the resolved scalar dissipation rate as a tabulation coordinate. A priori testing has been conducted on a H2/Air triple flame and shows that the multi-regime flamelet tabulation captures correctly the triple flame structures.

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*Speaker

†Corresponding author: samuel.dillon@centralesupelec.fr

Flame stability analysis in domestic cooking burners – Effect of hydrogen addition

Rajalakshmi Ravichandran *† [1,2], David Honoré‡ [1,3], Corine Lacour§ [1,3], Sylvain Marc [2], Michel Lecoeur [2], Stephane Carpentier [4]

[1] Complexe de recherche interprofessionnel en aérothermochimie – Université de Rouen Normandie, Institut national des sciences appliquées Rouen Normandie, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR6614 – France
[2] Krampouz – Krampouz – France
[3] Institut national des sciences appliquées Rouen Normandie – Institut National des Sciences Appliquées, Normandie Université – France
[4] ENGIE – ENGIE Lab CRIGEN – France

The stabilization mechanisms of small partially premixed flames are investigated with a focus on burners with self-aspirating combustion technology commonly utilized in cooking appliances. Krampouz company specializing in manufacturing crepe makers, employs these burners with power outputs ranging from 2 to 5 kW. An experimental characterization is performed to understand the physical phenomena entailed in the formation of the fuel/air premixture and flame stabilization mechanism with hydrogen-enriched methane-air flames in these burners. Gas sampling revealed a rich operating equivalence ratio of approximately 1.8 under nominal conditions, indicating a fuel-rich environment. However, a noticeable shift in the equivalence ratio was observed as the thermal power varied. Also, a consistent trend of decreasing equivalence ratio was observed with the addition of hydrogen to the premixture. This decrease in equivalence ratio with increasing hydrogen content highlights the altering stoichiometry of the fuel-air mixture with hydrogen. Furthermore, a flame stability map was created, describing the interplay between thermal power and equivalence ratio in methane-air flames with varying proportions of hydrogen. This study aimed to identify crucial operational thresholds, such as the boundaries of stable flame regions, flame lift-off regions, flame blow-off, and flashback regions. This finding highlighted a significant correlation where higher concentrations of hydrogen enhanced flame stability, while simultaneously expanding the boundaries of blow-off limits but also expanded the risk of flame flashback, as observed around 40% hydrogen addition with an equivalence ratio near 1.0. This highlights the dual challenge of stabilizing flames while mitigating the risk of flashback associated with the higher laminar flame speed of hydrogen. To further characterize these flames, OH* chemiluminescence imaging revealed that lifted flames appeared at higher thermal powers for pure methane-air flames, with a noticeable increase in total OH* signal intensity. Introducing hydrogen into the premixture resulted in a clear boost in the OH* signal alongside a decrease in flame length, at constant thermal power. This OH* signal intensity increase highlights its diverse impact on flame behavior. These findings drive forward the research of facilitating the use of hydrogen in domestic appliances for a low-emission society

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[*] Speaker

[†] Corresponding author: rajalakshmi.ravichandran@insa-rouen.fr

[‡] Corresponding author: david.honore@coria.fr

[§] Corresponding author: corine.lacour@coria.fr

Harnessing the enigmatic ortho-para isomeric conversion for energy-efficient and low-carbon production of liquid hydrogen

Paula Mendoza-Moreno *† [1], Ewa Marek * ‡ [1]

[1] Department of Chemical Engineering and Biotechnology, University of Cambridge – United Kingdom

Liquid hydrogen (LH) is considered an attractive replacement for hydrocarbon fuels, but the energy-intensive production of LH hinders its uptake in industry. The efficient use of energy for LH production depends on the relative content of the ortho-hydrogen (o-H) and para-hydrogen (p-H) isomers upon storage after liquefaction. At LH temperature, the o-H isomer spontaneously transitions to up to 99.6% p-H, releasing enough heat to vapourise the LH product in the process. Promoting the ortho-para conversion (OPC) to completion (99.6% p-H) during liquefaction allows eliminating vapourisation losses over long storage (> 1.8 years) but requires up to 57% higher upfront energy expenditure. Our work offers unexplored solutions to LH competitiveness by applying partial, instead of full, OPC while still attaining loss-less, time-specific storage. Our experimental results demonstrate that attaining full OPC (99.6% p-H2) with a commonly used OPC catalyst is impractical, while detailed simulations of hydrogen liquefaction highlight that the energy and environmental costs associated with full OPC are excessive especially if LH were used as a fuel or energy vector. We also consider a suboptimal OPC approach that accounts for previously unexplored non-idealities of the catalytic conversion compared to the conventional idealisation. Our approach reveals that considering only modest non-idealities results in 1-9% higher energy consumption than expected when OPC follows the thermodynamically dictated o-H/p-H composition. Such an energy increase for liquefaction extrapolates to an additional global energy demand of 0.4-3.8 GW/year by 2050 - currently unaccounted for in idealised studies. Considering higher but more realistic non-idealities would increase the required energy input, overstraining the relevant energy supply. Our life-cycle assessment highlights the imperative for such supply to be of renewable nature to ensure the sustainability of the LH2 carrier. Through tuneable OPC (*i.e.,* controlled p-H% in LH), we reduce energy expenditure in liquefaction by 8-13%, showing that LH with 83-95% p-H content attains loss-less storage for 1-7 days - sufficient for applications with day-scale storage, such as aviation. This, combined with wind-powered LH production, leads to 20x lower CO2 emissions than jet-fuels. We propose capitalising on potential energy savings by avoiding unjustifiably excessive OPC to capitalise on the CO-free combustion of LH for decarbonisation.

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*Speaker

†Corresponding author: pvm21@cam.ac.uk

‡Corresponding author: ejm94@cam.ac.uk

Heavy oil, Mazut Properties definition for Combustion in Numerical Simulations

Seyed Mohammadali Najafi *† [1], Hojat Ghassemi [1]

[1] Iran University of Science and Technology [Tehran] – Iran

Heavy fuel oil (HFO) properties are very dependent to temperature. In some applications which involve severe temperature variations, it is needed to know how temperature could change the properties. A thorough comprehensive definition of properties for a kind of HFO, Mazut, was performed using wide measurements and theoretical relations which can be used in various applications and was not available in previous studies. The relations were successful in simulating an HFO combustion in a combustion chamber. A numerical 3D Eulerian-Lagrangian simulation model for an HFO combustion and gasification has been developed on entrained flow chamber. A parametric study was performed to investigate the effect of equivalence ratio on temperature, specie concentration and efficiency. Syngas production efficiency and overall efficiency were maximum at Er=0.4.

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*Speaker

†Corresponding author: mohamadalinajafi2@gmail.com

Hydrogen combustion in a packed bed of quartz sand

Aki Fujinawa *† [1], Ewa Marek [1]

[1] Department of Chemical Engineering and Biotechnology, University of Cambridge, Philippa Fawcett Drive, CB3 0AS, United Kingdom – United Kingdom

To achieve net-zero emissions by 2050, a transition away from fossil fuel-based energy systems is required. While green hydrogen (H2) is a promising alternative fuel, the high formation rates of nitrogen oxides (NOx), risk of flashback, and flame instabilities, make large-scale power generation through the combustion of H2 challenging (1). The combustion of H2 in a fluidised bed of quartz sand has been proposed (2), where the key advantage is that the sand particles in the bed efficiently absorb the energy released in combustion, owing to their high heat capacities. This enables low operating temperatures, preventing NOx formation.

While the combustion of gases inside bubbles of fluidised beds might be adequately described by homogeneous gas-phase chemistry, the rate of heterogeneous chemical reactions in the particulate phase, such as radical quenching, recombination, and desorption at sand particle surfaces, must be quantitatively investigated to fully understand the multi-phase reactive flow in fluidised beds. This work reports experimental measurements of fuel conversion in H2-air mixtures through an empty reactor tube and a packed bed of quartz sand for a range of reactor temperatures, to study the effect of surfaces of quartz sand particles on H2 combustion. Experimental measurements are compared to model predictions incorporating homogeneous and heterogeneous reaction mechanisms.

In the empty reactor tube, a sharp increase in the yield of water vapour at 600◦C was observed, showing good agreement with simulations of H2-air combustion in a plug-flow reactor incorporating homogeneous chain-branching kinetics of H2 combustion from Alekseev et al.(3). In the packed bed, H2 conversion was observed at the lowest investigated temperature of 400◦C, suggesting that the onset of H2 conversion could have been even lower. The consideration of only homogeneous chemistry did not capture the experimental measurements in the packed bed reactor. In addition to the radical quenching and recombination mechanism proposed by Aghalayam et al. (4), the surface dissociation of H2 and O2 into H and O radical species, and the atomic desorption of radicals were deemed necessary to reach satisfactory predictions of low-temperature conversion of H2 in the packed bed.

References:
(1) S. Verhelst, T. Wallner, Hydrogen-fueled internal combustion engines, Progress in Energy and Combustion Science 35 (6) (2009) 490–527.
(2) J. Baron, E. Bulewicz, S. Kandefer, M. Pilawska, W. Zukowski, A. Hayhurst, Combustion of hydrogen ˙ in a bubbling fluidized bed, Combustion and Flame 156 (5) (2009) 975–984.
(3) V. A. Alekseev, M. Christensen, A. A. Konnov, The effect of temperature on the adiabatic burning velocities of diluted hydrogen flames: A kinetic study using an updated mechanism, Combustion and Flame 162 (5) (2015) 1884–1898.

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[*] Speaker
[†] Corresponding author: af793@cam.ac.uk

(4) P. Aghalayam, P.-A. Bui, D. G. Vlachos, The role of radical wall quenching in flame stability and wall heat flux: hydrogen-air mixtures, Combustion Theory and Modelling 2 (4) (1998) 515–530.

Igniting Hydrogen: Unveiling Combustion Dynamics in Fluidised Beds of Inert Silica Sand

Yujia Wang * [1], Ewa Marek† [1]

[1] Department of Chemical Engineering and Biotechnology, University of Cambridge, Cambridge CB3 0AS, United Kingdom – United Kingdom

Hydrogen, a promising net-zero fuel, is known for properties like low ignition energy, wide flammability range, high flame temperatures, and fast burning speed during conventional combustion of premixed H2 and air. Safety becomes a major concern in its application. In past research on hydrocarbon combustions (1-3), fluidised beds (FBs) have shown promise in improving control over combustion by flattening the temperature distributions and quenching radicals participating in chain-propagation and branching reactions. However, the application of FBs to hydrogen combustion remains underexplored. Apart from Baron *et al.*'s study (4), which is the sole publication in this area, little to no information about H2 ignition and combustion mechanisms in FBs is available. This study investigates the ignition point and combustion behaviour of dilute non-premixed H2/O2 gases, conducted in a fluidised bed of SiO2 sand (250-300 μm) at temperatures ranging from 100 to 800◦C. Special attention was paid to eliminating any possible catalytic materials in the quartz tube reactor. To avoid preignition, 5vol% H2 in N2 and 5vol% O2 in N2 were fed separately into the reactor and mixed above the distributor. Equivalence ratios, which represent the ratio of the fuel and air flowrates compared to flowrates at the stoichiometric conditions, of H2/O2 were changed to obtain fuel-rich (*i.e.* = 1.5, 2) or fuel-lean (*i.e.* = 0.125, 0.25, 0.5) mixtures. These mixtures can be considered non-flammable because either the H2 concentration is lower than the lower flammability limit (LFL) or the amount of O2 is below the limiting oxygen concentration (LOC) (5-6). Surprisingly, the results showed that auto-ignition was initiated at temperatures between 530◦C-580◦C varied with equivalence ratios. Combustion was self-sustained for lean mixtures, but unstable for rich mixtures. At temperatures above 600◦C, combustion remained stable at all equivalence ratios. An ignition point of 530◦C at stoichiometry was 55◦C lower than the predicted value from a kinetic model of a perfectly mixed H2/O2 stream, determined using Cantera. This low ignition temperature was unexpected because the offset of ignition in fluidised beds is usually delayed, with dilute gases flowing through an inert bed of sand acting as a flame arrestor. Therefore, the early ignition in this experiment implies a reaction mechanism that significantly differs from conventional H2/O2 combustion. The ongoing work investigates what other factors influence the ignition temperature and the location of H2 combustion in FBs.

References:

(1) Dennis, J. S., Hayhurst, A. N., & Mackley, I. G. (1982). The ignition and combustion of propane/air mixtures in a fluidised bed. Symposium (International) on Combustion, 19(1), 1205–1212. https://doi.org/10.1016/S0082-0784(82)80297-X

(2) Baron, J., Bulewicz, E. M., Zukowski, W., Kandefer, S., & Pilawska, M. (2002). Combus-

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[*] Speaker

[†] Corresponding author: ejm94@cam.ac.uk

tion of hydrocarbon fuels in a bubbling fluidized bed. Combustion and Flame, 128(4), 410–421. Scopus. https://doi.org/10.1016/S0010-2180(01)00359-5

(3) A simple model for explosive combustion of premixed natural gas with air in a bubbling fluidized bed of inert sand. Combustion and Flame, 134(4), 399–409. https://doi.org/10.1016/S0010-2180(03)00139-1

(4) Baron, J., Bulewicz, E. M., Zukowski, W., Kandefer, S., & Pilawska, M. (2002). Combustion of hydrocarbon fuels in a bubbling fluidized bed. Combustion and Flame, 128(4), 410–421. Scopus. https://doi.org/10.1016/S0010-2180(01)00359-5

(5) PD ISO/TR 15916: 2015 Basic considerations for the safety of hydrogen systems (Version 2). (2015). BSI. https://bsol.bsigroup.com/Bibliographic/BibliographicInfoData/000000000030298670
(6) BS EN 1839:2017 Determination of the explosion limits and the limiting oxygen concentration (LOC) for flammable gases and vapours. (2017). BSI. https://bsol.bsigroup.com/Bibliographic/BibliographicIn

Influence of Ethanol and Iso-butanol Addition on the Combustion Chemistry of Toluene Reference Fuel

Doha Kdouh * [1], Sylvie Gosselin [1], Nathalie Lamoureux [1], Kanika Sood [1], Laurent Gasnot† [1], Luc-Sy Tran‡ [1]

[1] Univ Lille, CNRS, UMR 8522 – PC2A – Physicochimie des Processus de Combustion et de l'Atmosphère, F-59000 Lille, France – Univ Lille, CNRS, UMR 8522 – PC2A – Physicochimie des Processus de Combustion et de l'Atmosphère, F-59000 Lille, France – France

The effort to reduce fossil fuel dependence and CO2 emissions from spark-ignition engines has sparked interest in oxygenated biofuels including alcohols. The addition of these biofuels to gasoline can significantly impact the combustion chemistry including emissions of pollutants like soot, PAHs, and aldehydes. Thus, this impact is necessary to be investigated. While some studies have investigated the combustion chemistry of Toluene Reference Fuel (TRF) (1)(2)(3) and TRF/alcohol mixtures (4)(5), quantitative analysis of chemical species under flame conditions remains limited. To address this lack, atmospheric premixed laminar flames by blending ethanol and iso-butanol with TRF under fuel-rich flame conditions using a McKenna burner have been studied.
In this study, three different flames were examined: TRF with an equivalence ratio () of 1.82, TRF-E (TRF blended with ethanol) with =1.82, and TRF-B (TRF blended with iso-butanol) also with =1.82. These flames were analyzed using gas chromatography (GC) to determine the mole fractions of various types of compounds including saturated and unsaturated aliphatic compounds, aldehydes, ketones, and aromatic species. Four GCs utilized for this purpose encompassed the determination of oxygen (O2), nitrogen (N2), and carbon monoxide (CO), followed by the sequential identification of small hydrocarbons, oxygenated hydrocarbons, single aromatics, and polycyclic aromatic hydrocarbons (PAHs). Additionally, two different methods were used to measure the flame temperatures: NO- LIF (Laser Induced Fluorescence) thermometry (NO was excited around 225 nm, and fluorescence was collected along entire (0,2) vibrational band) (6) and thermocouple temperature measurements (7). A thermocouple with a wire diameter of 0.2 mm was used for the latter method. Adding biofuel to the TRF flame caused significant changes in the amounts of certain substances. Figure 1 represents a comparison of the three studied flames for selected species. Some species like C2Hx, C3Hx, C4Hx, mono-aromatics, and naphthalene decreased, while others, like aldehydes, increased. Special change like in methanol and acetone upon adding either ethanol or iso-butanol is observed. However, the maximum flame temperature didn't change much.

(1) E. Hu, Z. Xu, Z. Gao, J. Xu, and Z. Huang, "Experimental and numerical study on laminar burning velocity of gasoline and gasoline surrogates," *Fuel*, vol. 256, p. 115933, Nov. 2019, doi: 10.1016/j.fuel.2019.115933.

(2) C. Shao, G. Kukkadapu, S. W. Wagnon, W. J. Pitz, and S. M. Sarathy, "PAH forma-

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[*] Speaker

[†] Corresponding author: laurent.gasnot@univ-lille.fr

[‡] Corresponding author: luc-sy.tran@univ-lille.fr

tion from jet stirred reactor pyrolysis of gasoline surrogates," *Combustion and Flame*, vol. 219, pp. 312–326, Sep. 2020, doi: 10.1016/j.combustflame.2020.06.001.

(3) S. Park, Y. Wang, S. H. Chung, and S. M. Sarathy, "Compositional effects on PAH and soot formation in counterflow diffusion flames of gasoline surrogate fuels," *Combustion and Flame*, vol. 178, pp. 46–60, Apr. 2017, doi: 10.1016/j.combustflame.2017.01.001.

(4) A. Khosousi *et al.*, "Experimental and numerical study of soot formation in laminar coflow diffusion flames of gasoline/ethanol blends," *Combustion and Flame*, vol. 162, no. 10, pp. 3925–3933, Oct. 2015, doi: 10.1016/j.combustflame.2015.07.029.

(5) P. Dirrenberger *et al.*, "Laminar burning velocity of gasolines with addition of ethanol," *Fuel*, vol. 115, pp. 162–169, Jan. 2014, doi: 10.1016/j.fuel.2013.07.015.

(6) K. K. Foo, N. Lamoureux, A. Cessou, C. Lacour, and P. Desgroux, "The accuracy and precision of multi-line NO-LIF thermometry in a wide range of pressures and temperatures," *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 255, p. 107257, Nov. 2020, doi: 10.1016/j.jqsrt.2020.107257.
(7) J. Elias *et al.*, "Thermocouple-based thermometry for laminar sooting flames: Implementation of a fast and simple methodology," *International Journal of Thermal Sciences*, vol. 184, p. 107973, Feb. 2023, doi: 10.1016/j.ijthermalsci.2022.107973.

Influence of turbulent inflow conditions on the Large-Eddy Simulation of a non-premixed hydrogen-air jet flame

Félicia Garnier * [1], Thomas Jaravel [1], Alexis Boudin [1], Davide Laera [2], Thierry Poinsot [1,3]

[1] CERFACS – CERFACS – France
[2] Politecnico di Bari – Italy
[3] Institut de mécanique des fluides de Toulouse – Institut National Polytechnique [Toulouse], Université Toulouse III - Paul Sabatier, Centre National de la Recherche Scientifique : UMR5502, Institut National Polytechnique (Toulouse), Centre National de la Recherche Scientifique – France

Hydrogen jet flames take part in numerous safety scenarios raised by the use of hydrogen throughout multiple industry sectors. For instance, in case of ignition during an accidental leak or an overpressure venting operation, a large turbulent diffusion flame may establish and anchor at the hydrogen outlet rim, potentially causing mechanical destruction. This study aims at achieving a fine physical understanding of such flames, particularly their response to turbulent inflow conditions.
The Large-Eddy Simulation (LES) methodology is applied to the turbulent non-premixed hydrogen-air flame investigated by Barlow and Carter (1,2). The jet flame is stabilized at the outlet of a pipe of diameter D = 3.75 mm, where pure hydrogen flows at Re = 10,000 into air, yielding a flame of visible length L = 180D (Fig. 1).

In the reference computation, the turbulent hydrogen jet is modeled by injecting synthetic anisotropic nonhomogeneous turbulence on a pipe inlet. The pipe length is kept short (2.6D) to limit computational cost. Even though it results in partially developed turbulence at the pipe exit, results show that the turbulent fluctuations are sufficient to correctly capture the jet destabilization and the flame structure over its whole length. The mixing process is found to be tightly coupled to the jet destabilization mode, which is strongly sensitive to the inlet conditions (3,4,5). In the jet flame LES, the hydrogen jet destabilizes under the combined effects of Kelvin-Helmoltz instability, driven by shear, and turbulent fluctuations, convected from the injection tube.

The LES is able to retrieve finite rate chemistry and differential diffusion effects, which are expected in such flames (6,7). Results also show a fair agreement with the mean and RMS experimental dataset, including common safety metrics such as flame length. In particular, the rate of decay of axial velocity and mixture fraction is well-predicted, indicating that the mixing rate is correctly captured. The flame structure fairly agrees with temperature and intermediate species measurements throughout the flame. Furthermore, the numerical results suggest the occurrence of local extinction events in the flame base region, associated with locally high scalar dissipation rate.
In order to quantify the sensitivity of jet stability and flame structure to the turbulent inflow conditions, a supplementary LES is performed where the hydrogen turbulent inlet is supplied by a precursor periodic pipe simulation. At the hydrogen injector exit, the turbulent flow is

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fully developed with higher levels of fluctuations than in the synthetic turbulence injection case. Discrepancies between both injection methods seem to prevail in the flame base. As the mixing process in the near field influences the far field, the flames are compared downstream of the potential core breakup. The numerical results seem to indicate that the far field is sensitive to jet exit conditions to a lesser extent than the near field, as the discrepancies observed at the flame base are smeared out by the far field smoother gradients.

Investigating the onset time of puffing/micro-explosion in rapeseed oil/water emulsion droplets under forced convection: A parameter analysis

Zhaoping Ying * [1]

[1] Interdisciplinary Center for Scientific Computing, Heidelberg University – Germany

The disruption behaviours of fuel/water emulsion droplets enhances atomization and improves spray combustion efficiency. The phenomenon of emulsion droplets puffing or micro-explosion under forced convection is not extensively researched. A novel framework is used to predict the puffing/micro-explosion onset time of rapeseed oil/water emulsion droplets under forced convection. This study examines a benchmark scenario with the following conditions: droplet radius of 1.8e-3 m, droplet temperature of 293.15 K, ambient gas temperature of 975 K, initial volume fraction of rapeseed oil in the emulsion droplet at 0.9, and the droplet is stationary but air motion is at 2 m/s. The impact of different initial conditions on the onset time of rapeseed oil/water emulsion droplets puffing/micro-explosion is systematically investigated. This includes analyzing parameters such as air velocity, initial droplet temperature and size, and the concentrations of droplet components. The numerical results indicate that increasing air velocity significantly improves heat transfer to droplets, resulting in a notable decrease in the time it takes for puffing/micro-explosion to occur. Higher initial droplet temperatures and smaller droplet radii accelerate droplet disruption due to reduced thermal energy requirements for boiling nucleation of the less volatile component (water). Conversely, decreasing the volume fraction of the more volatile component (rapeseed oil) prolongs the onset time of disruption for the same reason. Therefore, optimal atomization and combustion performance in biofuel/water droplets spray is achieved with increased ambient air velocity, elevated initial droplet temperature, reduced droplet radius, and higher volume fraction of biofuel component within practical application constraints.

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[*] Speaker

LES of a differentiated injection NH3-H2 swirled flame: preliminary NOX analysis

Héctor José Vargas Ruiz * [1,2], Davide Laera [2,3], Ghislain Lartigue [1], Syed Mashruk [4], Agustin Valera Medina [4], Laurent Gicquel [2]

[1] TotalEnergies – TotalEnergies OneTech – France
[2] Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique – Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique - CERFACS – France
[3] Polytechnic University of Bari / Politecnico di Bari – Italy
[4] Cardiff University – United Kingdom

Gas turbines are one of the most reliable and cost-efficient power sources. However, energy production is a major source of greenhouse gases (GHG), particularly carbon dioxide and methane. The decarbonization of gas turbines can be foreseen through the adoption of ammonia-hydrogen blends. In this context, unconventional setups, such as the differentiated injection burner, are being investigated to achieve low-NOX NH3-H2 combustion. NOX production in such flames needs to be understood and mitigated if the aforementioned fuels are to be implemented at an industrial scale. In an effort to understand the mechanisms leading to the formation of nitrogen oxides, Large Eddy Simulations of the partially-premixed ammonia-hydrogen flame experimentally studied by Mashruk et al. at Cardiff University are performed (Fig. 1). A novel experimentally validated Analytically Reduced Chemistry, able to reproduce NH3-H2-N2 flame properties and NOX levels, is used. The Multi-Fuel Thickened Flame model (MF-TFLES) coupled with Charlette's efficiency function is used to take flame-turbulence interaction into account. The origin of NOX is retrieved from the simulation results based on the nitrogen atom chemical pathway and the topology of the reactive zone. This preliminary study will serve as the basis of a more detailed pollutant analysis which will help characterize the emission performance of the differentiated injection technique and identify the features of the configuration required to minimize NOX production.

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Laminar Burning Velocity of NH3/NO/N2 mixtures: an experimental and numerical study

Noé Monnier *† [1], Nathalie Lamoureux [2], Seif Zitouni [3], Pierre Bréquigny [3], Christine MounaÏm-Rousselle [3]

[1] Laboratoire pluridisciplinaire de recherche en ingénierie des systèmes, mécanique et énergétique – Université d'Orléans : EA4229, Institut National des Sciences Appliquées - Centre Val de Loire : EA4229, Université d'Orléans, Institut National des Sciences Appliquées - Centre Val de Loire – France
[2] Physicochimie des Processus de Combustion et de l'Atmosphère - UMR 8522 – Université de Lille : UMR8522, Centre National de la Recherche Scientifique : UMR8522, Université de Lille, Centre National de la Recherche Scientifique – France
[3] Laboratoire pluridisciplinaire de recherche en ingénierie des systèmes, mécanique et énergétique – Université d'Orléans : EA4229, Institut National des Sciences Appliquées - Centre Val de Loire : EA4229, Université d'Orléans, Institut National des Sciences Appliquées - Centre Val de Loire – France

Ammonia (NH3) is not only a hydrogen carrier but also promising carbon-free fuel. The understanding of its combustion kinetic is crucial, especially its interaction with key nitrogen chemistry species such as nitric oxide (NO). To improve the understanding of NH3/NO interaction on all levels, experimental measurements were carried on NH3/NO/N2 mixtures to determine fundamental combustion parameters such as the laminar burning velocity and Markstein length. The experiments were conducted in a spherical combustion vessel under normal pressure and temperature for different equivalence ratio and oxidizer mixtures (%NO ranging from 40 to 70 in N2). Experiments showcased a shifting behaviour of maximum laminar burning velocity from rich to lean mixtures with increasing %NO in the oxidizer mixture. Furthermore, the Markstein length becomes less dependent upon equivalence ratio with NO addition. After appraisal of a dozen recent mechanisms from literature, Han et al. (2021) was chosen as one best accurate kinetic model for NH3/NO/N2 combustion to provide kinetics analysis. The numerical simulations were conducted using the open software CANTERA to evaluate additional fundamental parameters such as the Lewis number, which details the transport mechanism of species in the flame front and the Zel'Dovich number which corresponds to the dimensionless overall activation energy. In addition, appraisal of the reaction mechanisms revealed an unusual behaviour with respect to temperature and heat release rate profiles. A 2-step variation was for first time observed Based on the kinetics analysis, it was found that the 1st increase of temperature corresponds to the location in the flame front where major reactions lead to heat release and the 2nd one to an excess of NO undergoing conversion to N and N2 in a reverse thermal-NO mechanism, releasing energy at a much slower rate than during the temperature increase. This reduces NO emissions even at lean conditions.

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[*] Speaker

[†] Corresponding author: noe.monnier@etu.univ-orleans.fr

Low-Temperature Oxidation of Tetrahydropyran in a Jet-Stirred Reactor

Caroline Lewin * [1], Jiabiao Zou [2], Jeremy Bourgalais† [1], Olivier Herbinet [1], Frédérique Battin-Lelcerc [1], Aamir Farooq [2]

[1] Laboratoire Réactions et Génie des Procédés – Université de Lorraine, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR7274 / UPR3349 – France
[2] King Abdullah University of Science and Technology [Saudi Arabia] – Saudi Arabia

In the context of transitioning to renewable and carbon-neutral fuels in the transportation sector, biomass-derived fuels emerge as a promising alternative. Tetrahydropyran (THP), a simple lignocellulose-derived biofuel, has been extensively studied at high temperatures (1-3); however, its low-temperature oxidation has not been as extensively explored. This necessitates comprehensive experimental measurements to elucidate the influence of the ether group in the intricate kinetics governing its oxidation chemistry in the low to intermediate temperature regime (4,5).
The low-temperature oxidation of THP was studied in a jet-stirred reactor (JSR) from 450 to 900 K. Equivalence ratios of 0.25, 0.50, and 1.0 were investigated. Residence time, pressure, and fuel inlet mole fraction were maintained at 4 s, 800 Torr, and 0.5%, respectively. The main products and stable species were identified and quantified by connecting the JSR to two gas chromatographs (GC) equipped with flame ionization detectors (FID). For species identification, a GC coupled to a mass spectrometer (GC-MS) was used. Experimental results were compared to the predictions of a detailed kinetic mechanism developed in this study.

A variety of species was quantified, including olefins, C1-C4 carbonyl compounds, and cyclic ethers. As shown in Fig. 1, fairly good agreement between experiments and simulations was obtained for the mole fraction profiles of THP and main products such as dihydropyran. Additionally, a pronounced negative-temperature coefficient (NTC) region was observed for fuel-lean conditions. At low-temperatures, depending on the H-abstraction site of the THP molecule, chain branching reactions become favorable and the formation of ketohydroperoxides enhance the reactivity. As the temperature increases, the major contribution of these pathways is replaced by the formation of less reactive species, ring-opening and decomposition reactions, leading to the observed NTC behavior.

References:

(1) L.-S. Tran, R. De Bruycker, H.-H. Carstensen, et al., Pyrolysis and combustion chemistry of tetrahydropyran: Experimental and modeling study, Combust. Flame 162 (2015) 4283-4303.

(2) P. Dagaut, M. McGuinness, J. Simmie, et al., The ignition and oxidation of tetrahydrofuran: Experiments and kinetic modeling, Combust. Sci. Tech. 135 (1998) 3-29.

(3) N.J. Labbe, V. Seshadri, T. Kasper, et al., Flame chemistry of tetrahydropyran as a model heteroatomic biofuel, Proc. Combust. Inst. 34 (2013) 259-267.

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*Speaker

†Corresponding author: jeremy.bourgalais@cnrs.fr

(4) B. Rotavera, C.A. Taatjes, Influence of functional groups on low-temperature combustion chemistry of biofuels, Prog. Energy Combust. Sci. 86 (2021) 100925.
(5) L.-S. Tran, O. Herbinet, H.-H. Carstensen, et al., Chemical kinetics of cyclic ethers in combustion, Prog. Energy Combust. Sci. 92 (2022) 101019.

Modeling of mass and heat transfers in multicomponent droplet phase change

Aymeric Vié * [1], Artur Carvalho Santos [2], Fernando Luiz Sacomano Filho [3]

[1] Laboratoire d'Énergétique Moléculaire et Macroscopique, Combustion – CentraleSupélec, Université Paris-Saclay, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UPR288 – France
[2] Laboratoire d'Énergétique Moléculaire et Macroscopique, Combustion – CentraleSupélec, Université Paris-Saclay, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UPR288 – France
[3] Universidade de Sao Paulo – Brazil

Decarbonating aviation will require alternative fuels, such as biofuels or e-fuels. Among them, liquid fuels composed of hydrocarbons are still a preferred option, as they can still be used in today's engine architectures. In the objective of performing simulations of the combustion chamber with these fuels, an important step is the prediction of the vaporization of the liquid droplet. The most standard approach for kerosene is to consider the liquid fuel as a unique surrogate species. The required evaporation model is thus single-component, the most famous being the one by Abramzon and Sirignano (1), widely used in the combustion community. However, identifying the differences between conventional and alternative fuels requires discriminating the droplet species. Unfortunately, there is no consensus on the best modeling strategies. In the present work, we will highlight recent advances in the modeling of multi-component phase change, focusing on the transport phenomena of heat and mass in the gas phase. Specifically, a general formulation for the energy equation has been proposed, independent of the diffusion velocity closure for the species equation (2), and thus enables to account for differential diffusion of enthalpy. For the mass transfer, a formulation allowing both evaporation and condensation has been developed along with a robust algorithm (3). Finally, a new formulation based on the Stefan-Maxwell equations for the diffusion velocities has been proposed (4). All models are extended to account for convection effects following the strategy of Abramzon and Sirignano (1). All models are compared in various cases relevant to combustion applications, showing their forces and weaknesses and thus opening new perspectives for multi-component droplet phase-change modeling (2-5).

(1) B. Abramzon and W. A. Sirignano (1989), Droplet vaporization model for spray combustion calculations, Int. J. Heat Mass Transfer, Vol. 32, No.9 pp. 1605-1618.

(2) F. L. Sacomano Filho, A. C. Santos, A. Vié, G. C. Krieger Filho (2022), A new robust modeling strategy for multi-component droplet heat and mass transfer in general ambient conditions, Int. J. Heat Mass Transfer, Vol. 194, pp. 123102.

(3) A. C. Santos, F. L. Sacomano Filho, A. Vié (2023), The general formulation of the energy equation and the impact of enthalpy diffusion on multi-component droplet heat and mass transfer, Int. J. Heat Mass Transfer, Vol. 210, pp. 124172.

(4) A. C. Santos, F. L. Sacomano Filho, A. Vié (2024), A reference formulation for comput-

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[*] Speaker

ing mass transfer rates of multi-component droplets undergoing general phase-change, Int. J. Heat Mass Transfer, Vol. 222, pp. 125185.

(5) F. L. Sacomano Filho, L. E. A. P. Carvalho, A. C. Santos, A. Vié, J. A van Oijen (2024), Impact of multi-component description of hydrophilic fuel droplets in propagating spray flames, Combustion and Flame, Accepted.

Numerical simulation of aluminium combustion

Jean Villard * [1]

[1] Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique – CERFACS – France

As society is moving away from hydrocarbons, there is a need for a clean way to store and transport energy over the globe. For this need, metal fuels are very attractive and excellent candidates as alternative carbon-free and renewable fuels. Due to their high energy density, availability, stability and low cost, metals and especially aluminium are able to replace hydrocarbons in many applications. In addition, metal oxides are solid and may be easily collected and recycled (1). Aluminium is already well known as a fuel, used for many years in space propulsion. However, the detailed understanding of the combustion of aluminium particles remains a challenge which requires to combine sophisticated experiments with numerical simulation. The modelling of aluminium combustion then must take into account all existing phenomena, from melting and evaporation of the metal particle to gaseous and heterogeneous oxidation and finally condensation and solidification into metal oxide particles. In this work, a complete model for burning aluminum particles has been developed and implemented in the massively parallel Navier-Stokes compressible solver AVBP in order to compute a stabilized laminar flame. The model includes the dual composition of the aluminium particle with an alumina cap, heterogenous surface reactions and condensation of the combustion products, nucleation of products into particles following Finke et al. (2). The Lagrangian tracking of these product particles is an original feature of the model, with regards to the literature where an Eulerian formulation is mostly reported. It offers the possibility to give more details about the formed metal oxide particles, in particular their size. This model was used to compute. Results and analysis of the 2D stabilized aluminum laminar flame obtained with this model confirm experimental observations and give detailed explanation of the various mechanisms at play.

(1) J.M. Bergthorson, S. Goroshin, M.J. Soo, P. Julien, J. Palecka, D.L. Frost, and D.J.

Jarvis. Direct combustion of recyclable metal fuels for zero-carbon heat and power.

Applied Energy, 160:368–382, December 2015

(2) Jannis Finke and Fabian Sewerin. Combining a population balance approach with detailed

chemistry to model the condensation of oxide smoke during aluminum combustion in
spatially homogeneous reactors. Combustion and Flame, 248:112510, February 2023.

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*Speaker

PLASMA-ASSISTED COMBUSTION FOR ENERGY INTENSE INDUSTRY

Nerijus Striūgas* [1], Raminta Skvorčinskienė [1], Andrius Tamošiūnas [2], Rolandas Paulauskas † [1]

[1] Laboratory of Combustion Processes, Lithuanian Energy Institute Breslaujos st. 3, LT-44403 Kaunas – Lithuania

[2] Plasma Processing Laboratory, Lithuanian Energy Institute Breslaujos st. 3, LT-44403 Kaunas – Lithuania

The effective decarbonisation of the entire glass sector as soon as possible requires the development of new methods and technologies and the search for environmentally friendly alternatives to natural gas as a carbon-neutral alternative fuel. This paper presents the vision and latest results of the Horizon Europe project GIFFT (Sustainable Glass Industry with Fuel-Flexible Technology), whose overall objective is to develop a sustainable, hybrid and biofuel-flexible heat generation technology and process that can be integrated into industrial glass production through the efficient use of plasma combustion and gasification systems.

The GIFFT process provides high flexibility in fuel use and more dynamic operation in response to changes in energy and fuel markets. By combining available surplus electricity with alternative fuels such as hydrogen and biomass-derived syngas in a plasma combustion mode, up to half of the heat can be recovered from the electricity in the form of flame. This significantly extends the possibilities for achieving higher electrification of the process and, thus, lower CO2 emissions. Preliminary results of combustion tests will be made available to demonstrate the validity of the theoretical assessment. This work evaluates the effect on the flame geometry by varying the fuel inlet parameters and the plasma-forming gases. In the present case, hydrogen is taken as an alternative gas for substituting natural gas. The oxidiser is pure oxygen. The flame geometry formed by the plasma-assisted burner is compared with the original methane-oxygen and hydrogen-oxygen combustion cases.

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*Corresponding author: Nerijus.Striugas@lei.lt

†Speaker

Pyrolysis and combustion experiments on a wood pellet under low or high heating ramps and associated gaseous emissions

Alain Brillard *† [1], Guillaume Gerandi [2], Valerie Tschamber [2]

[1] Laboratoire Gestion des Risques et Environnement, Université de Haute Alsace – Université de Haute Alsace - Mulhouse : EA2334 – France
[2] Laboratoire Gestion des Risques et Environnement, Université de Haute Alsace – Université de Haute Alsace - Mulhouse : EA2334 – France

Wood pellets are commonly used for heat and energy production in domestic or industrial boilers. When they fall into the combustion zone, they first go through a pyrolysis stage before the combustion one. They are submitted to high temperature ramps. The overall combustion process leads to gaseous and particulate emissions that may be harmful to residents living close to the exhaust. For the present study, pyrolysis and combustion experiments were performed on a single wood pellet in a drop tube furnace. A temperature ramp of approximately 5 ◦C/min was applied and the sample mass was continuously recorded. The mass and mass rate curves were compared to that obtained for pellet sawdust in a thermobalance under the same temperature ramp. In the pyrolysis case, kinetic modeling was performed coupling the Extended Independent Parallel Reaction model and a thermal model to take into account the thermal diffusional limits inside the pellet. In the combustion case, the pellet is being degraded in a unique stage. Pyrolysis and combustion experiments were also performed under isothermal temperatures between 400 and 900 ◦C and different oxygen concentrations. During both pyrolysis and combustion experiments, the main gaseous emissions were continuously measured. From these experiments and analyses, it is possible to determine the optimal experimental conditions that lead to minimal emissions.

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[*] Speaker

[†] Corresponding author: alain.brillard@uha.fr

Speed-up drivers for H2-enriched flames in Porous Media Burners

Enrique Flores-Montoya *† [1], Pierre-Alexandre Masset [2], Thierry Schuller [1], Laurent Selle [1]

[1] Institut de Mécanique des Fluides de Toulouse, Université de Toulouse, CNRS, 31400, Toulouse – Institut de Mécanique des Fluides de Toulouse, Université de Toulouse, CNRS – France
[2] LE2H - Commissariat à l'Energie Atomique (CEA), Bâtiment 460, CEA Saclay, Gif-sur-Yvette, 91191 – Commissariat à l'énergie atomique et aux énergies alternatives – France

The storage of excess renewable energy in the form of hydrogen is a viable path for the reduction of CO2 emissions. The subsequent use of H2 as a fuel requires addressing specific challenges such as flame stabilization and NOx mitigation. Porous Media Burners (PMBs) are a fuel-flex, low pollutants and broad power range combustion technology with a great potential to address the specificities of H2 combustion. When a flame is stabilized within the voids of a solid porous matrix, the enhanced solid conductivity recirculates heat from the burnt gases to the fresh reactants. As a result, the incoming flow is preheated and the flammability range of the mixture is extended. An experimental study on the influence of porosity and hydrogen enrichment on the stabilization of premixed CH4-Air flames in PMBs is presented. Flame stabilization is analyzed via direct flame front tracking, which is made possible by a novel experimental apparatus. The use of additive manufacturing for computer-generated topologies allows making optically-accessible PMBs featuring see-through directions. This methodology also enables topology tailoring which is here exploited to study the influence of porosity on burner's performance. Flame front tracking reveals a different stabilization trend in highly H2-enriched flames. A comparison with a theoretical model is used to remove the effect of preheating and focus on other fuel properties. This suggests a flame-speed enhancement mechanism driven by Lewis number effects in $Le < 1$ mixtures. Together with recent 3D Direct Numerical Simulations, these results provide evidence that preferential diffusion effects are key in the stabilization of flames in PMBs. These phenomena, not considered in state-of-the art 1DVolume Averaged Models, remain crucial for the design of efficient PMB using hydrogen as a fuel

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[*] Speaker

[†] Corresponding author: enrique.floresmontoya@imft.fr

Study of the effect of equivalence ratios and biofuel amounts on the formation of aromatics in biofuel-fuel mixture premixed flames

Kanika Sood * [1], Sylvie Gosselin [1], Laurent Gasnot [1], Luc-Sy Tran† [1]

[1] Univ Lille, CNRS, UMR 8522 – PC2A – Physicochimie des Processus de Combustion et de l'Atmosphère, F-59000 Lille, France – Univ Lille, CNRS, UMR 8522 – PC2A – Physicochimie des Processus de Combustion et de l'Atmosphère, F-59000 Lille, France – France

Transport fuels are now subjected to blending mandates with biofuels and other biomass-derived fuels to facilitate the transition towards a sustainable transportation sector by curbing carbon emissions while maintaining most of the current vehicle fleet (1). One of the main components of biomass i.e., lignin, earlier considered as a waste product in the pulp and paper industry, was recently found to be a source of variety of valuable chemicals and fuels (i.e., "lignin-based biofuels") (2). Despite the potential presented by these biofuels, their combustion processes are likely to modify the formation of aromatic compounds (oxygenated and non-oxygenated), which may further impact the properties of the formed soot particles. In order to achieve safe integration of these biofuels into our energy system, it is necessary to quantitatively assess the impact of the change in biofuel amount and equivalence ratio on the formation of these aromatics in flame conditions.

This study reports the quantitative results on the evolution of the mole fractions of aromatics in the form of a detailed parametric study. Five laminar premixed flames of anisole (a surrogate for lignin-based biofuels) and hydrocarbon fuel blends stabilized at atmospheric pressure were investigated using Gas Chromatography (GC) setups. A custom-built GC equipped with a pre-concentration device enabled to trap sufficient material to quantify Polycyclic Aromatic Hydrocarbons (PAHs and Oxy-PAHs) even at ppb levels. Nearly 80 intermediate species were overall quantified in this work. Out of these five flames, two different series of measurements were studied. The first set of series consisted of three flames, namely F1 (0% anisole, =1.82), F2 (10% anisole, =1.82), and F3 (15% anisole, =1.82) where the equivalence ratio was fixed to a constant value of 1.82 while the amount of anisole increased, which allowed to investigate the influence of added anisole amounts. To demonstrate the effect of the change in the equivalence ratio, three flames comprising the second set of series were studied, namely F4 (10% anisole, =1.70), F2 (10% anisole, =1.82), and F5 (10% anisole, =1.90), where the equivalence ratio increased, meanwhile the percentage of anisole in the total fuel mixture for the three flames was constant (10%). Figure 1 reflects how the quantitative impact on the different aromatic species is sensitive to the equivalence ratio to different extents. On the other hand, increasing the anisole amount elevated the production of nearly all aromatics to a similar extent. These results are thoroughly discussed in the present study.

References:

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[*] Speaker

[†] Corresponding author: luc-sy.tran@univ-lille.fr

(1) Kohse-Höinghaus K, Oßwald P, Cool TA, Kasper T, Hansen N, Qi F, et al. Biofuel combustion chemistry: from ethanol to biodiesel. Angew Chem Int Ed 2010;49:3572–97. https://doi.org/10.1002/anie.2
(2) Ma J, Shi S, Jia X, Xia F, Ma H, Gao J, et al. Advances in catalytic conversion of lignocellulose to chemicals and liquid fuels. J Energy Chem 2019;36:74–86. https://doi.org/10.1016/j.jechem.2019.04.026.

Study on spectral characteristics from plasma-assisted flames of ammonia-biogas mixtures with different NH3 content

Ernest Bykov * [1], Rolandas Paulauskas [1], Adolfas Jančauskas [1], Ignas Ambrazevičius [1]

[1] Laboratory of Combustion Processes, Lithuanian Energy Institute, Breslaujos st.3, Kaunas, LT-44403 – Lithuania

The shift towards a carbon-free energy landscape by 2050 is increasingly necessary due to dwindling fossil fuel resources and stringent CO2 emissions regulations amidst a global rise in energy demand. Alternative fuels like hydrogen, biogas, and ammonia emerge as promising candidates in the use of low/zero carbon fuels. However, ammonia combustion due to low flame speed and high nitrogen content is complicated and requires techniques to improve combustion stability and efficiency. For these reasons, this work focus on plasma-assisted combustion of ammonia-biogas mixtures and spectral characteristics from the flames using UV-VIS and NIR spectrometry.

The experiments were performed in a premix burner coupled with a gliding arc plasma application at fuel equivalence ratios ϕ = 0.83, 0.71 and 0.625, respectively. The mixtures were prepared in the mixing chamber by mixing biogas (CH4-CO2/60-40vol%) with NH3 (20, 40, 60 and 80 vol%). The thermal power of the burner was kept constant (1.32 kW) for all the cases. Non-thermal plasma was generated with a Redline Technology G2000 generator with a constant driving frequency of 120 kHz and with three applied voltages: 4.6, 6.6 and 8.33 kV, respectively. Time-resolved OH*, C2*, CH* and NH2* chemiluminescence data have been captured alongside the measurements done with UV-VIS (200-1000 nm) and MIR (2000-5500 nm) emission spectroscopy.

Examining the data obtained from MIR, it was determined that plasma started influencing the combustion process more intensively, forcing it to generate more significant amounts of three-atomic gases from the mixture that contained 30% NH3. Potentially, higher activity in H2O and CO2 generation (maximum peaks were observed at 2856 nm, where mixed water vapour/CO2 peak is placed) could indicate plasma positive influence on the combustion process due to complete processing and oxidation of fuel. For mixtures that contained 10 and 20% ammonia, the plasma assistance didn't show a noticeable effect. Biogas-ammonia mixtures containing 30,40,50,60,70 and 80% of NH3, respectively, showed the biggest impact when 8.33 kV voltage was applied with an increase in the emission intensities at 2856 nm by 9, 18, 9, 10, 12 and 7% compared to the regime without plasma assistance for Φ=0.83. The significant effect by the plasma assistance was observed with the mixture containing 40% of NH3 at ϕ =0.83. It led to increased intensity of H2O/CO2 by 3.41, 9.57 and 18.15%, respectively, at 4.6, 6.6 and 8.33 kV, respectively. While switching to leaner conditions, like ϕ = 0.71 or ϕ =0.625, the effect was not intense due to decreased flame temperature. MIR emissions on the same wavelength for ϕ =0.625 were more negligible, compared to ϕ =0.83, reaching up to 58.4% of the emission intensity under the same voltage and mixture when compared to fuel richer conditions.

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*Speaker

The UV spectroscopy showed the same trend in general. OH*, NH, CN, CH, C2, NH2 and H2O radicals were detected respectively at the wavelength of 308, 335, 357, 384, 430, 523, 590 and 928 nm. The biggest influence of the plasma application on each ϕ and voltage was observed for OH* and NH2* radicals, respectively. According to the obtained values, mixtures that contained 30 and 40% of NH3 showed the most significant reaction on plasma assistance. OH radical, in this case, increased by 25-65% for ϕ =0.83 and by 19-54% for ϕ =0.71 compared to the regime without assistance. NH2* increased by 46-82% for ϕ =0.83 and by 31-75% for ϕ =0.71 compared to the regime without assistance. Such a reaction of OH* and NH2* radicals could be the marker of the combustion intensification. The highest influence of the plasma, as well as for MIR spectroscopy, was observed at 8.33 kV. Investigation of the mixtures of the CH4 in the CO2 stream with NH3 that is combusting under plasma assistance showed promising results due to the prolonged blow-off limit of the mixtures (mixtures without plasma assistance at the Φ=0.625 were not able to achieve self-sustaining combustion, extinguishing after a couple of seconds). There is a relatively considerable (up to 70%) intensification in the radical emissions, as well as an increase in three-atomic gas generation, which could possibly indicate the enhanced combustion characteristics after the plasma process. It was determined that spectral data of biogas-ammonia mixtures that contained 30 and 40% of NH3 under plasma-assistance resulted in the closest spectral data of natural gas which in turn shows such mixture and technique suitability in industrial applications.

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The evolution of 3D surfaces and properties of turbulent spherical flames of methane and hydrogen mixtures

Simone Hochgreb * [1], Yutao Zheng [1], Shaik Pervez Ahmed [2]

[1] University of Cambridge – United Kingdom
[2] Rolls Royce PLC – United Kingdom

We analyse a recent set of experiments on turbulent premixed spherically expanding flames (SEFs) of methane and hydrogen mixtures using fast 3D flame interface scanning measurements using Mie scatter (1). The flame reconstruction allows for the determination of the volume burned, flame surface location and volume growth rate of mixtures of lean methane and hydrogen at different pressures and temperatures.

In this presentation, we give an overview of the methodology and the following results as a function of time or radius: (a) 3D flame volume growth rate, (b) flame area, (c) flame surface density, (d) flame brush thickness in 3D and 2D, (e) flame curvature distribution compared to 2D distributions.

We compare the growth rate of the 3D and 2D extrapolated flame volumes to find good agreement between the time evolution of the measured 3D volumetric radius and the equivalent 2D radius based on the half-way point of progress of reaction, . The 3D flame brush thickness was found to grow linearly with the volumetric radius, with a slope weakly dependent on the turbulence level, with values between 0.5 and 2.0. The flame area was determined to be dependent on the volumetric radius as a power law, with an exponent between 2.3 and 2.9, also weakly dependent on turbulence levels or mixture type.

For the first time, 3D flame surface densities and principal curvatures are determined for the flames. 3D and 2D flame surface densities were found to decrease with flame radius with a power law of exponent of order unity; 2D flame surface significantly overpredicted the true 3D values. We observe that the values for hydrogen were significantly higher than those for methane. This is expected from the higher propensity to instabilities for the lean hydrogen mixtures, which generates additional flame surface area.

3D principal curvatures were for the first time estimated from eigenvalues of the second fundamental forms of the reconstructed surfaces, allowing the determination of the statistics of mean and Gaussian curvatures as a function of time and thus flame mean radius. The mean 3D flame curvature was found to be inversely proportional to flame radius, and relatively insensitive to turbulence intensity, even in the case of larger, more planar flames. Mean 3D curvatures across the flame brush were determined to be positive (convex) towards the reactant mixture at the leading edge, and negative (concave) towards the trailing edge, as predicted from DNS measurements. The mean and probability distributions of 3D curvatures were found to be significantly different than 2D curvatures extracted from the central planes, with the 3D measurements showing much narrower distributions and lower mean values. Differences between mean 3D and 2D

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measurements were different by an order of magnitude in the case of hydrogen flames, possibly owing to the onset of thermodiffusive instabilities which affect the local fine structure of the flame.

- Ahmed, B. Thorne, M. Lawes, S. Hochgreb, G. V. Nivarti, R. S. Cant, Three dimensional measurements of surface areas and burning velocities of turbulent spherical flames, Combust. Flame 233 (2021) 111586.

Thermal Radiation Acceleration Effects in premixed Steam-Diluted Hydrogen Flames

Julie Ben Zenou * [1], Ronan Vicquelin [1]

[1] Laboratoire d'Énergétique Moléculaire et Macroscopique, Combustion – CentraleSupélec, Université Paris-Saclay, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UPR288 – France

Hydrogen combustion is considered in the medium term to neutralize the carbon emissions of several industrial processes and means of transport. Dilution of hydrogen flames with steam is one of many strategies to enhance flame stability and mitigate nitrogen oxide emissions. In general, combustion simulations of free flame properties do not consider thermal radiation. However, the significance of thermal radiation in these diluted flames, due to the presence of participating species that not only emit but also reabsorb radiation in both the burnt and fresh gases, calls for further exploration.

This research focuses on the intricate coupling of thermal radiation with combustion in premixed H2-Air-Steam flames, highlighting the impact of thermal radiation on laminar flame speed as well as on flame structure and dynamics. 1D laminar flame calculations are performed by coupling a reactive fluid solver with a semi-analytical thermal radiation code. Both a grey gas approximation for preliminary understanding and an accurate CK narrow-band model for realistic simulations that account for spectral-dependent gas properties are considered.

Three main effects of thermal radiation are found: a decrease in burnt gas temperature due to emission, a preheating of the fresh gases before the flame front caused by steam reabsorption, and an increase in laminar flame speed. This increase is quantified for a wide range of conditions via an in-depth parametric study involving variations in domain length, equivalence ratio, dilution level, and pressure. The observed flame acceleration is significant for most conditions, particularly for lean and very lean flames, which can be up to 500% faster if thermal radiation is considered. Even for more practical flames with adiabatic laminar flame speeds around 20 cm/s, the effect of radiation can exceed 50%. The impact of different conditions (domain length, pressure, dilution level, and equivalence ratio) on this quantitative effect of radiation on flame speed is thoroughly understood and explained.

Furthermore, dimensionless coupling numbers derived from characteristic time ratios for convection, chemistry, and radiation are introduced for each condition studied. These metrics facilitate the classification of radiation-combustion coupling into three distinct regimes: near-adiabatic, where thermal radiation's effects are minor; weakly coupled, where radiation affects the fresh and burnt gases but does not interact within the flame front; and strongly coupled, where radiation competes with chemical reactions within the flame front. More than just a gradual, quantitative change in the effects of radiation, these regimes denote a fundamental change in the physical nature of the coupling. This classification enhances the understanding of radiation-combustion interactions, providing a framework for the rational inclusion of thermal radiation effects in combustion models. The study also introduces an iterative two-layer model to efficiently estimate the impact of thermal radiation on flames, which shows high accuracy except in the strongly coupled regime. Finally, it introduces a predictive model that quickly determines a

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flame's coupling regime using only an adiabatic simulation, helping to decide whether to neglect, approximate, or fully integrate radiation in simulations of premixed diluted flames.

Turbulent Partially Cracked Ammonia/air Premixed Spherical Flames

Seif Zitouni *† [1], Pierre Bréquigny [1], Christine Rousselle [1]

[1] Laboratoire pluridisciplinaire de recherche en ingénierie des systèmes, mécanique et énergétique – Université d'Orléans : EA4229, Institut National des Sciences Appliquées - Centre Val de Loire : EA4229, Université d'Orléans, Institut National des Sciences Appliquées - Centre Val de Loire – France

The combustion of ammonia requires, for most energy conversion systems, a combustion promoter such as hydrogen to guarantee the start-up, stability and combustion efficiency. Partially cracked ammonia (PCA) can provide sufficient hydrogen concentrations to enhance the burning velocity in comparison with pure ammonia. However, little work exists on the use of PCA blends operating under relevant turbulent conditions. To that end the outwardly propagating spherical flame configuration was employed to determine the laminar and turbulent flame propagation characteristics of PCA (NH3/(H2+N2)) and corresponding binary (NH3/H2) mixtures across various turbulent combustion regimes. First, PCA and ammonia-hydrogen blends exhibit similar flame propagation rates under various turbulent intensities, even for laminar case. The highest turbulent burning velocity was observed at leanest conditions, as opposed to laminar flames which exhibited highest flame speed at conditions above stoichiometry. Under rich conditions, no substantial flame enhancement due to turbulence was measured irrespective of the hydrogen content. This lack of flame enhancement under turbulent conditions is attributed to the effect of preferential diffusion with good agreement observed with trends in measured Markstein numbers. The normalized turbulent flame speed is dominated by the enhanced molecular diffusivity afforded by the presence of hydrogen up to 15% enrichment, prior to decreasing upon further hydrogen addition under lean and stoichiometric conditions. This 'bending' phenomenon may be the contribution of several factors including; the transitioning between combustion regimes associated with low Damköhler numbers (Da) and flame thickening; merging of flamelets due to the presence of ammonia enhancing wrinkling; and combined changes in laminar burning velocity and preferential diffusional behavior. Furthermore, good agreement for turbulent flame speed is observed with a correlation that includes the influence of turbulent stretch (Ka) and non-equidiffusion (Le), with the agreement reducing with decreasing chemical to turbulent time scale ratios ($Da << 1$).

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[*] Speaker

[†] Corresponding author: seif-eddine.zitouni@univ-orleans.fr

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