



## Book of Abstracts



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# Session 1: Combustion of metals

Chair: Laurent Selle

Keynote: Fabien Halter

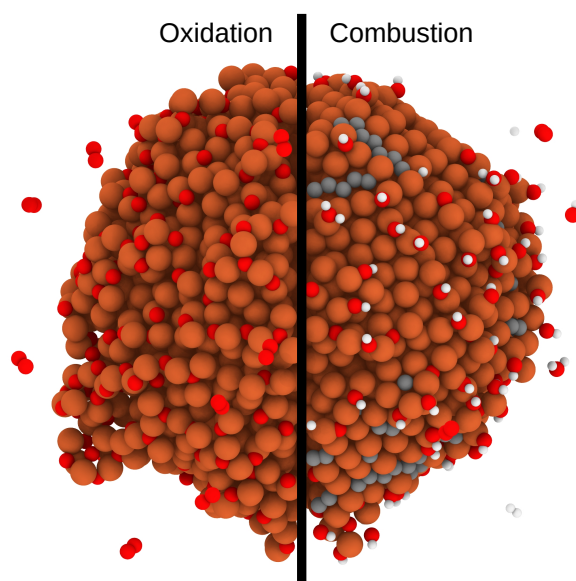
Recyclable metal fuels as future zero-carbon energy carrier

After obtaining a PhD in Mechanical Engineering in 2005, he worked on combustion phenomena in IC engines. He was appointed as full Professor at University of Orléans in 2014, where he developed canonical set-ups to experimentally investigate gaseous and multiphase combustion processes. He co-authored more than 100 papers and advised more than 20 PhD students. He is a member of the Editorial Board of Combustion and Flame and has served as colloquium co-chair for the two previous International Symposium on Combustion. He is currently the director of a Research Federation involving several laboratories in Orléans, with focus on energy-related research. He has led several national and international projects in the field of energy. He has co-organized several international workshops on premixed laminar flames and is actively working since several years in the research of new energy carriers, such as metal fuels.

# Reactive molecular dynamics investigation of the oxidation of iron-based nanofuel for next generation low-carbon engines

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Reactive molecular dynamics simulations are performed to investigate the use of iron nanoparticles as fuel substitute or additive in heavy hydrocarbon fuels, in order to achieve low- or zero-carbon emissions in next generation combustion technologies. Iron nanoparticles have been selected as energetic materials since they combine many advantageous characteristics, such as low production cost, very low toxicity and high burning rates. The effects of externally applied electrostatic fields on the oxidation and combustion processes are also investigated as relevant for new thermal-electrical hybrid engines. Both constant temperature and constant energy simulations are performed in order to match the conditions of a typical combustor, and study the ignition and transient behaviour of iron nanoparticles. This study suggests that iron nanoparticles can be used as fuel substitute or additive to reduce carbon emissions. In addition, the interaction of electrostatic fields with nanomaterials can offer new possibilities for the control of the reaction process as well as for the synthesis of tailored nanoparticles.

Simulations of nanoparticle oxidation consist of an iron nanoparticle surrounded by oxygen molecules at different temperature and pressure conditions. The burning rate of the nanoparticle increases with higher temperatures and densities, which can lead to significant energy release. As the oxidation layer is formed on the surface of the nanoparticle, further oxidation is being hindered. Therefore, the oxidation rate is governed by the inward diffusion of oxygen atoms towards the core of the nanoparticle. Results under externally applied electric fields show that the oxidation rate of iron nanoparticles is not significantly affected in the initial stages. However,

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when strong electric fields are applied, an increase in the burning rate can be noted after the first nanosecond. Analysis of the chemical composition of the nanoparticle’s surface suggests that the shell composition is affected by the external Coulomb force. The absorbed oxygen atoms get negatively charged and diffuse along the surface of the nanoparticle to counteract the externally applied electric field. This species rearrangement leads to an anisotropic shell thickness with varying chemical composition. As a result, oxygen atoms gather on the nanoparticle’s hemisphere with normal opposite to the electric field lines, leading to a rapid melt. The nanoparticle’s melt can even lead to detachment of iron molecules from this surface region. On the contrary, there is a shortage of oxygen atoms on the nanoparticle’s hemisphere with normal parallel to the electric field lines. This shortage permits further oxidation. Such oxidation layer variations increase the burning rate of iron nanoparticles when an electric field is applied. Simulations with an iron nanoparticle surrounded by oxygen and n-dodecane molecules are also performed. N-dodecane was selected as a single-component surrogate for common aviation fuels, such as the Jet A-1 and JP-8. Results suggest that iron nanoparticle additives significantly accelerate the fuel and oxidizer consumption. The decomposition of n-dodecane is initiated at the nanoparticle’s surface by hydrogen abstraction and a subsequent absorption of the hydrogen and carbon atoms. This dehydrogenation reaction path occurs faster than the common pyrolysis and oxidation paths of n-dodecane. Hydrogen and oxygen compound products are formed in the nanoparticle’s shell and are released back into the gas phase, demonstrating a catalytic behaviour of the nanoparticle. It is noteworthy that no carbon species are emitted back in the gas phase, but remain trapped on the surface. Therefore, iron nanoparticles can be used as additives in conventional fuels to achieve faster heat release and lower carbon gas emissions. Additionally, the application of an external electrostatic field further increases the n-dodecane consumption rate. A rise in the number of product species was also observed due to the overall accelerated kinetics of the system. Analysis of the system’s kinetic energy suggests that the increased reactivity under an external electric field occurs due to an increase in the translational energy of the molecules. The absorbed species diffuse along the surface of the nanoparticle to counteract the externally applied electric field.

# A Lagrangian framework for the numerical simulation of aluminum particle combustion

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Aluminum is an energy carrier with a large energy density per mass and volume, which is used in several applications such as rocket boosters and explosives. Its combustion does not produce carbon dioxide so it has some potential as a low-carbon energy carrier. The modelling of aluminum combustion involves many physical phenomena that make its integration in CFD solvers quite challenging. First, the fuel is initially in solid phase, usually in the form of a powder, which requires a two-phase flow framework. Then, the main reaction product, alumina  $\text{Al}_2\text{O}_3$ , is also in a condensed phase, which raises the issue of nucleation and condensation. Last but not least, there is a large variety of combustion regimes (e.g. group vs isolated, heterogeneous vs homogeneous), depending on the oxidiser, the particles' diameter and ambient conditions. The general objective of this project, which is a collaboration between CEA and IMFT, is to validate a simulation framework for aluminum flames in the compressible solver AVBP. The condensed phases are treated as Lagrangian particles and in order to bypass the problem of nucleation, the flow is seeded with alumina particles of negligible mass to serve as nuclei for the condensation of combustion products. The combustion is modelled using a kinetic scheme, developed by E. Washburn *et al.* [1], which has been restricted to oxygen. The stiffness of the numerical solution is handled via a Godunov-type numerical scheme, called HLLC.

The overall framework is validated on 0D, 1D and 2D cases of increasing complexity. The reference experimental validation is a bunsen-type flame studied by R. Lomba [2], which is computed in 2D. The computational domain contains approximately 300 000 triangular cells, with a spatial resolution of  $60\mu\text{m}$  in the flame region. The injection of particles and air is at 300K, in stoichiometric proportions. Specific attention is devoted to the ignition of this flame, which turns out to be a challenge, both experimentally and numerically. The associated initialisation procedure is described in details. Finally, flame- front speed and thickness are successfully compared to the experiment, giving a global validation of the simulation framework.

E. B. Washburn, J. N. Trivedi, L. Catoire, and M. W. Beckstead. The simulation of the combustion of micrometer-sized aluminum particles with steam. *Combustion Science and Technology*, 180(8):1502–1517, 2008.

R. Lomba, P. Laboureur, C. Dumand, C. Chauveau, and F. Halter. Determination of aluminum-air burning velocities using PIV and Laser sheet tomography. *Proceedings of the Combustion Institute*, 37(3):3143–3150, 2019.

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# Effects of condensed-phase oxidation kinetics on the ignition characteristics of fine iron particles

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Iron is an excellent fuel for long-term storage and long-distance transport of renewable energy owing to its carbon-free nature, high energy density, and potential for non-volatile combustion in air. To develop real-world technologies of iron combustion, a better understanding of the fundamentals underlying the combustion process of fine (i.e., micron- to hundreds-of-micron-sized) iron particles is required. Ignition of iron particles in an oxidizing environment marks the onset of a self-sustained combustion. The objective of this study is to examine the theoretical predictions of iron particle ignition characteristics using two different kinetic models for the rate of condensed-phase iron oxidation that have been in the literature: (1) A first-order O<sub>2</sub>-concentration-dependent linear rate law (i.e., independent of oxide-layer thickness) proposed by Hazenberg and van Oijen [1]; (2) A parabolic rate law that is inversely dependent of oxide-layer thickness and independent of gaseous O<sub>2</sub> concentration, which was obtained from metallurgical studies and applied by Mi *et al.* [2] to model the ignition process of iron particles. Calculations using these kinetic models will be performed to estimate the critical gas and particle temperatures required to trigger a thermal runaway (namely, the ignition temperature) and ignition delay time of isolated particles, suspensions of particles under isobaric and isochoric conditions, and particles in propagating flames. The outcome of this study will inform us whether condensed-phase kinetics play a significant role in modeling flames, constant-volume explosion, and detonations of iron-particles suspension.

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Hazenberg, T. and van Oijen, J.A., 2021. Structures and burning velocities of flames in iron aerosols. *Proceedings of the Combustion Institute*, 38(3), pp.4383-4390.

Mi, X.C., Fujinawa, A., and Bergthorson, J.M., 2022. A quantitative analysis of the ignition characteristics of fine iron particles. *Combustion and Flame*, 240, pp. 112011.

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# Towards full understanding of single iron particle combustion

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Metal fuels, powders of micron-sized metal particles are gaining attention as promising energy carriers [1]. Most of them have high energy densities, are inherently carbon free, recyclable, compact and some of them are also cheap and widely available. Iron is considered as a promising metal fuel since it possesses all aforementioned advantages and is expected to burn heterogeneously, without the formation of nano-sized iron-oxide products [1]. In turn, these particles can be captured and reduced using solar and wind energy [1, 2], thereby enabling a carbon-free energy cycle.

Understanding the burning process of a single iron particle and knowing how much iron is evaporated during combustion is of key to use iron as a metal fuel within a circular process. In this work, 2D axial symmetric simulations of an iron particle burning in a O<sub>2</sub>-N<sub>2</sub> atmosphere are presented and discussed [3]. By resolving the full boundary layer, mass and heat transfer are accurately modelled, including Stefan flow. We only consider the conversion of Fe to FeO, since FeO is the most relevant oxide up to the maximum particle temperature [4, 5]. An evaporation model is implemented to investigate the forming of nano-sized iron-oxides products. The formation and evolution of the iron oxide nano-particles are investigated by using a sectional model.

The model is validated by comparing the time to maximum temperature and the maximum temperature of a 40 and 50  $\mu\text{m}$  particle in an O<sub>2</sub>-N<sub>2</sub> atmosphere with the laser-ignitions experiments as performed by Ning et al. [6]. It is shown that even though the particle temperature stays below the boiling temperature of Fe(l) and FeO(l), a small but not negligible amount of mass is evaporated, which limits the maximum temperature of the particles [3].

## Funding

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J. Bergthorson, "Recyclable metal fuels for clean and compact zero-carbon power," *Prog. Energy Combust.*, vol. 68, pp. 169–196, 2018.

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T. Hazenberg and J. van Oijen, "Structures and burning velocities of flames in iron aerosols," *Proc Combust. Inst.*, vol. 38, no. 3, pp. 4383–4390, 2021.

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# The utilisation of Fe<sub>2</sub>O<sub>3</sub>, CuO and SrFeO<sub>3-δ</sub> oxygen carriers in chemical looping combustion of biomass char

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Among different Bioenergy with Carbon Capture and Storage (BECCS) options, chemical looping combustion with biomass fuel stands out as an attractive technology due to the inherent separation of CO<sub>2</sub> from N<sub>2</sub>. A stream containing only CO<sub>2</sub> and H<sub>2</sub>O is produced because the oxygen to reaction is provided by a solid metal oxide particle, referred to as an ‘oxygen carrier’. This research focuses on the combustion of biomass char carried out in fluidised beds of various oxygen carriers. Particles of biomass char were combusted in a bubbling fluidised bed (i.d. 30 mm) of inert bed, SiO<sub>2</sub> (as a reference), or an active bed of oxygen carrier: (1) Fe<sub>2</sub>O<sub>3</sub> prepared from a nature ore, pyrite, (2) CuO supported on mayenite, (3) SrFeO<sub>3-δ</sub>, strontium ferrite perovskite. In the temperature range investigated in this work, copper oxide and strontium ferrite but not iron oxide thermally decompose, releasing gaseous O<sub>2</sub> (so-called ‘chemical looping oxygen uncoupling’, CLOU). Hence, to make the combustion conditions comparable with various oxygen carriers, all experiments were performed with a fixed partial pressure of O<sub>2</sub>,  $p_{O_2}$ ,  $\sim 0.015$  bar. Despite the same  $p_{O_2}$  in all experiments, the presence of the oxygen uncoupling reaction throughout the bed reduced the influence of the external mass transfer to the char particle, resulting in a significant increase in the char combustion rate. The time needed to fully burn 0.1 g of biochar particles in different beds at 1165 K followed the trend CuO < SrFeO<sub>3-δ</sub> < Fe<sub>2</sub>O<sub>3</sub>  $\approx$  silica sand. The difference in the performance of CuO and SrFeO<sub>3-δ</sub> was ascribed to the lower oxygen availability in the perovskite. Despite the observation that combustion in a bed of iron oxide particles results in a comparable burnout time to an inert bed of SiO<sub>2</sub>, iron oxide played an active role in the process, reacting with CO formed during char combustion, resulting in a nearly CO-free gas stream at the outlet. Therefore, iron oxide is a good candidate also for oxygen carrier-aided combustion (OCAC) in air, as it allows for efficient combustion of volatiles already in the bed.

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\*Speaker

# Modeling Effects of Liquid Droplets on Premixed Laminar Acetone Flames

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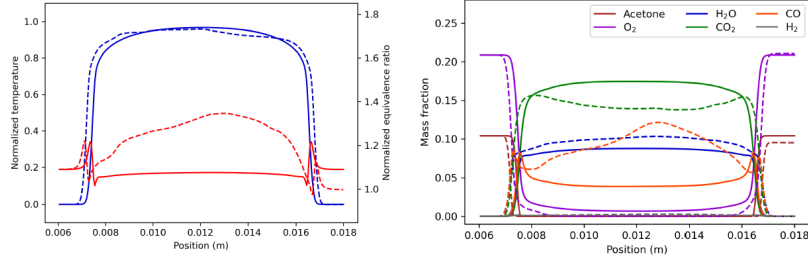


Figure 1: Temperature (blue) and phi (red) (left) and species mass fractions (right), as a function of distance from the left hand side nozzle (zero and 0.024 m are the two sides of the emerging droplet). Solid lines correspond to the symmetric baseline gas phase without droplets, dashed lines to the case with vapour and droplets emerging from the right hand stream. Conditions are:  $\phi = 1.1$ ,  $T_0 = 423$  K,  $K = 340$  s<sup>-1</sup>, liquid fraction 0.10, and monodisperse droplet size  $D_{32} = 42.6$   $\mu$ m.

We report on the effect of liquid droplets on the structure and propagation speed of laminar opposed premixed flames using acetone and air as a fuel. Acetone is one of many oxygenated compounds such as ethers and alcohols, which can be sustainably synthesized from biomass, and are therefore of interest to low carbon combustion. Conveniently, acetone has a boiling point close to ambient temperature and pressure, and it is therefore easily generated in either vapour or liquid form for purposes of the current investigation on the role of droplets in gas-phase combustion.

Spray combustion is important in the chemical conversion of liquid fuels. There are many models for spray combustion, yet there is little direct experimental verification of the interaction of fuel droplets with flames. In this study, we use the well-understood opposed premixed twin flame platform to investigate the interaction of droplets and flames, with the variation that one of the streams contains only vaporised mixture, and the other, both vapour and droplets. Previous studies have numerically simulated the role of water droplets on methane-air laminar impinging flames, as well as the effect of addition of acetone droplets to methane flames, the latter both experimentally and numerically.

Simulations were performed using the commercial platform Ansys Fluent, for a geometry consisting of axisymmetric twin 14 mm diameter nozzles separated by 24 mm, surrounded by annular gaps of 10 mm, on a mesh of 134,400 cells. The droplets are not spatially resolved internally, but interact with the flow in the form of sources or sinks of momentum, mass and energy. The inner nozzles delivered fuel/air mixtures with or without droplets, and the outer shielding flows delivered nitrogen. Top hat velocity profiles of bulk velocity of mixtures were imposed at the

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nozzle outlet into the domain, and constant pressure outflow conditions were imposed for the outflow.

Equivalence ratios of 0.8 to 1.2 were simulated for the mixture, at atmospheric pressure and temperature of 293 K. A liquid fraction of 0.10 was used, and monodisperse droplet sizes of Sauter mean diameter  $\{D\}_{32} = 42.6 \mu\text{m}$ , and 2 and 3 times the baseline value, for comparisons with experiments with polydisperse mixtures with the same Sauter mean diameter. The chemical model used by Pichon et al. has been validated against experimental flame results over a few studies, but uncertainties still remain in the rich region.

Figure 1 shows major species profiles for the show mass fractions of main species for a liquid mass fraction of 0.1, and droplet size  $D_{32} = 42.6 \mu\text{m}$ . The droplets are observed to vaporize before reaching the symmetry plane. The effects of the addition of droplets are interestingly felt across both sides of the opposed flame. The temperatures decrease on the droplet side, owing to evaporation of the droplet fuel, and the overall equivalence ratio goes from stoichiometric (because the fuel did not evaporate) to rich (after the droplets evaporate in the burned zone). This appears to affect the gas side of the flame as well, with both flames shifting upstream, indicating faster flame speeds.

The species profiles show that significantly more CO and water are produced. The increased CO mass fractions can be explained by the lower temperatures and richer mixtures arising from the droplet evaporation in the product gas, the increase in water levels remains to be explained in detail. We notice that equilibrium conditions are not reached in the burned gas, even in the gas-only case, at these strain rates.

The effects change significantly with equivalence ratio: for lean mixtures, the effect is primarily one of cooling the mixture, and the flame speeds are lowered by the presence of droplets relatively to the undisturbed gas-only levels. For richer mixtures, the effects are mixed, as there are countervailing effects of the droplets corresponding to both cooling and enrichment of the mixture.

The effects of increased droplet size appear both in a higher resistance to evaporation, and in the fact that the larger droplets actually cross the symmetry line and are subsequently dragged back into the original stream, creating an oscillatory motion of the droplets, which are eventually carried away by the bulk flow.

Based on the simulations, the paper concludes with considerations of whether and under what conditions it may be possible to create simple models for the combustion of droplet-laden flows by using the simple stretched flame model paradigm.



# Session 2: CO<sub>2</sub> Capture and re-utilization - Hydrogen 1

Chair: Corine Lacour

Keynote: Kevin Van Geem

Process intensification of CO<sub>2</sub> capture and CO<sub>2</sub> utilization

Kevin Van Geem is full professor in the Faculty of Engineering and Architecture at Ghent University (UGent). He is director of the Center of Sustainable Chemistry and director of the board of the Laboratory for Chemical Technology of Ghent University. His main research interest is thermochemical reaction engineering in general, with a focus in particular the transition from fossil to alternative resources such as biomass, CO/CO<sub>2</sub> and plastic waste. He is a former Fulbright Research Scholar of MIT and visiting professor at Stanford. He is in charge of the pilot plants for chemical recycling, oxidative coupling of methane, steam cracking, biomass pyrolysis and super dry reforming. He is the author of more than two hundred scientific publications, has 3 patents and he is managing director of his own spin-off company on modeling steam cracking. He is involved in electrification, process intensification, machine learning data mining, product formulation, drug discover, scale-up and process modeling.

# Numerical Investigation of Heavy Duty Diesel Engine powered by Syngas from Waste Gasification

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Syngas can be obtained by gasification and pyrolysis processes of different waste streams and comprised of mainly five gases (CO, H<sub>2</sub>, CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>) along with few minor components. The composition of CO,H<sub>2</sub> in Syngas can be controlled by operating conditions and composition of different feed-stocks. In the current study, the different composition of Syngas obtained by oxygen controlled gasification process has been used for operating heavy duty diesel piloted dual fuel engine and the effect on its performance and emissions have been investigated by numerical simulations. The sector based reactive numerical simulations are performed by using CONVERGE-CFD, with moving mesh modelling for compression and power stroke. The small amount of diesel fuel was injected to ignite compressed syngas-air mixture. The numerical investigation on performance and NO<sub>x</sub>, soot emissions are performed for different syngas compositions. For validation of the simulation natural gas and diesel piloted operation was used. The syngas composition obtained by oxygen controlled gasification process will be used for engine operation. The method development and parametric study in this study will provide pathway to further optimize the application oriented operations of gasification system for efficient performance and low emission.

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\*Speaker

# Numerical Validation and Investigation of Fuel-Lean Premixed Catalytic Hydrogen/Air Flame Under Laminar Condition

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Premixed combustion of fuel lean Hydrogen/air over Pt catalyst is numerically investigated in a planar channel reactor, aiming to extend the model for developing cost effective catalytic and low NOx emission hydrogen combustion system. Computations are carried out in two-dimensional reactor in which two 300 mm long walls are Pt coated and placed 7 mm apart. Steady laminar model is examined in conjunction with elementary heterogeneous and homogeneous chemical reaction schemes and validated with available established experimental results [C. Appel et. al. (2002)]. It shows that the onset of homogenous ignition is independent of inlet flow and equivalence ratio. However, a parametric study of equivalence ratio by reducing its value to hydrogen lower flammability limit is carried out to develop a stability map showing the dominant homogenous and heterogenous combustion regime. Moreover, the stability map of the onset of homogeneous ignition as a function of wall temperature in present model is studied. Finally, A comparison is made with radiation and NOx model to investigate the thermal effect and NOx emission characteristics in same configuration.

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# Experimental investigation of ignition delays in RCM for lean H<sub>2</sub>/air mixtures under ICE conditions

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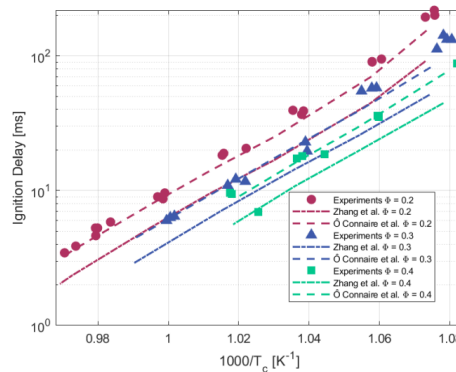


FIGURE 1 – Ignition delay time data for H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> mixtures at  $P_c = 30$  bar and varying equivalence ratio and comparison with predicted results using the Zhang et al. mechanism (2021) and Ô Conaire et al. mechanism (2004).

In order to use Hydrogen (H<sub>2</sub>) as a fuel for Internal Combustion Engines (ICEs), the study of fundamental combustion properties is necessary. Compression Ignition Engines (CIEs) require spontaneous combustion and therefore short ignition delays whereas Spark Ignited Engines (SIEs) need longer delay to avoid knock and flashback issues. Ignition delay measurements are required in order to validate kinetic mechanism, especially in unexplored conditions representative of ICE operations.

Numerous autoignition studies on H<sub>2</sub> mixtures have been conducted using Rapid Compression Machine (RCM). *Mittal et al. (2006)*, studied the autoignition of H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub>/Ar mixtures for low-to-intermediate temperatures (950 K - 1100 K) and high pressure (15 bar - 50 bar). *Das et al. (2012)* studied the autoignition of dry and moist H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> mixtures for low-to-intermediates temperature (907 K - 1048 K) and high pressure (10 bar - 70 bar). *Kéromnes et al. (2013)* studied the autoignition of H<sub>2</sub>/CO/O<sub>2</sub>/N<sub>2</sub>/Ar mixtures for low-temperatures (929 K - 1014 K) and high pressures (8 bar - 32 bar).

All these studies have shown that autoignition delay times decrease with an increase in equivalence ratio. It is noted, that all the aforementioned studies employed Argon as a diluent and

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at stoichiometric conditions. As such, in order to ensure application for ICEs, the study of autoignition delay of lean H<sub>2</sub>/Air mixtures at high pressures and low-to-intermediate temperatures is required to have NO<sub>x</sub> emission as low as possible and to anticipate knock for SIE.

Fuel ignition properties were determined experimentally employing a rapid compression machine, with detailed description of the apparatus available in *Pochet et al. (2020)* and volume compression profiles are measured from non-reactives mixtures. Equivalence ratio studied are 0.2, 0.3 and 0.4. Initial pressure (990 - 1020 bar) and initial temperature (85 - 130 °C) were chosen to reach a compression pressure  $P_c$  of 30 bar and a compression temperature  $T_c$  of 920 - 1030 K.

Experimental data was compared to numerical simulations in order to appraise chemical kinetic reaction mechanisms, through the use of CHEMKIN and employing closed-homogeneous reactor model. Volume compression profiles are computed from non-reactives test for each mixture and used for the simulations. Simulations were performed with an absolute tolerance and a relative tolerance of 10<sup>-21</sup> and 10<sup>-9</sup>, respectively, as convergence criteria and with a timestep of 10<sup>-3</sup> s. Simulations were directed with two kinetic mechanisms, from *Zhang et al. (2021)* (11 species and 32 reactions) and from *Ô Conaire et al. (2004)* (10 species and 19 reactions).

Fig.1 displays that ignition delays times decrease with increasing temperature. The trends are linear, thus no negative temperature coefficient zones are visible for these conditions. Experiments and simulations have the same trend as a function of the equivalence ratio for lean mixtures. As the equivalence ratio increases (up to  $\Phi = 0.4$ ), the ignition delays decrease. Experimental results are in good agreement with *Ô Conaire et al. (2004)* kinetic mechanism prediction. However, a difference of at least a factor two is observed between the experimental results and those from the simulations led by *Zhang et al. (2021)* kinetic mechanism. Several explanations will be investigated such as the dead volume length, uncertainties of pressure measurements or the kinetic mechanism precision for lean combustion at high pressure and low-to-intermediate temperatures. Simulations revealed, with OH peak, that when the equivalence ratio increases, mixtures become more reactive and so on, ignition delays times decrease.

Ignition delay experiments for H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> for lean regimes ( $\Phi = 0.2, 0.3$  and  $0.4$ ), for varying  $T_c$  (920 K - 1030 K) at  $P_c = 30$  bar using a RCM were conducted to investigate the impact of lean stoichiometry. The study revealed that for lean regimes, when the equivalence ratio increases, delays decrease. This decrease comes from the fact that the amount of hydrogen make the mixture more reactive. This reactivity will be studied in details. Future work includes testing to higher equivalence ratios (up to  $\Phi = 0.6$ ) as well as varying the compression pressure. Moreover, the impact of water addition of future mixtures will be studied for dilution operation in ICE.

# Impact of Hydrogen on Soot Formation in Hydrocarbon Diffusion Flames

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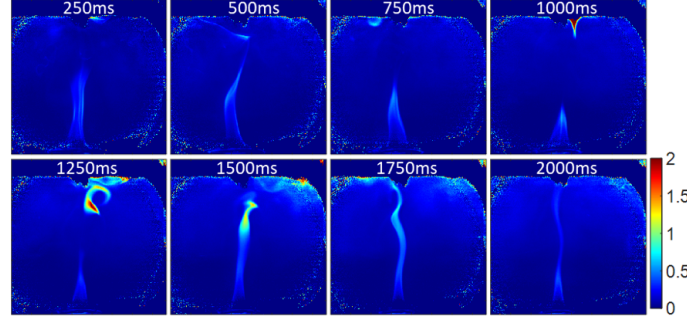


Fig. 1 Temporal development of soot optical thickness KL during combustion of iso-octane liquid fuel films within a 3-bar air environment. Times in each image represents the time after the initiation of the flame. Image size: 73.7 x 73.7 mm<sup>2</sup>.

Replacing conventional hydrocarbon fuels with zero-carbon fuels, such as hydrogen, is critical for reducing net CO<sub>2</sub> emission and tackling global climate change. In the near term, it is more likely that the zero-carbon fuels are utilized in blend with conventional hydrocarbon fuels instead of on their own. It is therefore of significant importance to investigate the pollution emissions, such as soot, in the combustion process of these fuel blends. This in-progress study aims to quantitatively characterise the impact of hydrogen on soot generation in hydrocarbon diffusion flames, such as in flames of liquid fuel film and in turbulent jet flames. The measurement technique used in this study is diffuse back-illumination extinction imaging (DBIEI), which provides line-of-sight information of spatial distribution of soot concentration in flames. Flames of liquid fuel film will be initiated on a metal fuel plate, which is enclosed by a constant volume chamber; the amount of hydrogen-in terms of its volume fraction-in the environmental gas mixture in the chamber is varied to investigate its influence on the soot formation in fuel film combustion. This, to some extent, mimics the combustion of fuel films in a direct injection engine, which intakes lean hydrogen/air mixtures. Fig. 1 presents an example for the temporal evolution of soot optical thickness KL in the combustion of iso-octane fuel films, with the ambient gas being pure air and the ambient pressure of 3 bar absolute. For turbulent jet flames, hydrogen will be blended with a gaseous hydrocarbon fuel, such as methane, and the impact of hydrogen concentration on soot generation in the flame will be examined with DBIEI.

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# Stirred reactor calculations of NOx emission from hydrogen gas turbine combustors

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Hydrogen combustion is expected to play a significant role in the decarbonisation of aviation. Nevertheless, a question arises as to whether a hydrogen-fuelled jet engine would have lower, higher or the same emissions of nitrogen oxides (NOx) as conventional technologies using kerosene. This study addresses this question from a preliminary design standpoint by relying on thermodynamic cycle, kinetic and mixing computations that consider gas turbine operability and NOx emission propensity at a range of operating conditions. Results using the well-stirred reactor model, assuming a premixed air-fuel mixture at the combustor inlet, show that lower NOx can be expected while maintaining cycle efficiencies similar to kerosene systems. Further, the analysis indicates that the thermodynamic cycle cannot be overlooked, especially when selecting a hydrogen combustor's equivalence ratio and residence time. A higher NOx estimate may be obtained by selecting only specific operability criteria to match a kerosene system, such as adiabatic flame temperature or laminar burning velocity; hence, much care is needed when comparing fuels. Attention is also needed in the combustion system design to achieve quick mixing so as to burn only at the required equivalence ratio that ensures low NOx emission. The effects of incomplete mixing are here evaluated using the Imperfectly Stirred Reactor (ISR) model with various unmixedness levels at the combustor inlet, core and outlet, based on theoretical estimates. The results indicate that simple approaches combining mixing and chemical reaction effects, such as the ISR approach, can assist the preliminary design of future non- or partially-premixed hydrogen combustion systems by identifying suitable mixing scenarios without solely relying on computationally expensive computational fluid dynamics simulations.

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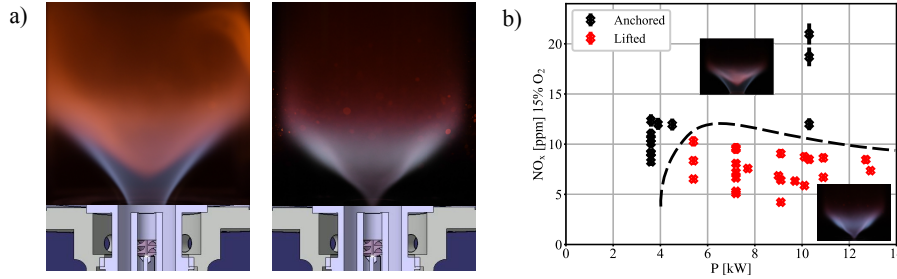
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# Interplay between NOx emissions and flame stabilization in a dual swirl H2/air burner

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Ensuring low NOx emissions and preventing flashback is challenging in combustors powered by hydrogen. A burner called HYLON, for HYdrogen LOw NOx burner, has been developed at IMFT in which hydrogen and air are injected separately in a coaxial injector to avoid flashback. Hydrogen is injected through a central lance equipped with an axial swirl vane and featuring a small recess relative to the annular channel outlet through which swirled air is flowing. This H2/air injector allows two different flame stabilization modes. In the first one, the flame is anchored on the lip of the central hydrogen lance. In this regime illustrated on the left in Fig. 1(a), combustion takes place along a diffusion reaction layer from the hydrogen injector rim to the top of the flame. A second diffusion reaction layer also develops at the top, in the center of the flow, where hydrogen burns with vitiated air. In the second regime, the flame is stabilized aerodynamically a few millimeters downstream the central hydrogen lance as shown on the right in Fig. 1(a). In this case, the swirled hydrogen and air streams mix and combustion takes place in a partially premixed mode. Figure 1(b) shows that NOx emissions are strongly impacted by the stabilization mode, which itself depends on the level of swirl conferred to the hydrogen central stream. It is found that swirling the hydrogen flow yields aerodynamically lifted flames with low NOx emissions. NOx emissions of lifted flames also reduce for increasing hydrogen injection velocities indicating a better mixing between the hydrogen and air streams before combustion. Effects of the central hydrogen swirl and hydrogen injector recess on flame stabilization are examined. It is found that swirling the hydrogen flow is necessary, but is not sufficient to lift the flame from the hydrogen central lance. A small recess to the central injector widely extends the operability range of the burner with aerodynamically stabilized flames. It is also shown that flame stabilization is barely influenced by the air injection velocity, while the hydrogen injection velocity is the main parameter controlling flame stabilization.

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<sup>\*</sup>Speaker



# Large eddy simulation of swirling technically-premixed H<sub>2</sub>-Air flame with accurate NO<sub>x</sub> prediction

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The effects of climate change are leading to further restrictions applied by the government to contrast the excessive greenhouse gas production. Simultaneously, the persistent installation of renewable energy source plants, is demanding more efficient and reliable ways to store the excess energy.

In this context, Hydrogen has been pointed out as the main player for the energy transition towards zero emissions future. Indeed, it can be used as chemical storage through water electrolysis and directly used in fuel cells or directly burnt, e.g., in gas turbines to produce electricity. Even if the combustion of hydrogen does not produce CO<sub>2</sub>, thus reducing positively the greenhouse gas production, it may lead to large NO<sub>x</sub> emissions. Furthermore, its peculiar physical-chemical characteristics, such as high adiabatic temperature, high laminar flame speed, high reactivity, can trigger dangerous phenomena in real combustion applications (flashback, combustion instabilities, damaging heat transfer).

At the moment, only few works are present in the literature investigating lab scaled swirled stabilized burners fueled with neat H<sub>2</sub> by means of CFD. Nonetheless, none of them present a comprehensive study of the mixture formation and subsequently NO<sub>x</sub> dynamic formation. Being a light molecule, hydrogen introduces different complexities in the simultaneously solution of kinetics, convection and diffusion problems.

Hence, herein a numerical campaign on the 100% H<sub>2</sub> technically premixed swirled burner, designed at the Berlin Institute of Technology, has been carried out to study the H<sub>2</sub> flame structure with an accurate estimation of NO<sub>x</sub> production.

The swirled stabilized burner has been designed with peculiar features to efficiently burn hydrogen by keeping low the NO<sub>x</sub> pollution (< 10 ppm at 15% O<sub>2</sub>) with the aim to contrast flashback phenomena. It is characterized by high fuel injection momentum and an axial air jet.

To perform effective Large Eddy Simulations (LES) with the high fidelity AVBP solver, an analytical reduced kinetic mechanism for H<sub>2</sub>-air with NO<sub>x</sub> has been derived using CERFACS in-house code ARCANE. It consists of 15 transported species and 47 reactions for affordable LES calculations. Moreover, its laminar flame speed has been assessed on a wide range of temperature and pressure. NO<sub>x</sub> production validated against measurements on experimental diffusion flames.

Firstly, LES simulations of the cold case have been run to perform a grid sensitivity analysis. The core of burner is represented by the air flow splitting system, which has been studied

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<sup>\*</sup>Speaker

in detail. The axial air injection demonstrated to be slightly below the transonic regime and thus affecting the overall mixture formation. The latter has been analyzed by looking at the flow dynamics interaction between swirler, fuel injection and axial air jet.

To simulate the combustion process, the dynamic thickening flame model (DTFLES) has been used. One stable flame operating condition with global equivalence ratio equal to 0.6 has been investigated and the results compared with experimental PIV, OH-PLIF and OH\* data (Fig.1a). To accurately study the flame structure, a static mesh refinement (SMR) with Tekigo has been applied on an initial solution in the volume with the high flame location probability.

Both adiabatic and non-adiabatic flames have been studied by including the conjugate heat transfer (CHT) technique. For this purpose, the solid part has been discretized and the heat conduction problem has been solved with AVTP a thermal solver coupled with AVBP. A deep insight on the heat release zone pointed out the capability of the simulation in capturing preferential diffusion effect of light molecules ( $H_2$  and  $H$ ), even if species diffusion coefficients are affected by the thickening model (Fig.1b).

Finally, an analysis of the rich/lean spots dynamic formation and its correlation to the NO<sub>x</sub> production has been presented. A relation between lean/rich spots and the main NO<sub>x</sub> paths, namely the intermediate N<sub>2</sub>O and the diazenyl radical NNH paths, has been demonstrated downstream of the reaction zone. Finally, a global evaluation of the NO<sub>x</sub> downstream of the combustion chamber has been carried out numerically (Fig.1c).

# Session 3: Biomass Combustion

Chair: Terese Løvås

Keynote: Mirjam Röder

Assessing and maximising sustainability trade-offs of bioenergy systems

Mirjam Röder is a Reader at the Energy and Bioproducts Research Institute (EBRI) at Aston University. She leads the Systems Analysis research in EBRI and is the Topic Group leader for Systems in the UK's Supergen Bioenergy Hub.

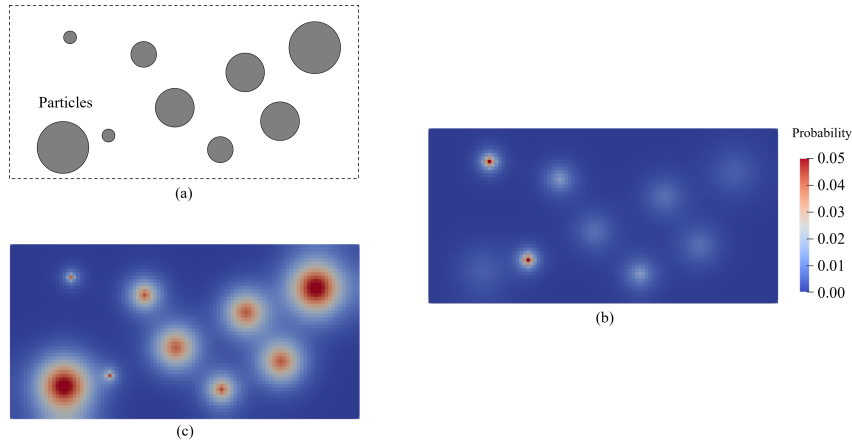
Her research interests focus on the role of bioenergy and bioproducts in the transition to a low carbon future. Her research are the sustainability of bioenergy, bioenergy in the context of global challenges and development, the role of bioenergy systems in climate change mitigation, including bioenergy with carbon capture and storage/utilisation (BECCS/U) and governance frameworks.

# Diffusion-based implementation of the kernel smoothing method used in the Eulerian-Lagrangian simulations of the biomass combustion

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<sup>2</sup> RISE Fire Research – Norway



The Eulerian-Lagrangian approaches can provide a comprehensive prediction of a transient combustion process with the tracking of individual fuel particles. To couple the continuum models for the gas phase and the discrete models for the solid phase, the key issue is to correctly transfer the information between the two framework models. In simulations of e.g. a fixed-bed combustor, the length scale of the fluid flow could be smaller than the particle size, and particular coupling schemes are required. The smoothing method with kernel functions is a widely used method to resolve such coupling problems.

In this study, a CFD/DEM (computational fluid dynamics/discrete element method) model with a new coupling scheme is developed to simulate the thermal conversion of biomass particles in a fixed-bed. In the proposed model, the Gaussian kernel is used both in filtering the fields of fluid properties and redistributing the discrete solid-phase properties and the source terms. A diffusion-based implementation is applied to calculate the discrete Gaussian kernel function with respect to the computational efficiency. As shown in Fig. 1, the particle size distribution and the particle shrinkage during the combustion process is considered in the new coupling scheme, and the bandwidth of the Gaussian kernel is dependent on the particle diameter for each particle. The new method has a good grid-independence performance, it allows the grid size to be much smaller than the particle size. The influence of the newly introduced parameter, the ratio of the bandwidth to the particle diameter, is analyzed by a detailed comparison between the simulation and a fixed-bed experiment.

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# Gaz and particle emissions of a domestic boiler fed with wood, miscanthus and straw pellet.

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Use and the study of new renewables energies is imposed by the need to find alternatives to fossil fuels. The biomass is one of the most promising alternatives. Biomass can be classified according to its origin, the woody biomasses are currently the most widely used. There are other types of biomass such as biomass of agricultural origin and energy crops. Their abundance makes them serious candidates to provide alternative source of energy. The use of alternative biomasses has not been properly exploited and it is known that this use can generate different behaviors in the combustion devices with possible impacts in terms of polluting emissions. For these reasons, there is a need to study the effect of the nature and composition of the biomass on its emissions during combustion.

In order to experimentally investigate the combustion of biomass, an experimental bench based on an instrumented domestic pellet boiler of 20kW has been set up with a control of the air and fuel inlets. Three biomasses have been used for this work, wood, miscanthus and straw. Gaseous and particulate pollutant emissions have been made in the smokes at the exhaust, for CO and NOx with a TESTO analyzer, particle mass concentration with a PPS (DEKATI), particle size distributions with a Scanning Mobility Particle Sizer (SMPS, TSI). A CPMA (Cambustion) was set up in tandem. configuration with the SMPS to evaluate the effective density of particles produced during the biomass combustion. TEM images were made from the aerosol produced by the combustion of wood and miscanthus.

Different parameters such as the feeding mode (pulsed or continuous), the air distribution within the furnace and the nature of the biomass are studied. The results obtained showed that CO emissions are strongly influenced by the feeding mode of the boiler. Particles and NOx can be less affected by this loading process. We were able to reduce the CO emissions of a conventional heater by about 40% by simply changing the feeding method. The impact of the position of air injection in the combustion chamber was also investigated. It was observed that small changes in the air distribution close to the fuel bed can have significant effects on the reduction of gaseous pollutant emissions. Also, the results obtained showed clear differences in the levels of gaseous emissions of the three types of biomasses, with wood being the lowest of the three. Finally, in terms of particulate emissions, there are clear differences in mass concentration and size distribution, MET images and effective density showed differences in the nature and shape of particles for miscanthus and wood biomasses.

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<sup>\*</sup>Speaker

# Pyrolysis kinetics of hydrochars derived from agricultural residues using thermogravimetric analysis

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Energy recovery has been shown to be a promising strategy for the management of agricultural wastes or residues. Thermochemical conversions such as pyrolysis, gasification, combustion, and hydrothermal processes can be used to generate energy from these materials. Hydrothermal carbonization (HTC) transforms wet biomass at low temperature ranging from 180°C to 250°C into a carbonaceous material named hydrochar that possesses attractive potential for energy production considered as a fuel. In the integrated valorization of hydrochars by combustion, pyrolysis, and gasification technologies, pyrolysis plays a key role in the overall process performance, as well as on the design of pyrolysis-based equipment and the characteristics of the final products.

To confirm the potential of the hydrochars as solid fuel, the pyrolysis process was investigated using thermogravimetric analysis (TGA). A comparative analysis was performed to evaluate the thermal decomposition, reactivity, and kinetics of raw biomass and hydrochars produced from HTC of olive pomace (OP) and *Agave Salmania* bagasse (AB) [1], [2]. From an experimental design, two types of hydrochars were selected, respectively those with the lowest (~ 20%) and highest (~ 35%) fixed carbon content, produced at 180°C (HC1), 250°C (HC2) and 30 min residence time. The raw biomass and hydrochar samples were heated to 1000°C at three different constant heating rates of 100, 400, and 800°C/min, in an inert atmosphere.

A model-free kinetic methodology was applied to the TGA data for estimating the conversion and activation energy to both raw (OP and AB) and derived hydrochars. Three common model-free (FWO, KAS, and Friedman) methods were applied to perform the analysis during this work. From the linear regression analysis, the values obtained from FWO model were considered as more reliable compared to Friedman and KAS methods.

To assess the effect of rapid heating on decomposition, literature data [3] for raw AB at lower heating rates (10, 20, 40 and 80°C/min) were used as a reference. By linking both studies, it was found that increasing the heating rates generally reduces the activation energy ( $E_a$ ). This methodology was afterwards used to estimate the  $E_a$  for AB hydrochars, as well as raw OP and its respective hydrochars. The kinetic analysis showed that HTC of OP improved the reactivity of hydrochars by decreasing the average activation energy from 76.18 kJmol<sup>-1</sup> for raw OP to 67.38 and 62.07 kJmol<sup>-1</sup> for HC1OP and HC2OP, respectively. Meanwhile, raw AB and derived hydrochars presented a more stable profile with average activation energies between 92.74 and

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\*Speaker

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161.61 kJmol<sup>-1</sup>, for raw AB and the 250°C derived-hydrochar, respectively. The activation energies were not similar for all conversion levels ( $\alpha$ ) ranging from 0.1 to 0.9. In the case of OP,  $E_a$  declined during the reaction stage of  $0.1 < \alpha < 0.6$  to reach a minimum value at  $\alpha = 0.6$  and subsequently increased during the reaction stage of  $0.6 < \alpha < 0.9$ . This two-staged trend of  $E_a$  could be attributed to the decomposition of hemicellulose and cellulose (between 150 and 400°C). In addition, as the reaction progresses the decomposition of the extractives demands more energy taking into account that lignin can also make the material more stable and thus more resistant to decomposition.

Therefore, depending on the biomass feedstock the kinetic analysis indicates that the HTC process can improve the reactivity of the hydrochars during the pyrolysis stage as a part of an overall thermochemical conversion process.

Keywords: Pyrolysis, kinetics, activation energies, hydrothermal carbonization, hydrochar, TGA.

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# Exhaust recycling as a CO<sub>2</sub> utilisation strategy in integrated biomass gasification power cycles

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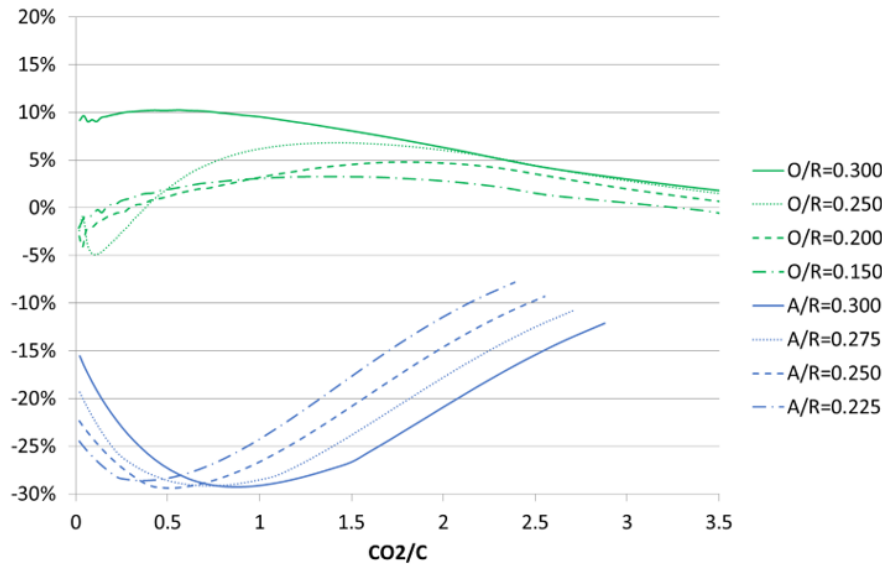
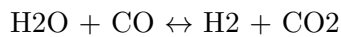
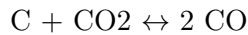


Figure 1: Effective CO<sub>2</sub> conversion in air (blue) and oxy (green) co-gasification with recycled exhaust

Using CO<sub>2</sub> as a gasifying agent to produce syngas is one potential scheme to valorise waste CO<sub>2</sub> streams that would otherwise be released to the atmosphere. Within a gasification system, the CO<sub>2</sub> agent reacts with char through the reverse Boudouard reaction while also influencing the water-gas shift and dry reforming reactions to generate the hydrogen and carbon monoxide product gas.



When this syngas is used as a fuel in a conventional power cycle, the overall system creates a cycling carbon dioxide utilisation (CDU) pathway (Hepburn, et al., 2019) since the final CO<sub>2</sub> emissions are released to the atmosphere. A similar strategy used for biomass gasification in a bioenergy with carbon capture and storage (BECCS) system would instead represent a closed

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CDU pathway. In both cases, the use of the CO<sub>2</sub> as a gasifying agent stands to improve the gasification process and overall system performance.

An interesting integrated system configuration that makes use of this principle supplies the CO<sub>2</sub> gasifying agent to the gasifier through recycling a portion of the exhaust from the power cycle. Such a direct CDU strategy takes advantage not only of the exhaust CO<sub>2</sub> material but also some waste heat rejected from the engine. This setup becomes a highly coupled system where the gasifier thermodynamic conditions are influenced by the recycled exhaust which is dependant on the engine's combustion performance which is in turn affected by the properties of the syngas generated from the gasifier.

To investigate the overall performance and CDU potential of this strategy, a representative numerical model is used to simulate this proposed system. Gasifier performance is simulated with a non-stoichiometric, thermodynamic equilibrium model to predict the syngas composition based on the supplied feedstock, gasifying agents, and operating conditions of the reactor (Chaiwatanodom, et al., 2014). The powerplant is simulated with a time dependant, zero-dimensional, internal combustion engine model. Model parameters are selected to simulate the combustion and heat transfer characteristics of a spark ignited engine run on syngas (Shivapuji & Dasappa, 2017).

Exhaust recycling CDU in an air-gasification power cycle is capable of marginally improving the indicated system efficiency from 28.13% to 29.24% for small amounts of exhaust recycling (Greencorn, et al., 2022). Although the CO<sub>2</sub> conversion under these conditions is poor, there is sufficient enhancement to the gasification system to allow for full char conversion at gasifier air ratios as low as  $\lambda=0.25$ , thus increasing the gasifier efficiency. Despite this advantage, significant limitations to the benefit of exhaust recycling CDU in this system arise due to build-up of inert diluents in the system. Diluted syngas blends with small heating values generate low exhaust temperatures which in turn cause low gasification temperatures and poor gasifier performance. Gasifier temperatures drop with increasing exhaust recycling, falling below 500°C for exhaust recycling ratios exceeding 1.5 moles of CO<sub>2</sub> per mole of feedstock carbon depending on air equivalence ratio. Nitrogen dilution alone is calculated to reduce the potential system efficiency by 2.5% from the ideal.

For oxy-combustion/oxy-gasification BECCS systems, this direct CDU strategy becomes more effective at converting CO<sub>2</sub> into syngas. Higher combustion temperatures in the oxy-combustion systems generate proportionately higher exhaust temperatures. Recycling the high temperature exhaust enhances the thermodynamic environment of the gasifier, providing favourable conditions for endothermic reactions that consume CO<sub>2</sub> as a reactant. The effect of exhaust recycling increases the indicated system efficiency from 23.35% to a peak of 26.89% due to lower O<sub>2</sub> demands in the gasifier, with best performance achieved at an oxygen equivalence ratio of  $\lambda=0.15$ .

While the gasification temperature is the major factor influencing gasifier performance, there is some degree of CDU attributable to the CO<sub>2</sub> transferring waste engine heat to the gasifier and to concentration-based equilibrium shifts. Even though the CO<sub>2</sub> appears to remain unreactive as a gasifying agent under some of these conditions, the gasifier requires the recycled exhaust to achieve full char conversion, particularly for low equivalence ratio conditions.

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## Session 4: Ammonia Combustion

Chair: Christine Rousselle

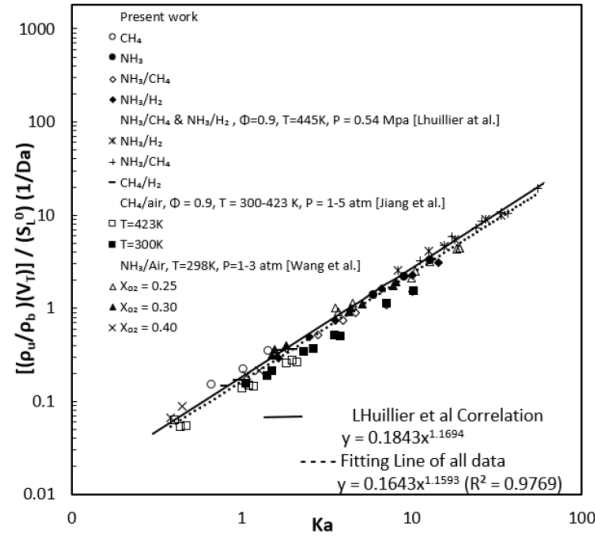
Keynote: Agustin Valera-Medina  
Ammonia for Net Zero Combustion

Agustin Valera-Medina is a Professor at Cardiff School of Engineering, U.K. He has participated as PI/Co-I in 29 industrial projects with multinationals including PEMEX, Rolls-Royce, Siemens, Ricardo, Airbus, and BP, attracting approximately £9.7M in research. He has published 178 papers (h-index 26), 46 of these specifically concerning ammonia for power. He has supervised 28 PhD students, 9 on ammonia-combustion related topics. Prof. Valera-Medina led Cardiff's contribution to the Innovate-UK "Decoupled Green Energy" Project (2015–2018) led by Siemens and in partnership with STFC and the University of Oxford, which aimed to demonstrate the use of green ammonia produced from wind energy. He is currently PI of the project SAFE-AGT (EP/T009314/1, £1.9M) to demonstrate the use of ammonia as an efficient gas turbine fuel. He leads the combustion work package of the H2020 project FLEXnCONFU (884157), a €12.7M project conceived to demonstrate ammonia power in large turbine engines. He is also PI and co-I of projects related to ammonia for transportation, propulsion, and heat/cooling (including OceanRefuel, MariNH3, Dock2Dock, Ammonia Optimization, Amburn, etc.). He has been part of various scientific boards, chairing sessions in international conferences and moderating large industrial panels on the topic of "Ammonia for Direct Use." He supported the preparation of two Royal Society Policy Briefings on "Green Ammonia". He is currently chair of the "Combustion and Emissions" working group of the Ammonia Energy Association, and co-Director of the Green Ammonia Working Group UK. He is the main author of the book 'Techno-economic challenges of ammonia as energy vector' (Elsevier).

# Turbulent Flame Speed Correlations for Pure Ammonia flames and Blends with Methane or Hydrogen

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**Fig.1:** Da-corrected  $S_T/S_L$  ratio against Ka. Literature data from spherically expanding flames of Lhuillier et al. (2021), Jiang et al., (2016) and Wang et al., (2021).

Ammonia (NH<sub>3</sub>) has been gaining recognition as a promising carbon-free fuel and hydrogen-energy carrier. Recently, considerable research has emerged on the challenges associated with NH<sub>3</sub> combustion (low-flame speed, high auto-ignition temperatures, high potential for detrimental emissions pollutants, i.e. NO<sub>x</sub>), however, there remain limited studies about turbulence-flame interaction for NH<sub>3</sub> as a fuel. The turbulent flame speed ( $S_T$ ) indicates the level of reactivity of a flame, influenced by flow properties, flame chemistry, laminar and turbulent transport properties, and is of key importance for practical industrial applications. As such, the aim of this work is to provide insight into various turbulent flame speed correlations and to determine appropriate correlations to use for NH<sub>3</sub> combustion and its blends with Methane (CH<sub>4</sub>) and Hydrogen (H<sub>2</sub>). To that end, using the spherical expanding flame configuration, the turbulent flame speeds of stoichiometric NH<sub>3</sub>/air, NH<sub>3</sub>/CH<sub>4</sub> (60% CH<sub>4</sub> vol.%), and NH<sub>3</sub>/H<sub>2</sub> (30% H<sub>2</sub> vol.%) were evaluated at various turbulent intensities, with flame propagation recorded using Mie-Scattering tomography. By assuming a spherical flame, the surface equivalent flame radius ( $R_s$ ), defined as  $R_s = (A/\pi)^{1/2}$ , where A represents the burnt gases area was evaluated, with an equivalent flame propagation velocity derived as  $V_T = (dR_s)/dt$ .

The majority of turbulent flame speed correlations are based upon laminar flame properties (laminar flame speed,  $S_L$ ; laminar flame thickness,  $\delta$ ), properties of the turbulent flow (root-mean-squared turbulence intensity,  $u'$ ; integral length scale,  $LT$ ), and dimensionless numbers (Karlovitz number,  $Ka$ ; Damköhler number,  $Da$ ; Reynolds number,  $Re$ ; Lewis number,  $Le$ ). In

<sup>\*</sup>Speaker

this study, the correlations proposed by Bradley, Zimont, and a modified version of Muppala, were employed. Overall, the Zimont correlation showed good agreement with the presented dataset, as well as previous experimental measurements found within the literature. A modified version of the Muppala correlation, updated to include the influence of flame-stretch interactions (through the use of  $Ma$ ), demonstrated reasonable agreement, underlining the prominent role of stretch upon the combustion of ammonia-based mixtures. Finally, a proportional relationship between  $ST/SL$  and  $DaKa$ , in the form of  $ST/SL = aDa.Ka^b$ , exhibits very good agreement with the present and previous datasets (see Fig. 1) and collapses well into the empirical formulation, underlining that  $NH_3$ -based fuels maybe be described using the usual turbulent combustion models.

Fig.1:  $Da$ -corrected  $ST/SL$  ratio against  $Ka$ . Literature data from spherically expanding flames of Lhuillier et al. (2021), Jiang et al., (2016), and Wang et al., (2021).

Acknowledgments: This project has received funding from the European Union’s Horizon 2020 research and innovation program agreement No. 884157

# Uncertainty Quantification of the Combustion Characteristics of NH<sub>3</sub>/H<sub>2</sub> Fuel Blends

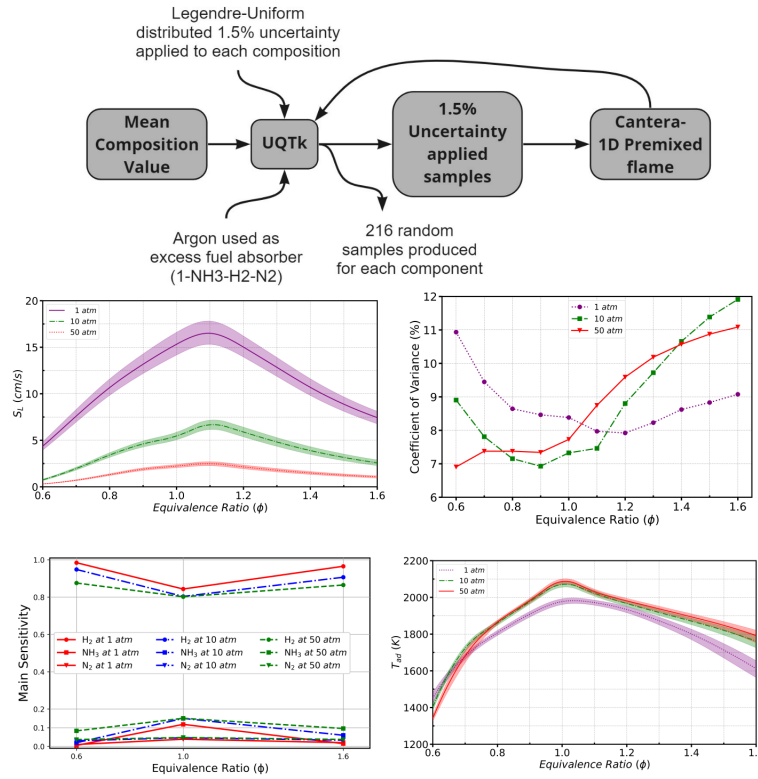
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Ammonia is a promising hydrogen carrier but the reactivity of pure NH<sub>3</sub> is low. Blending it with hydrogen can increase reactivity. However, blended fuels are often associated with high compositional uncertainty, leading to severe problems such as flame instability and excessive emissions [1]. It highlights the importance of performing uncertainty quantification and the minimisation of unwanted combustion uncertainties by identifying the leading sources. So far, almost all studies on the combustion of ammonia blends assumed prior-known conditions [2,3], while the effects of compositional uncertainty on the fundamental combustion characteristics are largely ignored.

The overall effects of compositional uncertainties on the flame temperature, the flame speed, and the formation of emissions can be determined using global sensitivity analysis (GSA). In general, a large number of parameters is needed in this analysis, making it extremely expensive.

<sup>\*</sup>Speaker

As a remedy, other global sensitivity methods can be developed to reduce computational costs. Polynomial chaos expansion (PCE) is one of the numerous GSA methods based on probabilities [4]. In the present work, PCE-based UQ analysis is conducted using Uncertainty Quantification Toolkit (UQTK) [5] and Cantera open-source library, see Fig. 1a. The effects of 216 uniform random samples (associated with  $\pm 1.5\%$  uncertainty assuming 3D Legendre-Uniform polynomials) on 1D premixed flames are evaluated for different blend compositions. The extensively validated chemical kinetic mechanism of Han et al. [6] is employed for calculating the combustion properties of blended fuel.

Specifically, this investigation explores the effects of compositional variability on the combustion properties of  $\text{NH}_3/\text{H}_2/\text{N}_2/\text{Ar}$  blends at various initial pressures (1, 10, 50 atm) and temperatures (298, 500, 700 K). It also examines the effect of the Argon (Ar) as a passive species to absorb the rest of the uncertainties ( $\text{Ar}=1-\text{NH}_3-\text{H}_2-\text{N}_2$ ). Lastly, the point after the flame front is determined to evaluate flame properties by referencing practical residence time for 1D premixed combustion. The results indicate that 1.5% uncertainty in each fuel composition causes uncertainty of up to 70% for  $\text{NO}_x$  emission and 12% for the laminar flame speed ( $SL$ ). Further, 5% uncertainty of  $T_{ad}$  at various initial pressures ( $P_i$ ) along with 30% variations in  $\text{NO}_x$  emission and 11% in  $SL$  are observed. The analysis also reveals 3% uncertainty in  $T_{ad}$  at different initial temperatures ( $T_i$ ). It is further found that the uncertainty effects are maximal for  $\text{NO}_x$  emission at richer combustion. The trend of uncertainty effect defined by the coefficient of variation ( $CV$ ) is fluctuated after equivalence ratio  $\text{ER}=1.1$ , while no fluctuation is observed in  $CV$  for near stoichiometric combustion conditions for different  $P_i$  and  $T_i$ . Fig. 1b presents the effects of different initial pressures upon the uncertainty of  $SL$ , showing that the uncertainty is higher for atmospheric combustion. Further, it is observed that 1.5% uncertainty in the fuel composition leads to 12% uncertainty in  $SL$ . As shown in Fig. 1c, the uncertainty effects vary considerably with  $\text{ER}$  and different initial pressure ( $P_i$ ). Yet, adiabatic flame temperature ( $T_{ad}$ ) appears to be a less affected property with a max of 5% uncertainty, which is around 100 K at  $\text{ER}=1.6$ . It is also reported that the contribution of  $\text{H}_2$  to the  $T_{ad}$  is higher at all  $\text{ER}$ s, but it decreases in stoichiometric conditions while that of  $\text{NH}_3$  increases. This is probably because of the increase in  $\text{NH}_3$  heat release rate at  $\text{ER}=1.0$ , as seen in Fig. 1d. The conducted UQ analysis shows that the main contributor to all of the flame characteristics is  $\text{H}_2$ . The current study can provide a guide for uncertainty reduction by providing quantified uncertainty originated from the compositional variability.

**Fig. 1.** (a) Schematic diagram uncertain system. (b) and (c) Effects of fuel variability on the  $SL$  at  $T_u=298$  K for  $\text{NH}_3/\text{H}_2/\text{N}_2/\text{Ar}$ . (d) and (e) Fuel variability effect on the adiabatic flame temperature of  $\text{NH}_3/\text{H}_2/\text{N}_2/\text{Ar}$  at  $T_u=298$  K for various  $P_i$ .

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# A brief understanding of the chemiluminescence signature of premixed ammonia-air flames

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Ammonia has become one of the top contenders amongst other fuels in a conquest to reduce carbon emissions as it is a zero-carbon fuel, can be easily stored and transported and, has a high-octane rating which is favourable in spark-ignition engines. However, ammonia-air flames are characterized by low flame speeds leading to an early blow-off, low heat release and, narrow flammability limits. To enhance the combustion process, it is important to understand the inner flame structure and its response to change in equivalence ratio or even a perturbation in the flow. It is known that ammonia-air flames are thicker than most hydrocarbon flames [1]. Studies on ammonia blended with methane and hydrogen flame structures are available in the literature [2-5]. Determining the position of the highest heat release rate (HRR) is essential in industrial systems in order to characterize flame stability. Viguera-Zúñiga et al. in their paper [6] obtained chemiluminescence from various species which was used to study radical formation in high-temperature reactions for NH<sub>3</sub>/CH<sub>4</sub> blends in swirl flows both experimentally and numerically and also to determine the location of the highest HRR. To the authors’ knowledge, no information on HRR is available for pure ammonia/air flames. The work presented here uses chemiluminescence of excited species and 1D Chemkin simulations of the counterpart non-excited species to compare the behaviour of these species and also, to determine possible HRR markers. The experiments were performed on a Bunsen burner at atmospheric conditions for  $\phi = 0.9-1.4$ . The premixed laminar flame speed calculator of Chemkin-*Pro* was used to simulate 1D freely propagating ammonia-air flame. The kinetic scheme of Stagni et al. [7] was used upon previous comparison and validation against experimental results among different kinetic schemes [8].

Excited species of interest in this work for ammonia-air flames were identified as NH<sub>2</sub>\* at 632 nm and NH\* at 337 nm. The respective filters were used to obtain the chemiluminescence. The position of each species within the flame front has been determined by finding the distance of each of the species from the fresh gas surface. On choosing a position at which the strain rate for these flames can be considered as negligible; a comparison with the structure of simulated unstretched freely propagating flames was proposed. The 1D simulation provides the temperature evolution, the position of the maximum HRR, and the concentration of the non-excited species along the domain. The experimental and the numerical results can be superimposed.

It was seen that both NH<sub>2</sub>\* and NH\* were quite close to their counterpart non-excited species

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\*Speaker

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which allows us to assume that both the excited species are formed mostly as a result of unreactive collisions. It was observed that the max HRR was in between both the excited species showing that the product of  $\text{NH}_2^*$  and  $\text{NH}^*$  is a good indicator of determining the maximum HRR experimentally.

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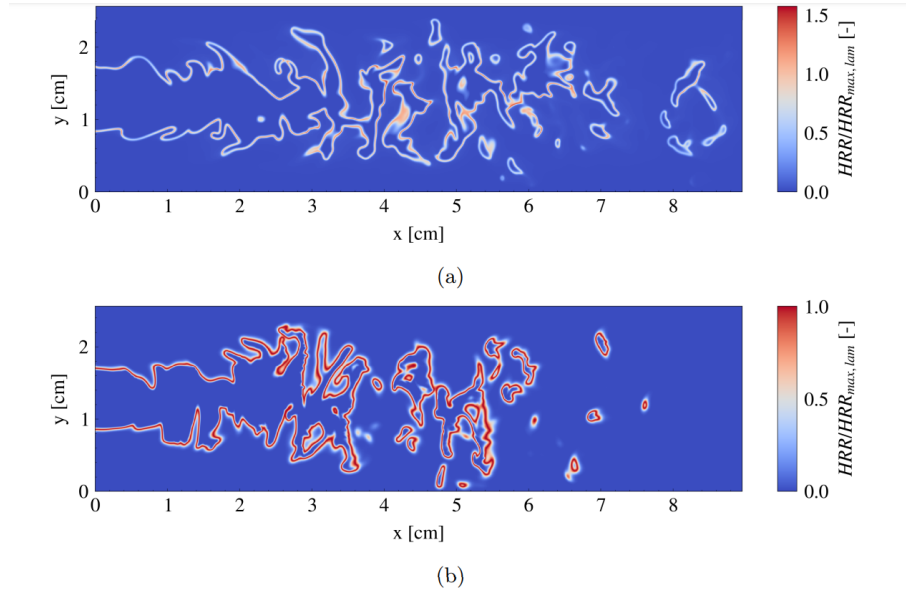
# Direct numerical simulation of a premixed turbulent ammonia/hydrogen-air flame in a slot burner configuration

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In this study, a 3-D premixed ammonia/hydrogen-air flame is investigated using direct numerical simulation (DNS) in a slot burner configuration. Ammonia ( $\text{NH}_3$ ) is a promising hydrogen ( $\text{H}_2$ ) carrier but has a low laminar burning velocity, not suitable for combustion systems. Therefore, ammonia-based fuels such as ammonia/hydrogen mixtures are a promising solution for carbon-free combustion. These mixtures can be tuned to match the laminar flame properties of representative methane-air flames with the intent to replace the fuel in gas engines without design modification. The  $\text{NH}_3/\text{H}_2$  mixture is optimized using 1-D premixed flame simulations with Cantera to reach a laminar flame speed (SL) at the same equivalence ratio and reactants' initial temperature as a methane-air flame. For the optimization a methane-air flame at an equivalence ratio of 1 and initial temperature of 300K in the fresh gases with a laminar flame speed of 0.38 m/s is chosen. The same laminar flame speed of 0.38 m/s is reached for a mixture ratio of 91% of  $\text{NH}_3$  and 9% of  $\text{H}_2$  in mass fraction. The thermal laminar flame thickness of the  $\text{NH}_3/\text{H}_2$  blend is ( $\delta_L$ ) is 450  $\mu\text{m}$ . In the 3-D DNS setup, fresh gases are continuously injected

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in the center of the inlet at a height of  $H = 8.5\text{mm}$  and a velocity of  $U = 25\text{m/s}$ . The domain size is  $10.5H \times 3H \times 1.5H$  in the streamwise, transverse, and spanwise directions respectively. A synthetic Passot-Pouquet spectrum is used for turbulence injection with a root mean square velocity fluctuation ( $u'$ ) corresponding to 10% of the inlet velocity and an integral length scale (LT) of  $H/4$ . The resolution is 11 points in the thermal flame thickness, leading to a grid of  $2191 \times 627 \times 314$  points. The simulation was performed over two flow-through times for a duration of 8 ms. We obtain  $u'/SL \approx 6.6$  and  $LT/\delta L \approx 4.7$ . DNS results will help understand the structure of the premixed turbulent  $\text{NH}_3/\text{H}_2$ -air flame in comparison to an unstretched laminar flame: the flame length, flame surface, stretch factor, curvature, turbulent flame speed will be computed. The flame surface and flame length of the  $\text{NH}_3/\text{H}_2$ -air flame is similar to a  $\text{CH}_4$ -air flame under the same conditions. However, the heat release rate of  $\text{CH}_4$ -air flame is of the same order than for the laminar unstretched flame, but for the  $\text{NH}_3/\text{H}_2$ -air flame, the heat release rate is higher than one of a laminar unstretched flame as illustrated Fig. 1. Detailed post-processing will discuss the role of fast hydrogen diffusion in the mixture and its potential impact on the increased heat release rate.

# Effect of Adding Ammonia on the Internal Nanostructure of Soot Particles Formed in Ethylene Laminar Flames

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Low carbon combustion has been of interest in marine applications which could allow the partial blending of hydrocarbons (HCs) with zero-carbon fuels such as ammonia (NH<sub>3</sub>) to reduce greenhouse gas (GHG) emissions [1]. In such blends, the propensity of NH<sub>3</sub>-HC combustion to form soot emissions is reduced [2] which could be in part due to changes in the reactivity of the soot particles, influenced by their nanostructure. The graphitization of the soot internal structure impacts the soot reactivity towards oxidation due to the formation of larger layer planes with few carbon atoms at edge sites, where they are more reactive, relative to in plane sites [3]. In this study, the internal structure of young and mature soot particles formed in ammonia-ethylene (NH<sub>3</sub>-C<sub>2</sub>H<sub>4</sub>) laminar diffusion flames is analyzed to identify how NH<sub>3</sub> addition affects soot at different growth stages. Soot particles are sampled from the centerline of 0%, 20%, and 40% NH<sub>3</sub> (by volume) blended C<sub>2</sub>H<sub>4</sub> flames with fixed carbon flow and their nanostructure is examined using lattice fringe analysis of soot high resolution images obtained using transmission electron microscopy (HRTEM) and electron energy loss spectroscopy (EELS) analysis. Elemental analysis of the soot surface was done using x-ray photoelectron spectroscopy (XPS) to identify the tendency of ammonia to react with the particles in the flame. Changes in the distribution of the length and tortuosity of fringes analyzed in HRTEM images indicates the effect of NH<sub>3</sub> addition on the soot particle graphitization. The results show that young soot particles become more amorphous as the percentage of NH<sub>3</sub> increased as the fringes become shorter and more tortuous. Mature soot is more graphitic compared to young soot [4]; it also exhibits the same effect where the degree of soot graphitization decreases by adding more NH<sub>3</sub>. However, the impact of NH<sub>3</sub> on mature soot is less pronounced. In addition, electron energy loss spectroscopy (EELS) is used as a complementary technique to study the degree of graphitization based on the ratio of sp<sup>2</sup> to sp<sup>3</sup> in soot. A similar trend is observed from the EELS analysis indicating a reduction in the degree of graphitization of young and mature soot due to NH<sub>3</sub> addition. Moreover, the bonding between carbon and functional groups resulting from the decomposition of NH<sub>3</sub> such as amines (NH<sub>2</sub>) is detected using XPS at the surface of the soot particles with the atomic percentage of nitrogen linearly increasing with the addition of NH<sub>3</sub>. Consequently, soot formed in NH<sub>3</sub> blended flames could be more reactive due to its reduced graphitization which leads to higher availability of carbon atoms at edge sites and increased potential for oxidation. This could be caused by the C-NH<sub>2</sub> bonds formed at the particle surface which may inhibit the binding of carbon layer planes leading to less graphitized nanostructure during soot growth. The increased soot reactivity could play a role in reducing the sooting propensity of NH<sub>3</sub> blended flames.

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<sup>\*</sup>Speaker

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# Enabling ultra-lean combustion of ammonia-hydrogen in porous media burners

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Lauren Simitz <sup>2</sup>, Bassem Akoush <sup>1</sup>, Priyanka Muhunthan <sup>1</sup>, Matthias  
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To mitigate climate change caused by the anthropogenic release of carbon dioxide and methane in the atmosphere, many industries must transition to carbon-free renewable energy sources within the next decades. One of the possible fuels considered for this task is ammonia. It is a carbon-free fuel that can be synthesized from green hydrogen and whose combustion does not emit any greenhouse gases. Several challenges must however be addressed before this fuel can be widely deployed in practical systems: ammonia-air flames have a significantly slower flame speed, higher ignition temperature and larger flame thickness than conventional hydrocarbon flames. Ammonia combustion can also generate significant amounts of pollutants such as nitric oxides and unburnt ammonia. Porous media have been used to address similar combustion challenges and allow the stabilization of very lean flames for applications such as gas turbines, jet engines and radiant heaters for industrial processes. In this work, we extend previous studies and examine the stabilization of ammonia-hydrogen-air flame in a porous media burner, with a particular focus on lean mixtures. Flames are stabilized at the interface between two open-cell ceramic foam with different pore size. Heat is recirculated by conduction and radiation in the ceramic matrix, thereby preheating the fuel and enhancing the flame consumption rate. We demonstrate experimentally that an adequately designed porous media burner can stabilize flames over a wide range of operating conditions: (1) from pure ammonia to a 40% hydrogen volume fraction; (2) very lean (equivalence ratio of 0.5) to rich (equivalence ratio of 1.4); and (3) with a turn-down ratio greater than 15:1. Power densities in excess of 90 MW.m<sup>-3</sup> can also be achieved. Finally we report the nitric oxide and unburnt ammonia emissions of this porous media burner and find that operation in the ultra-lean regime can lead to a good compromise between low nitric oxides and low unburnt ammonia emissions.

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\*Speaker

# High pressure combustion of ammonia blends in an industrial model burner

Mario Ditaranto <sup>\*</sup> <sup>1</sup>, Inge Saanum <sup>1</sup>, Jenny Larfeldt <sup>2</sup>, Karl-Johan Nogenmyr <sup>2</sup>

<sup>1</sup> SINTEF Energy Research – Norway

<sup>2</sup> Siemens Energy – Sweden

Hydrogen from renewables or reformed natural gas with CO<sub>2</sub> Capture and Storage (CCS) can be used as fuel to achieve CO<sub>2</sub> free power production. Because of the challenges related to transport and storage of H<sub>2</sub>, NH<sub>3</sub> has been proposed as a hydrogen carrier as it can be stored in liquid form at moderate pressures and temperatures. NH<sub>3</sub> could be used as a fuel directly, but its low reactivity, flame speed, and a high propensity to generate NO<sub>x</sub> make combustion stability challenging in conventional gas turbine combustors. As no solutions are commercially available today, a transitional approach is to only replace part of the natural gas with NH<sub>3</sub> to limit the change in the combustion properties, although this only partly decarbonizes the fuel. Alternatively, ammonia could be decomposed back to a mixture of hydrogen and nitrogen which has better combustion properties, but at the expense of an endothermal reaction. A trade off could be a partial decomposition where the end use fuel is a mixture of ammonia, hydrogen, and nitrogen. The presented work investigates experimentally combustion of various blends of CH<sub>4</sub>/NH<sub>3</sub> and NH<sub>3</sub>/H<sub>2</sub>/N<sub>2</sub> in an industrial downscaled Dry Low Emission (DLE) burner at high pressure. The effects of fuel composition and equivalence ratio on the emissions of NO<sub>x</sub>, CO, CH<sub>4</sub>, HCN, N<sub>2</sub>O, and NH<sub>3</sub> are studied at different pressures and power. It shows that introduction of NH<sub>3</sub> in the fuel results in unacceptably high NO<sub>x</sub> emissions in a conventional combustor and the flame stability limits the maximum NH<sub>3</sub> content in the fuel. One recognized way to limit NO<sub>x</sub> formation in NH<sub>3</sub> combustion is to limit the oxygen availability in the flame by operating fuel rich. The high pressure combustion facility used allows for operation in a two-stage combustion strategy with a rich primary zone, where this effect is quantified. In addition, it is observed that increasing pressure has a strong and favourable effect on NO<sub>x</sub> formation.

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<sup>\*</sup>Speaker



## Session 5: Biofuels combustion

Chair: Alison Tomlin

Keynote: Olivier Herbinet

Towards a better understanding of biofuels' oxidation chemistry

Olivier Herbinet is Associate Professor at University of Lorraine since 2007. He is a specialist in the use of continuous flow reactors (e.g., jet-stirred and flow tube reactors) for the study of gas phase reactions (oxidation and pyrolysis) of organic compounds, using a wide range of diagnostics from gas chromatography to mass spectrometry with ionization using synchrotron radiation. These studies led to 94 peer-reviewed publications (H-index = 39 (WoS)). He was vice leader of the Working Package 1 of the Cost Action Smartcats (2015-2019).

# Diethyl ether cool flames: The impact of ozone-seeding on the reactivity

Thomas Panaget <sup>\* 1</sup>, Killyan Potier <sup>2</sup>, Sebastien Batut <sup>2</sup>, Amaury Lahccen <sup>2</sup>, Yann Fenard <sup>2</sup>, Laure Pillier <sup>2</sup>, Guillaume Vanhove<sup>† 2</sup>

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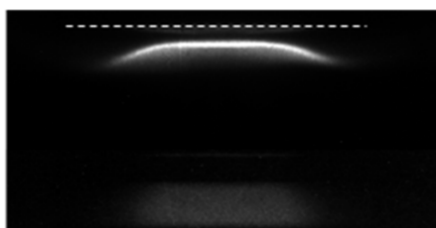


Fig. 1. Raw  $\text{CH}_2\text{O}^*$ -chemiluminescence image of the diethyl ether cool flame (the burner plate is represented with a white dashed line)

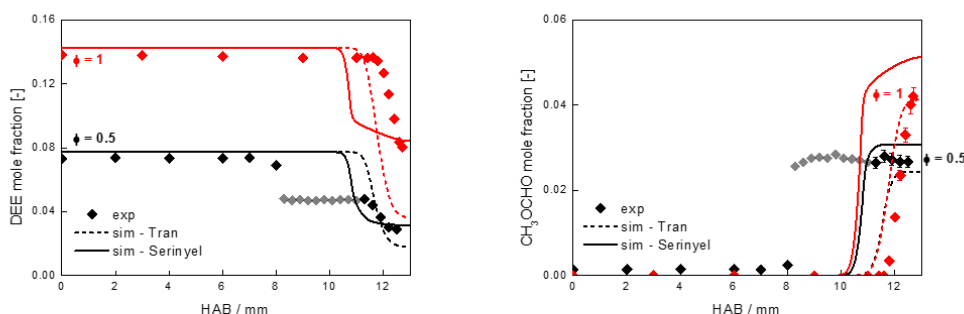


Fig. 2. Fuel (left) and acetaldehyde (right) mole fraction profiles in both flames,  $\phi = 0.5$  (black) and  $\phi = 1$  (red), and simulations with the Serinyel *et al.* model (full line) and the Tran *et al.* model (dashed line)

From their discovery in the beginning of the 19th century to the present day, the chemistry behind the formation of cool flames has raised many questions within the combustion community. Considering their importance in the realization of advanced combustion technologies, cool flames were also extensively studied during the last two decades.

Because of their longer induction times in comparison with hot flames and limited stability domain, ozone or plasma are widely used to stabilize cool flames in laboratory-scaled burners. The aim of such chemical sensitization is to provide reactive species *in-situ* which will accelerate the H-abstraction reactions [1,2]. When ozone is seeded, its decomposition upstream from the flame front will yield atomic oxygen O. It has however been observed that, in the case of dimethyl ether (DME), ozone addition could modify the relative distribution of the decomposition pathways of  $\text{RO}_2$  radicals [2,3]. While ozone-seeded and spontaneous cool flames have been studied

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in the past, direct comparisons of spontaneous and ozone-seeded cool flames have never been performed.

In this work, diethyl ether cool flames were stabilized and studied in a stagnation plate burner. Two conditions were selected, enabling the assessment of the impact of ozone seeding on the cool flame: In the first case, ozone was seeded to stabilize a lean cool flame with an equivalence ratio of 0.5, and in a second case a stoichiometric flame was stabilized without O<sub>3</sub> addition. Chemiluminescence emission of excited formaldehyde (Fig. 1) was used to measure the cool flames position in the burner. Detailed temperature and mole fraction profiles of stable reactants, intermediates and products of the oxidation of the diethyl ether in the cool flame were established for both conditions (Fig. 2.). Relevant and recent detailed kinetic models from the literature, respectively developed by Tran *et al.* [Tran *et al.*, *Proc. Comb. Inst.* 2019, 37, 511-519] and Serinyel *et al.* [Serinyel *et al.*, *Combust. Flame* 2018, 193, 453-462], were used in order to improve the understanding of the low temperature oxidation kinetics of this ether, as well as the effect of ozone addition on the species distribution after the cool flame.

Despite of the equivalence ratio variation, experimental results show that ozone plays an important role in the cool flame temperature, which is higher in the lean case, seeded with ozone, in comparison to the stoichiometric case. Ozone seeding also greatly influences the fuel conversion in the cool flame. The predictions of the main products by the Serinyel *et al.* model agree fairly well with experimental measurements, while some minor intermediates species are widely underestimated, namely 2-methyl-1,3-dioxolane and ethyl vinyl ether. Interestingly, the ozone addition marginally affects the main reaction pathways of DEE in the cool flame. The most significant impact relies on the  $\cdot$ OH atom production, yielding H radicals, which are mainly responsible of the fuel conversion in these conditions. Finally, these results suggest that there may be missing pathways leading to the formation of minor species in the low temperature range.

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# Reaction kinetics of the consumption mechanism of Oxygenated Polycyclic Aromatic Hydrocarbons (OPAHs)

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Laurent Gasnot <sup>1</sup>, Florent Louis <sup>1</sup>, Abderrahman El Bakali <sup>1</sup>, Luc-Sy  
Tran <sup>1</sup>

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This research focuses on the study of the gas-phase reaction mechanism of oxygenated polycyclic aromatic hydrocarbons (OPAHs) by using theoretical methods. OPAHs are formed during the incomplete combustion processes of hydrocarbons, biofuels and biomass. Recent studies show a significantly higher toxicity for OPAHs than for conventional PAHs. Despite this concern, the fundamental principles of OPAHs chemistry are still not well understood, which explains why current combustion kinetic models do not incorporate an adequate mechanism of their formation and decomposition, and are rather oriented towards the formation of small OPAHs (2-3 cycles). Thus, the aim of our project is to study the different decomposition pathways of representative OPAHs, starting by the addition reactions on the double bond and/or H-abstraction reactions, both by H or OH free radicals, followed by cyclization reactions on the resulting cyclic intermediates. The latter would allow the production of larger or different OPAHs than the ones currently detected.

The presentation will cover a first part where we have studied the H-abstraction reactions of some OPAHs (two benzofurans and two benzodioxins) by H-atoms in a systematic way. The thermo-kinetic data have been obtained by the CCSD(T)-F12/CBS//CAM-B3LYP/6-311++G(d,p) method.

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# Automatic reduction of HEFA bio-jet fuel: From detailed composition to CFD compatible reduced kinetics

Quentin Cazères <sup>\*† 1</sup>, Théo Ogier <sup>2</sup>, Thomas Lesaffre <sup>2</sup>, Eléonore Riber <sup>2</sup>,  
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The ongoing climate crisis demands for new energy resources in all economic sectors. For aviation, one of the most promising technology is the use of bio-derived fuels that are able to replace conventional kerosene. Such fuels already exist and are produced via several processes such as Alcohol-To-Jet-Synthetic-Paraffinic-Kerosene (ATJ-SPK) or Hydrotreated- Esters-and-Fatty-Acids-Synthetic-Paraffinic (HEFA-SPK). In order to complete the experimental evaluation of these fuels, in particular concerning their pollutant emissions, reliable CFD is needed and must include fuel effects through accurate chemistry descriptions. Detailed chemical mechanisms with hundreds of species have been developed in the last decade and are able to model the kinetic behaviour of fuel oxidation as well as CO and NOx production. However, they stay far too expensive for 3D computations of realistic cases. As a consequence, several techniques and methodologies have been developed to reduce these mechanisms.

This work demonstrates how all the existing reduction techniques can be combined in a practical and automated workflow allowing to fully reduce a kinetic mechanism of HEFA, starting from its detailed composition to a final Analytically Reduced Chemistry (ARC) suited for CFD and more particularly Large Eddy Simulation (LES).

The first step consists in the definition of a surrogate fuel model that can be used with the detailed CRECK\_2003\_TOT\_HT\_LT mechanism *Ranzi et al.* (a) *Ranzi et al.* (b) *Bagheri et al.* containing 492 species and 17790 reactions.

The definition of the surrogate fuel model follows the work of *Narayanaswamy et al.* *Kim et al.*. The composition includes species selected among the ones available in the detailed mechanism, in proportions that allow to match measured physico-chemical properties such as carbon atom repartition inside hydro-carbon families obtained from gas chromatography, liquid density, distillation curve and other relevant properties for combustion. Then a lumping of the pathways involved in the pyrolysis is performed with the methodology of *Herbele et al.* for each of the surrogate component in order to keep a multi-component description of the fuel. Finally, DRGEP *Pepiot-Desjardins et al.* (a), Lumping *Pepiot-Desjardins et al.* (b) and Quasi-Steady State Assumption are applied. All these steps are performed with the code ARCANE *Cazères et al.* to obtain the final mechanism.

The reduced mechanism is then employed in a 1-dimensional spray flame configuration, from *Shastry et al.* computed with the code AVBP in order to study the flame structure and the validity of the reduction hypotheses. Emphasis is put on the pyrolysis lumping step by comparing

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with an ARC scheme obtained without this reduction step.

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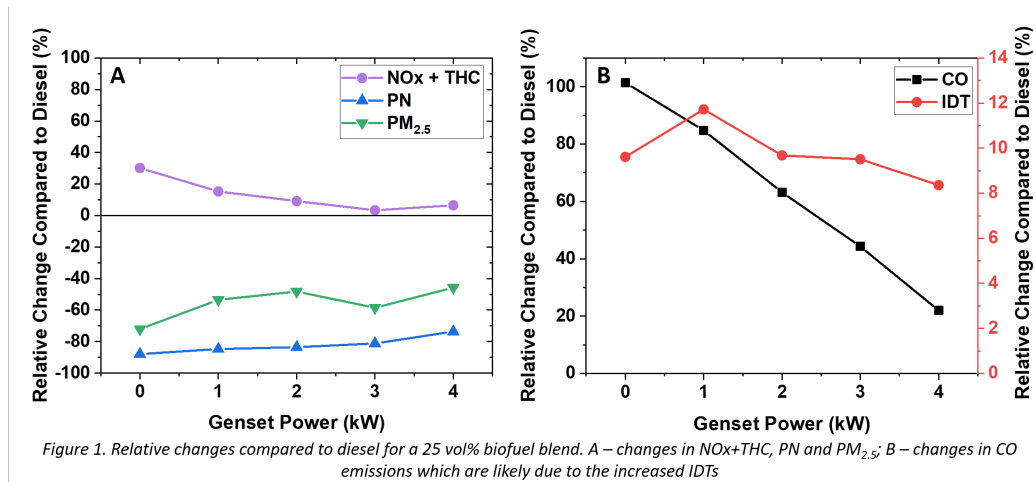
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# The Effects of Butyl-Based Three-Component Advanced Biofuel Mixtures on Compression Ignition Engine Emissions and Performance

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With the global population increasingly reliant on the shipping and haulage of goods, the need to rapidly decarbonise these parts of the transport sector is becoming increasingly pressing. In the UK, these sectors heavily rely on the use of diesel, which is likely to continue in the short term. Therefore, suitable low carbon alternatives need to be found. The use of biofuels as diesel alternatives is an ever-growing research area. This is in part due to legislation at European level which is mandating increased fractions of advanced biofuels used as blend components in fuels, resulting in developments in a range of production techniques (1).

Alcoholysis of biomass is one production technique of interest as it produces blends of potential fuel candidates (2). The primary products are an alkyl levulinate, a dialkyl ether, and the alcohol used (2). This blend composition could be tailored to ensure that properties in existing fuel standards, such as EN 590, can be met for blends of diesel and the three-component biofuel blend (2, 3). However, in addition, emissions standards for compression ignition (CI) engines must also be met. With the need to improve air quality in addition to reducing greenhouse gases (GHGs) emissions, emissions limits for air pollutants such as particulates and nitrogen oxides (NOx = NO+NO<sub>2</sub>) have been reducing with each version of the standards. Therefore, it is vital to understand the effects of biofuel blend compositions on engine emissions and performance.

This study investigated the impact of butyl-based biofuel blends with diesel on CI engine emissions and performance. The biofuel blends consisted of n-butyl levulinate (nBL), di-n-butyl

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ether (DNBE), and n-butanol (nBuOH). Biofuel blends which met the limits for flash point and viscosity set in EN 590, were shown to require at least 65 vol% nBL, up to 10 vol% nBuOH, and the remainder from DNBE, when blended at 10 vol% and 25 vol% in diesel (3). These fuel blends were tested in an air-cooled, direct-injection, four-stroke, single-cylinder Yanmar L100V CI engine. The engine was part of a generating set (genset), with the engine connected to a Hillstone load bank. The fuels were tested at steady-state for 20 minutes at five different genset loads: idle up to 4 kW. NO<sub>x</sub>, CO, and total hydrocarbon (THC) emissions were measured using a Horiba MEXA 7100D exhaust gas analyser. Particulate matter (PM) size distributions and particle number (PN) were measured using a Cambustion DMS500. PM<sub>2.5</sub> was captured on glass fibre filter papers and measured gravimetrically. A range of volatile organic compounds (VOCs), including formaldehyde and acetaldehyde, were measured using a Gasmeter Fourier Transform Infrared (FTIR) spectrometer. Ignition delay times (IDTs) were calculated using the in-cylinder pressure/crank angle profiles.

The engine maintained each steady state when fuelled with the selected blends. Although the cetane numbers (CN) of the blends are unknown, the increased IDTs indicate a reduction in the CN when compared to diesel. These increased IDTs contributed to changes in the emissions across all loads. As commonly seen for blends of low CN oxygenated biofuels with diesel, there was the expected reduction in PM<sub>2.5</sub> and PN, with reductions of up to 70% when using the blends, due to the increased IDTs increasing premixed combustion. This reduction in particulate emissions came with the trade-off of increased CO, NO<sub>x</sub>, and THC emissions, with increases of up to 100% for CO, 8% for NO<sub>x</sub> and 82% for THC individually, and 30% for NO<sub>x</sub>+THC combined, over the range of powers tested. As part of the increased THC emissions, there were increased VOCs detected by the FTIR. The increases in the CO, NO<sub>x</sub>, and THC emissions reduce with the increase in overall engine load, which combined with the reduced exhaust temperatures and pressures, is consistent with the findings of Frigo *et al.* (4).



## Session 6: Hydrogen 2

Chair: Simone Hochgreb

Keynote: Andy Brown

HyNet, demonstrating the reality of hydrogen as an energy vector

Andy started as a Student Apprentice with what was then the Central Electricity Generating Board, initially studying Electrical Engineering, but switched to Mechanical Engineering, in which discipline he is Chartered as a Fellow. During a 29-year career with the GEGB and successor companies he worked on coal, nuclear and gas turbine plant before moving to a role providing technical support to Business Development. Following privatisation, Andy joined Progressive Energy as Engineering Director at its inception in 1997. Progressive's pioneering of IGCC opportunities allowed Andy to develop further expertise (for which he was awarded the I.Chem.E's Hebden Medal) burning syngas and hydrogen in Gas Turbines, and CO capture, transportation and storage. He represents the UK in producing an ISO Standard for CO transportation. More recently extending this to hydrogen, he was responsible for the I.Chem.E's series on hydrogen (in recognition for which he was awarded their Ambassador medal). He has provided Engineering expertise across the many elements of the HyNet project. Andy co-chairs the Technical Working Group of the Carbon Capture and Storage Association and is the Energy Institute representative for CCUS.

# Investigation on the impact of hydrogen addition in a bluff body stabilized turbulent flame using high repetition OH PLIF-PIV and multiscalar measurements by spontaneous Raman scattering

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<sup>6</sup> Director of research – CNRS- CORIA – France

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We experimentally investigated the effect of hydrogen (H<sub>2</sub>) addition over the turbulence chemistry interactions in the lab-scale canonical non-premixed bluff-body burner. It is well known that, the non-premixed bluff-body burner possesses complex interactions between the central fuel jet, toroidal air recirculation vortex and extinction/re-ignition events. The objective of the present study is to follow up and provide further quantitative insights into the above-said processes as a function of hydrogen addition from methane turbulent flame up to full hydrogen one. This is accomplished through high-repetitive (5 kHz) simultaneous OH PLIF and PIV measurements. Results show the change in turbulent flame/flow interactions leading flame stabilization. In addition, combined OH\* chemiluminescence and 1D spontaneous Raman scattering have been implemented over some selected hydrogenated flames to determine instantaneous and simultaneous temperature and various species concentrations: CH<sub>4</sub>, H<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>, CO, CO<sub>2</sub> and H<sub>2</sub>O. The obtained measurements highlighted the significant influence of H<sub>2</sub> addition in the local extinction, re-ignition events and thus joint pdfs of species and temperature profiles.

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\*Speaker

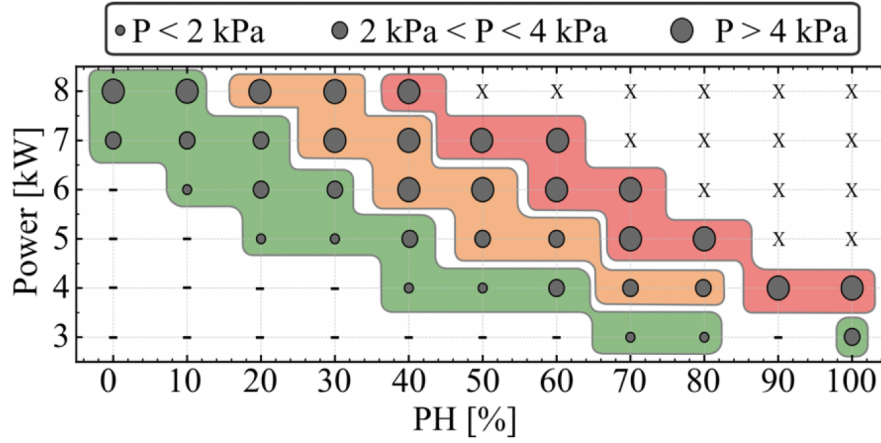
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# Impact of ignition strategy and back pressure on bluff body flame stabilization for hydrogen enriched mixtures

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In the drive to decarbonise large scale power generation, carbon free fuels such as green hydrogen offers a promising alternative to accelerate the energy transition towards zero emissions. Nevertheless, the success of this transition depends on the ability to build fuel flexible gas turbines capable to safely burn hydrogen enriched mixtures. In this context, a safe and reliable ignition process under a wide range of H<sub>2</sub> enrichment is of vital importance and must be taken into consideration at the design stage of the engine. The present work aims to elucidate the combustion dynamics during the ignition process when methane is replaced by hydrogen. It has been observed that the ignition dynamics alters the final stabilization mode of CH<sub>4</sub>-H<sub>2</sub> flames burning in a perfectly premixed mode. To further investigate these previous observations, ignition experiments were performed over a wide range of operating conditions from pure methane injection (PH0) to pure hydrogen injection (PH100). A perforated plate of porosity 0.17 is added at the combustion chamber outlet to increase the mean pressure drop of the system. The total pressure drop measured in cold flow conditions at  $U_b = 5$  m/s is 100 Pa and this small pressure drop leads to relatively high over pressures during ignition. In order to ensure the same thermal condition at ignition, a strict experimental protocol was followed. The burner was first preheated up to  $T = 470$  K measured at the center of a central bluff body. The chamber was then filled with the combustible mixture for 5 s to ensure a homogeneous fuel/air mixture throughout the combustion chamber. Finally, a flame kernel was initiated using a spark plug. Time-series of pressure, velocity and global heat release rate as well as flame images were recorded simultaneously to

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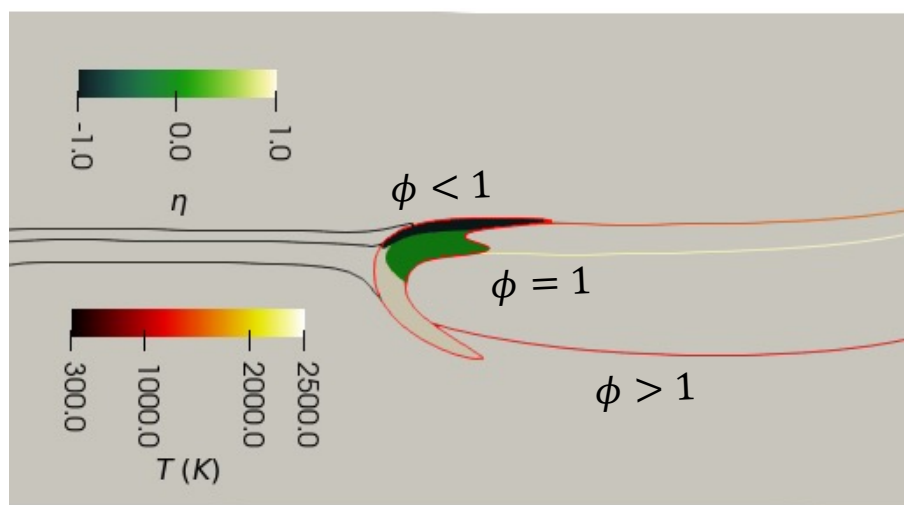
characterize the ignition dynamics during the ignition transient up to flame stabilization. Two ignition schemes were tested: In (I), the flame was first ignited for pure methane conditions at  $U_b = 5$  m/s and equivalence ratio of 0.7 and then the hydrogen content was slowly increased in quasi-static way up to the desired operating point. In (II), the flame was directly ignited at the equivalence ratio, flow velocity and hydrogen content of the desired operating point. The final state of the flame was found to be very sensitive to the ignition scheme (I) or (II). Three different scenarios were identified: (A) Soft ignition with direct stabilization, (B) transient flashback and (C) permanent flashback. It is shown that the propensity of the flame to flashback depends on both the amplitude of the over pressure inside the combustion chamber produced by ignition and the level of H<sub>2</sub>-content of the fuel blend (see Fig. 1). For a given thermal power, the operability range with final state (A) is significantly reduced with increasing hydrogen enrichment. For the same initial mean pressure drop, hydrogen enrichment amplifies the magnitude of the over pressure inside the combustion chamber due to its higher burning velocity. Furthermore, when H<sub>2</sub>-content is increased, flames close to the stability boundary could not be stabilized anymore with ignition strategy (II), whereas well stabilized flames were obtained with ignition strategy (I). Finally, an attempt is made to isolate effects of combustion properties from flow dynamics by keeping both the bulk injection velocity and laminar burning velocity fixed at 5 m/s and 0.25 m/s respectively for increasing levels of H<sub>2</sub>. For the same flow injection conditions, the ignition over pressure reached inside the chamber remained comparable and independent of the H<sub>2</sub>-content. Although the mean flow conditions and over pressures are kept constant the stabilization mode was found to be highly dependent on H<sub>2</sub>-content in the mixture.

# DNS analysis of triple flame speed of H<sub>2</sub>/air flames at high inlet temperature and high pressure

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Stabilization of hydrogen-air flames is a major concern in future engines. On one side, flashback risk dissuades the adoption of premixed combustion. On the other side, the separated injection of reactants generally leads to anchored flames dominated by pure diffusion regime. These flames, apart from generating unacceptable NO<sub>x</sub> emissions, can compromise the lifetime of materials because of too high heat fluxes transferred to the burner lip. Therefore, the key issue in most devices is to operate with partially premixed regimes exploiting aerodynamically stabilized flames. As result, it is crucial to understand mechanisms leading from lifted to anchored flames (and vice versa) across a mixture fraction gradient. Flames that propagate across a mixture fraction gradient are named triple flames (TF). They are characterized by three flame fronts as sketched in Fig. 1. A lean premixed (LP) branch develops on the lean side of the mixture fraction gradient. From the stoichiometric point to the flame periphery the local equivalence ratio gets smaller and smaller till the lower flammability limit is attained. The rich premixed (RP) side that develops on the opposite side of the flame is characterized by increasingly rich mixture up to the higher flammability limit. The streams of oxidizer / fuel in excess from the LP / RP side meet behind the premixed front, leading to a diffusion-controlled flame that corresponds to the tail of the triple flame. Integral theoretical analysis revealed that the laminar displacement speed  $V_{tr}$  of such flames is higher than the unstretched stoichiometric burning velocity by a factor equal to the square root of the volumetric expansion ratio. For a hydrogen-air triple flame, this displacement speed is high and reaches values of about  $V_{tr} \sim 7$  m/s. This high

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value may explain flame stabilization in partially premixed high flow velocity regions that are observed in some experiments. In this context we performed DNS of hydrogen/air triple flames and evaluate  $V_{tr}$  as function of the mixture fraction gradient, fresh gases inlet temperature and pressure. The displacement speed deduced from the simulations is compared to the theoretical relation and differences between the two are discussed in light of hydrogen characteristics.

# Stabilization of low-NOx hydrogen flames on a dual swirl coaxial injector

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The growing interest for a low-carbon transition has put hydrogen in the spotlight as a potential fuel to reduce the carbon footprint of numerous industries using combustion, among which the aeronautical and the energy generation sectors. However, the transition to hydrogen creates many challenges. The first challenge is to stabilize flames despite the unique combustion properties of hydrogen compared to conventional fuels. Then hydrogen combustion poses the risk of increasing other types of non-carbon pollution, namely nitrogen oxide (NOx) pollution, due to the higher combustion temperature of hydrogen. In addition, the high flammability of hydrogen poses an increased risk of flashback in premixed configurations commonly used to generate low-NOx flames. Thus, the search for a low-NOx strategy for hydrogen combustion is developing, and several technologies are being investigated. Among these technologies, we consider here a double swirl coaxial injector operated in non-premixed conditions. This is a likely solution for safe low-NOx hydrogen combustion thanks to its potential for high strain rate flow and enhanced mixing. The injector, housed in a square cross-section combustion chamber, is made of two coaxial channels. Hydrogen is injected into the central channel, and air is injected into the outer channel as the oxidizer. The inner channel is equipped with swirl vanes and the outer channel flow is swirled thanks to axial and tangential inlets. This defines two swirl numbers that can be independently controlled and contributes to the generation of multiple flame fronts that may be present simultaneously or not. Flow conditions then yield varying attached and detached flame structures that affect the thermal and chemical environment of the flame. A parametric investigation is undertaken to explore the topologies and the associated NOx emissions of hydrogen flames in this burner at atmospheric pressure. The flame structure is observed using OH\* chemiluminescence images collected by an intensified CCD camera equipped with a band-pass filter. Mole fractions of exhaust gas species (NO + NO<sub>2</sub> and O<sub>2</sub>) are measured using NDIR gas detectors and a paramagnetic sensor. Finally, the temperature is measured at the chamber wall and exit cross-section. The investigation involves varying the inner swirl number by changing the swirl vanes angle and the outer swirl number through variation of the axial to tangential injection ratio. The momentum flux ratio between the two channels of the injector is also varied by modifying the total air flow rate. This allows the exploration of a wide range of flame structures. The study reveals various stabilizations of hydrogen-air flames on the double swirl injector with five types of flame structures ranging from attached diffusion flames to fully lifted flames. The evolution of these structures following variation of inner and outer swirl levels and momentum flux ratio is studied, as well as the associated changes in chamber exhaust temperature and estimated chamber residence time is studied. These parameters are then used to interpret the variation in NOx emissions observed across variations in injection parameters and changes in structure. In addition, low-NOx flames are achieved under high swirl conditions, and hydrogen flames with an emission level under 10 ppm, have been observed.

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# An efficient numerical approach for estimating the flame describing function of hydrogen jet diffusion flames

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Confined flames are susceptible to thermoacoustic instabilities. These are caused by positive feedback between the acoustic field within the combustion chamber and the unsteady heat release rate of the flame. If acoustic waves within the chamber (i.e. weak pressure waves) are sufficiently in phase with the unsteady heat release of the flame, work is done on the fluid surrounding the flame and converted into acoustic energy. If this is not sufficiently damped, successively increasing acoustic pressure and heat release rate oscillation amplitudes occur and can lead to mechanical failure. It is therefore imperative, from an engineering point of view, to design out instability as early as possible within the design process.

A vast literature on the acoustic response of carbon-based fuels is available. However, as the world transitions to more sustainable technologies, hydrogen is likely to replace these fuels in some of their current applications. Hydrogen can be harvested and burnt with net-zero carbon emissions. Unfortunately, several studies suggest that combustors with hydrogen flames have an increased propensity to thermoacoustic instabilities. Furthermore, hydrogen’s unique properties, including its very low density, high mass and thermal diffusivities mean that simplified approaches which worked well for conventional fuels may no longer be sufficient for hydrogen flames.

This study focuses on the weakly nonlinear response of hydrogen jet diffusion flames to upstream velocity forcing. In past studies, the Burke-Schumann model with constant diffusivity and density was applied to conventional fuel mixtures to predict the flame dynamics under acoustic excitation. In the case of hydrogen, the effect of differential mass diffusion, density and heat capacity is thought to have a significant influence on the flame structure and heat release rate, therefore, a new formulation that accounts for some of these effects is here considered.

This study proposes a new numerical solver which can be used to efficiently estimate the flame describing function of hydrogen jet diffusion flames. The model still exploits the infinitely fast chemistry assumption, decomposing the combustion process into a mixing problem and a chemical reaction problem.

The mixing problem is solved by numerically integrating a diffusion-convection conservation equation derived from first principles and tailored to compressible gasses having a Lewis number close to 1, not allowing therefore to capture thermodiffusive effects. The flow velocity field required to solve the mixing equation is recovered by imposing mass continuity.

For the chemical reaction problem, the flame structure is obtained by solving the one-dimensional diffusion flame equilibrium problem.

The flame structure is then imposed over the mixing solution and the temperature field is inte-

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grated over the domain to predict the heat released by the flame.

By harmonically exciting the velocity boundary condition at the inlet of the jet flame, the flame describing function (FDF) of the flame can be obtained.

The solver has been validated against numerical simulations and experimental measurements showing good agreement. Flames obtained by burning pure hydrogen and perfectly cracked ammonia have been tested and the results are presented. The effect of the inlet temperature was investigated, as well as the effect of high water concentrations in the oxidiser stream.

Compared to direct numerical simulations, the reduced computational cost of this solver allows for extensive parametric studies, and if coupled with low order acoustic network solvers like OSCILOS, this solver can be used as a powerful tool in the early stages of combustion chamber design.

# A comparison of flame front extraction algorithms in OH-PLIF images of turbulent hydrogen-enriched methane-air flames

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Hydrogen has harnessed particular attention in the last decade, amid stringent environmental policies and growing sustainability concerns, as a flexible energy carrier of the future. Hydrogen/natural gas blends can be burnt with air in retrofitted combustors which can play a role in reducing carbon emissions while allowing stable operation over a wider range of lean conditions (Bell and Gupta 1997; Schefer 2003). Nevertheless, the addition of hydrogen, a non-unity Lewis number gas, to hydrocarbon fuels can, even at low quantities, alter flame characteristics and affect stability, combustion dynamics, and pollutant emissions (Schefer 2003; Halter et al. 2007). In the presence of turbulence, these flames can experience intense wrinkling leading to the formation of multiscale structures such as islands and pockets. Key geometric information about such flames (local curvature, flame surface density) can be obtained by locating the position of the flame front in planar laser-induced fluorescence or Mie scattering images. The complex flame shapes, multiscale structures, in addition to low signal-to-noise ratios inherent to high-speed diagnostics, pose a certain number of challenges for current contour detectors, which motivates the need for accurate flame front extraction algorithms.

In this work, we investigate the performance of typical flame front extraction techniques and apply them to high-speed OH-PLIF images of turbulent, premixed, hydrogen-enriched flames in a Bunsen burner. Three different techniques are tested: (a) a threshold-based method (Otsu segmentation), (b) a gradient-based method (Canny’s edge detector), and (c) a multiscale approach (complex wavelets). The differences between the flame fronts obtained are quantified and the algorithms are compared in terms of robustness, computational intensity, and sensitivity to conventional filters. The location of the flame front is traditionally determined from OH-PLIF images by locating the steepest gradients of OH intensity, assuming the OH and heat release peaks are coincident. A fundamental distinction is therefore made between segmentation-oriented (Otsu) and edge-oriented (Canny, wavelets) approaches (Papari and Petkov 2011). Flame fronts obtained using the former should be seen as approximations to flame fronts extracted using their edge-oriented counterparts, which highlight local maxima of OH intensity gradients. This is further demonstrated by the high sensitivity of Otsu thresholding to typical edge-preserving filters (anisotropic diffusion, bilateral filtering), which can yield errors larger than the flame thickness under high filtering conditions. An adaptive contrast enhancement method based on histogram equalisation is proposed to improve the robustness of Otsu thresholding. A combination of low/moderate filtering and adaptive contrast enhancement was found to significantly improve the accuracy and robustness of Otsu thresholding, even at high hydrogen-enrichment. Canny’s edge detector was then used to extract optimal flame fronts. A major limitation of this method, a priori knowledge of optimal thresholds, was partially overcome by applying a mask

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to the gradient map. The mask was calculated by morphological dilation of the Otsu contour to enclose the regions of interest. A local search method was then used to fill the small gaps in the obtained edges due to low signal-to-noise ratio regions in the OH-PLIF images. The edge linking method travels through pixels of maximum gradients in the 8-neighbourhood while minimising the search angle (Raghupathy 2004, Sweeney and Hochgreb 2009). Finally, a multiscale approach based on the  $\alpha$ -molecule framework (complex wavelets) was used for flame front extraction (Reisenhofer and King 2019; Grohs et al. 2016). Although the obtained contours were to an extent comparable to the edges found using Canny, the major increase in computational time and the need for further post-processing using this method was deemed unattractive for large data sets.

The result of this work highlights the performance of simpler, computationally inexpensive flame front extraction methods, provided that compatible smoothing filters are applied. Issues with contrast inhomogeneities, which often render the use of a global Otsu threshold impractical, can be overcome using adaptive contrast enhancement techniques. The obtained contours can serve as a good approximation with acceptable accuracy when computing location-independent statistics (i.e: global curvature statistics, flame surface densities). When investigations require high levels of accuracy in determining the flame front, edge-oriented approaches such as Canny should be used. The Otsu contour can be used as a tool to locate the relevant Canny edges and circumvent challenges related to hysteresis thresholding at low computational cost.

# POSTERS

## Toward Development of Machine Learned Techniques for Production of Compact Kinetic Models

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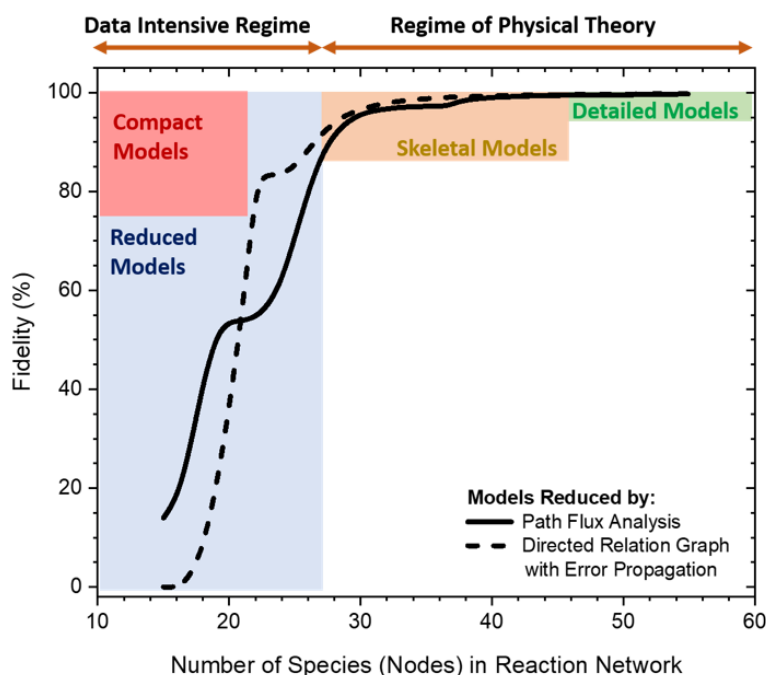


Figure 1. Dependence of fidelity of model calculation for methane combustion on complexity of reaction network, as indicated by number of species (or nodes), where *Detailed*, *Skeletal*, *Reduced* and *Compact Models* occupy different regions of detail-fidelity space. A series of skeletal and reduced models are produced by the Directed Relation Graph with Error Propagation reduction method via DoctorSMOKE++ and by the Path Flux Analysis method from the same detailed mode. The reduction and fidelity assessment were performed at: 1-40 atm, 1100-2000 K, methane/air mixture fractions 0.5 – 1.5, as described in the text.

Chemical kinetic models are an essential component in the development and optimisation of combustion devices through their coupling to multi-dimensional simulations such as computational fluid dynamics (CFD). Due to the significant level of detail contained within, detailed chemical kinetic models are computationally prohibitive for use in CFD. Therefore, low-dimensional kinetic models which retain good fidelity to the reality are needed, the production of which requires considerable human-time cost and expert knowledge.

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Here we present a novel compute intensification methodology to simplify the description of complex chemical reaction systems. This is demonstrated on the archetypal example of the methane combustion system. The coded algorithm, termed *Machine Learned Optimisation for Chemical Kinetics (MLOCK)*, allows for the production of minimally complex, high fidelity kinetic models, which we call "Compact Models" (i.e. minimised and optimised). The methodology is intentionally designed to require minimal starting information or other prior human knowledge. Instead, the MLOCK methodology emphasises the leverage of modern computing resources to perform large numbers of complex simulations quickly with minimal user input. The concept of MLOCK is to produce a data set, which is interrogable by objective data analysis methods, to automatically search the data set to find the optimum set (or sets) of numerical terms which results in an accurate replication of the target calculations.

MLOCK systematically perturbs each of the four sub-models of a chemical kinetic model to discover what combinations of terms results in an objectified good model. A virtual reaction network comprised of  $n$  species is first obtained using conventional mechanism reduction procedures. Once  $n$  is lower than a threshold value, the model performance is typically poor. To counteract this, the weights (virtual reaction rate constants) of important connections (virtual reactions) between each node (species) of the virtual reaction network are numerically optimised to replicate selected calculations across four sequential phases.

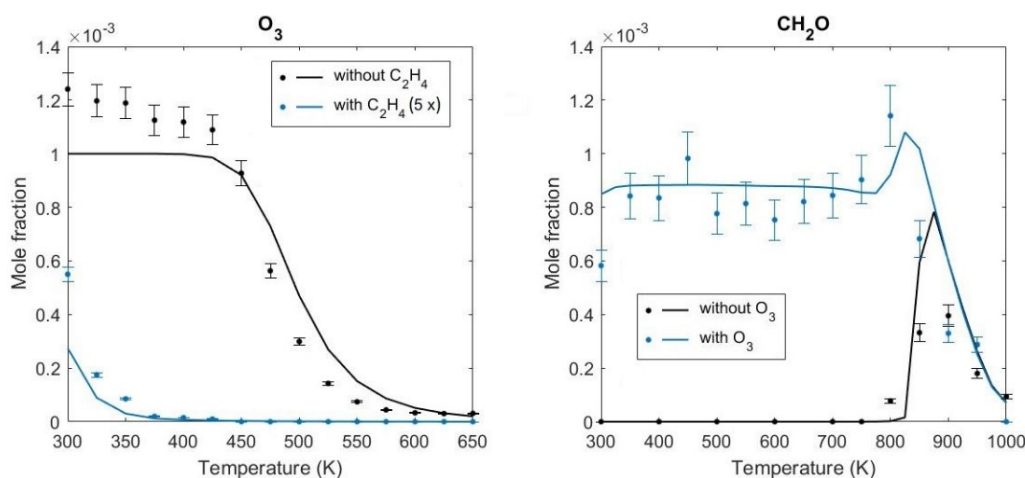
The first version of MLOCK, (MLOCK1.0) simultaneously perturbs all three virtual Arrhenius reaction rate constant parameters for important connections and assesses the suitability of the new parameters through objective error functions, which quantify the error in each compact model candidate's calculation of the optimisation targets, which may be comprised of detailed model calculations and/or experimental data.

In this study, the MLOCK algorithm is demonstrated by automatically creating compact models for the archetypal case of methane air combustion. It is shown that the NUGMECH1.0 detailed model comprised of 2,789 species is reliably compacted to 15 species (nodes), whilst retaining an overall fidelity of  $\sim 87\%$  to the detailed model calculations, outperforming the prior state-of-art.

# Experimental and Modeling Study of Ozone-Assisted Low-Temperature Oxidation of Ethylene in a Jet-Stirred Reactor

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Despite the rise of alternative propulsion technologies (e.g., battery-electric and hydrogen-powered fuel-cells vehicles), combustion will remain an important component of the future of both steady power generation and long-distance transport (aviation, trucks, ships). For these applications, the use of nonpetroleum-based fuels such as sustainably produced biofuels in conjunction with innovative combustion technologies like low-temperature combustion, is a key to ensure a clean and efficient energy conversion and a gradual transition to CO<sub>2</sub>-neutral operation. Plasma-enhanced combustion is a promising technique in the design of advanced air-breathing engines (enhancement of ignition time, flame stabilization and propagation) [1] and recently drew attention to ozone (O<sub>3</sub>), efficiently generated by electric discharge, as a low-temperature reaction promoter [2].

At very low temperature (300 – 600 K), below the thermal decomposition threshold of O<sub>3</sub>, the enhancement of O<sub>3</sub>-assisted alkene oxidation relies on the initial exothermic ozonolysis reaction which results in an abundant heat release, the formation of reactive species and radicals, including partially oxidized intermediates. A change in gas composition compared to the conventional low-temperature oxidation chemistry affects pollutant emission, transport properties, and dynamic characteristics of flame in practical O<sub>3</sub>-assisted combustion processes. Thus, detailed predictive kinetic models need to be developed for the optimization of the current technologies to further reduce soot/NO<sub>x</sub> formation and increase efficiency.

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However, research on the O<sub>3</sub>-assisted oxidation of fuels is scarce since it is a relatively recent field of investigation for the combustion community and with a much higher degree of complexity with alkenes due to the chemistry induced by the ozonolysis reaction. Questions regarding the identification of the low-temperature products and intermediates as well as the secondary reactions after the initial ozonolysis are still open. To address these questions, the ozonolysis of ethylene (H<sub>2</sub>C=CH<sub>2</sub>), the smallest alkene, serves as an ideal system to explore the kinetic networks in depth. The C<sub>2</sub>H<sub>4</sub>/O<sub>3</sub> detailed chemistry leading to room-temperature autoignition is still unclear (e.g. [3-5]).

This work studies the O<sub>3</sub>-assisted oxidation of C<sub>2</sub>H<sub>4</sub> in a jet-stirred reactor (JSR), commonly used for oxidation studies under operating conditions close to practical industrial applications. Residence time, pressure, equivalence ratio, and ethylene molar fraction were 2.5 s, 800 torr, 0.5, and 0.02, respectively. A temperature range of 300 to 1,000 K was covered to probe the different regimes that would be characterized by a unique chemical reaction network. Ozone was produced using an O<sub>3</sub>-generator fed with a O<sub>2</sub>/He gas mixture. O<sub>3</sub> was mixed with the fuel just before entering the JSR. An O<sub>3</sub> mole fraction of 1,000 ppm was introduced into the JSR for each reaction temperature and the O<sub>3</sub> mole fraction profile was obtained using an O<sub>3</sub> analyzer positioned downstream of the reactor. The mole fraction profile of the fuel and reaction products was obtained using the gas chromatography-mass spectrometry (GC-MS) technique.

Preliminary results show that without O<sub>3</sub> injection, C<sub>2</sub>H<sub>4</sub> is not reactive at temperatures below 800 K while a conversion of ethylene is observed from 300 K with an O<sub>3</sub> injection of 1,000 ppm. The formation of reactive species (e.g., carbon monoxide and formaldehyde) in non-negligible quantities is observed (see FIGURE 1). This figure also shows that without ethylene O<sub>3</sub> is almost not consumed before 450 K. The experimental product mole fractions are compared to the predictions of a recent kinetic model from the literature [4] (see FIGURE 1) providing insights into the dominant reaction pathways of the O<sub>3</sub>-assisted oxidation of C<sub>2</sub>H<sub>4</sub>.

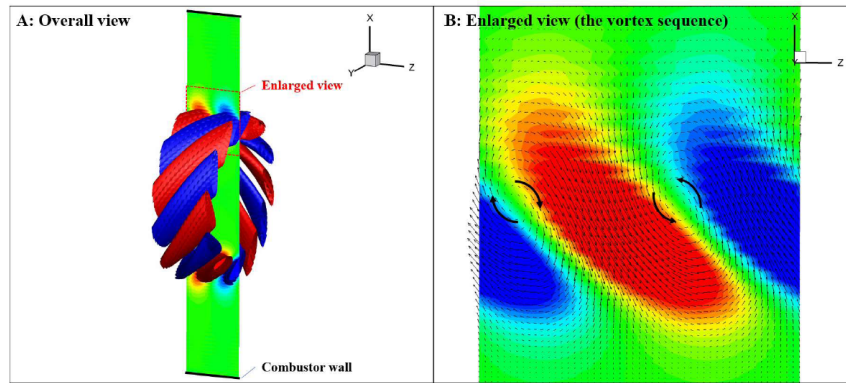
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# Hydrodynamic instability of swirling jet in a gas turbine combustor operating with lean premixed hydrogen-enriched biogas blends

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**Illustration:** Fig. A shows the three-dimensional structure of the dominating perturbation mode of the confined swirling jet. The iso-surface shows the axial velocity perturbation and the contour shows the amplitude of velocity perturbation in the axial-radial plane. Fig. B shows an enlarged view of the in-plane velocity perturbation, which manifests a vortex sequence that resembles the precessing vortex core.

Biogas, primarily consisting of methane, is a clean alternative for natural gas, as it produces net zero carbon emission. It has been shown that the biogas can be further improved by hydrogen addition, in terms of its kinetic and dynamic characteristics, such as flammability limit, flame temperature and combustion efficiency. In the present research, we investigate the dynamics of a gas turbine combustor operating with lean premixed hydrogen-enriched biogas blends. At lean combustion mode, thermoacoustic oscillation is one of the major issues for gas turbine combustors. The associated pressure fluctuation and unsteady heat release cause excessive wear to the combustor, or even structural failure. The present research aims to understand the contribution of hydrodynamic instability to the onset of thermoacoustic oscillation for a hydrogen-enriched biogas fuel. The concentration of hydrogen varies from 0% to 40% in the blend. The flow field and heat release rate of three distinctive thermoacoustic states, i.e., quiescent, intermittent and limit cycle, are measured by high-speed particle image velocimetry and chemiluminescence. The time-averaged flow field of the three scenarios is then analyzed by linear stability analysis to understand their characteristics of hydrodynamic instabilities. The measured flow field in the combustor consists of a confined swirling jet surrounding a recirculation zone, generated by an adverse pressure gradient as the swirl expands. The stability analysis reveals three discrete modes in the confine swirling jet. The dominating mode is an unstable helical mode of azimuthal wavenumber  $m = 6$ , which winds around the shear layer at the boundary of the recirculation zone. The corresponding time evolution of the three-dimensional perturbation field shows that

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the perturbation rotates at the centerline and propagates downstream. The perturbation velocity undulates in space and perturbs the swirl jet periodically, at a dominating frequency and wavelength of 410Hz and 1.1cm. The perturbation generates a sequence of downstream travelling vortices, which resembles the precessing vortex core as observed in the experimental measurement. The two other modes are found to be both decaying with time. One is located near the centerline of the swirl jet, at a higher frequency of 801Hz, and the other is found to be further outside the rigid-body rotation part of the swirl jet at a frequency of 413Hz. Notably, the second mode does not occur in an unbounded swirling jet, which might be associated with the boundary layer at the combustor wall. The stability analysis shows that the onset of PVC, which originates from hydrodynamic instability, follows the route of a super-critical Hopf bifurcation. This is in contrast with the subcritical bifurcation of thermoacoustic oscillation that occurs in the combustor. The different transition routes of hydrodynamic instability and thermoacoustic instability points to the role of flame that renders the system to nonlinearly unstable. **Keyword:** lean combustion, hydrogen combustion, swirling jet, thermoacoustic oscillation, hydrodynamic instability

# Performance of kinetic reaction mechanisms in predicting the laminar burning velocities of Ammonia-Hydrogen flames

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Energy from chemical fuels contributes to both domestic and industrial activities worldwide. However, over-reliance on hydrocarbon fuels has caused environmental drawbacks affecting human life and the ecosystem. Therefore, several studies are being carried out to find alternative carbon-free fuel sources. Ammonia has recently gained interest as one of these zero-carbon alternative sources. It offers several advantages, including its hydrogen carrier characteristics. However, the low burning velocity and high levels of nitrogen oxides (NO<sub>x</sub>) emissions of pure ammonia flames have led to the use of hydrogen-doped ammonia blends. To improve ammonia-based combustion technology, the ammonia chemistry and the chemical process of ammonia combustion should be deeply understood, thus requiring the knowledge of the essential combustion features and detailed chemical reactions. Therefore, the present work investigates the laminar burning velocity of the ammonia-hydrogen blend (70-30% vol). The four best performing kinetic reaction mechanisms for laminar burning velocity were identified from a total of 36 kinetic mechanisms from the literature. A chemical kinetic simulator (CHEMKIN-PRO) software was adopted to investigate the chemical kinetic of species in the gas phase under atmospheric conditions. The numerical results have been compared with experimental measurements from the literature. The results denote how the laminar burning velocity for this NH<sub>3</sub>-H<sub>2</sub> blend hits the maximum when the equivalence ratio is equal to 1.1. Also, both Gotama et al. (2021) and Stagni et al. (2020) provide a good agreement on lean conditions, while Nakamura et al. (2017) and Zhang et al. (2017) mechanisms are found to be more effective in estimating the laminar burning velocity at the rich region. These mechanisms were then analyzed based on reaction sensitivity and rate of production to identify the differences and key characteristics of these models. This analysis also demonstrated the important role of the reaction  $O_2 + H \leftrightarrow O + OH$  in ammonia oxidation. Furthermore, the dominant reaction in the decomposition of ammonia was found to be  $NH_3 + OH \leftrightarrow NH_2 + H_2O$ , and it has a negative sensitivity due to the consumption of active OH radicals.

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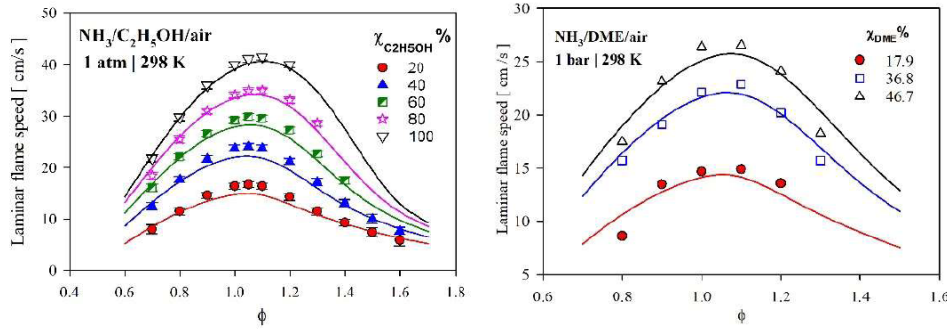
# Kinetic study on the influence of blending ethanol and dimethyl ether on the combustion behavior of ammonia

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**Figure 1:** Laminar flame speed of NH<sub>3</sub>/C<sub>2</sub>H<sub>5</sub>OH/air (left) and NH<sub>3</sub>/DME/air (right) at 1 bar/1atm and 298 K. Symbols: measurements, NH<sub>3</sub>/C<sub>2</sub>H<sub>5</sub>OH [2] and NH<sub>3</sub>/DME [3]. Lines: our kinetic model predictions.

$$\chi_{C_2H_5OH} = \frac{C_2H_5OH}{NH_3 + C_2H_5OH} \text{ and } \chi_{DME} = \frac{DME}{NH_3 + DME} \% \text{ (by mole).}$$

Ammonia (NH<sub>3</sub>) has excellent potential as a carbon-free fuel and ideal H<sub>2</sub> carrier for decarbonizing the industry and transportation sectors. Over the past few years, there have been significant efforts to explore the ways for clean, efficient, and effective utilization of ammonia on a large scale for combustion systems. However, ammonia combustion poses some unique challenges for its direct application in various practical combustion devices. There is a general belief that blending NH<sub>3</sub> with high reactivity fuels is an efficient way to overcome some of the inherent challenges of NH<sub>3</sub> combustion and meet carbon-neutrality at the same time. Renewable biofuels as combustion promoters look promising as they can be produced in a sustainable net-zero carbon cycle. Hence, co-firing NH<sub>3</sub> with renewable biofuels appears to be an amicable transition to a low-carbon society. To this end, ethanol (C<sub>2</sub>H<sub>5</sub>OH) and Dimethyl ether (DME, CH<sub>3</sub>OCH<sub>3</sub>) can be a promising candidate to promote NH<sub>3</sub> combustion for future sustainability. Both ethanol and DME are known to exhibit clean combustion. These isomers have different functional groups; therefore, they have different physical and chemical properties. Because of their remarkable combustion properties, they are attractive fuels to promote the combustion behavior of ammonia.

This work explores the blending effect of ethanol and DME on the combustion behavior of NH<sub>3</sub>. Our recent kinetic model (Shrestha et al. [1]) was employed to characterize the blends' combustion properties. Although ethanol and DME are part of our kinetic model [1], it was not

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validated for NH<sub>3</sub>/ethanol and NH<sub>3</sub>/DME blends earlier. Here, we conducted a detailed kinetic study to rationalize the similarity and differences of the enhancement effects of ethanol and DME on NH<sub>3</sub> combustion. Figure 1 shows the laminar flame speed of NH<sub>3</sub>/C<sub>2</sub>H<sub>5</sub>OH/air and NH<sub>3</sub>/DME/air at 1 bar and 298 K as a function of equivalence ratio. Symbols are experimental data reported in the literature, and lines are model predictions from this work. As seen, our model excellently captures the experimental data for the wide range of fuel blends. However, the model slightly underpredicts the laminar flame speed for  $\chi$ C<sub>2</sub>H<sub>5</sub>OH = 20, 40, and 60. We further investigated the laminar flame speed investigation of NH<sub>3</sub>/C<sub>2</sub>H<sub>5</sub>OH ( $\chi$ C<sub>2</sub>H<sub>5</sub>OH = 10 and 30), and NH<sub>3</sub>/DME ( $\chi$ DME = 10 and 30) blends under engine relevant conditions e.g.,  $\phi = 1.0$ ,  $T = 600$  K and  $P = 1$ -50 bar. Interestingly, despite having different molecular structures of the isomers, both isomers exhibited similar enhancement effects for the laminar flame speed of NH<sub>3</sub>.

We also investigated the ignition delay times behavior of NH<sub>3</sub>/C<sub>2</sub>H<sub>5</sub>OH and NH<sub>3</sub>/DME blends. We found that adding as little as 10% C<sub>2</sub>H<sub>5</sub>OH and DME shortens the ignition delay times of ammonia at  $\phi = 1.0$ ,  $P = 40$  bar and  $T = 1000$  K by a factor of 21 and 34, respectively. Below 1000 K, the blends of ammonia with the two isomers show a significant difference in the reactivity owing to their unique low- $T$  oxidation chemistry. The IDT of  $\chi$ C<sub>2</sub>H<sub>5</sub>OH = 10 was found significantly higher (lower reactivity) as compared to  $\chi$ DME = 10. For instance, the IDT of  $\chi$ C<sub>2</sub>H<sub>5</sub>OH = 10 is  $\sim 188$  ms and  $\chi$ DME  $\sim 17$  ms at  $\phi = 1.0$ ,  $P = 40$  bar and  $T = 800$  K. Such difference is not too surprising due to the active low-temperature chemistry of DME (higher OH radicals' concentration) as compared to ethanol. However, above 1000 K, both  $\chi$ C<sub>2</sub>H<sub>5</sub>OH = 10 and  $\chi$ DME = 10 exhibits similar ignition properties as that seen for laminar flame speeds.

# Measurement and simulation of sooting characteristics by an ATJ-SKA biojet fuel and blends with Jet A-1 fuel in laminar non-premixed flame

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We investigate the sooting propensity of an Alcohol-to-Jet-Synthetic Kerosene with Aromatics (ATJ-SKA) biojet fuel. The soot volume fraction and primary particle size in the pre-vaporised diffusion flames using ATJ-SKA biojet and blends with Jet A-1 at atmospheric conditions were measured experimentally and compared to numerical simulations. The measurements were conducted using extinction calibrated laser induced incandescence (LII). The soot volume fractions measured using the ATJ-SKA fuel do not show significant differences relative to measurements with Jet A-1. A comparison of the chemical composition of the fuels suggests that the Degree of Unsaturation (DoU) may not determine the sooting propensity of biojet fuels. The SEM analysis shows that diffusion flames using neat Jet A-1 produce finer soot particles and larger number density compared to the biojet and biojet surrogate. The soot model employs a semi-detailed chemical kinetic mechanism and a physical model which integrates the population balance equation governing the soot particle size distribution with an in-house reactive flow solver for multicomponent ideal gases. The model predicts the maximum soot volume fraction (SVF<sub>m</sub>) in the neat biojet case and the blended cases with Jet A-1 fuels within an error margin of 13% of the measured values. However, the predicted soot volume fraction distribution patterns differ from the measured one and the possible causes are discussed.

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# Progress in the study of the chemical kinetics of cyclic ethers in combustion

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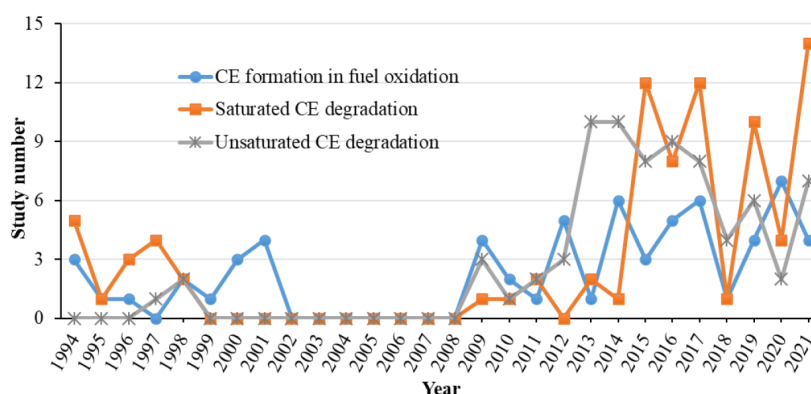
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Fig. 1 below is an exemplary figure, which presents an overview on the number of studies found in the literature over the years after 1994 related to CE formation and consumption chemistry.



**Fig. 1.** Number of studies found in the literature over the years after 1994 related to CE formation during fuel low-temperature oxidation and to the consumption of saturated and unsaturated CEs.

Cyclic Ethers (CEs) belong to a class of compounds of importance to understand the chemistry of both the auto-ignition of hydrocarbon fuels and the combustion of oxygenated biofuels. Our recent review article, which is under revision process, aims at systematically analyzing the application of up-to-date methods to unveil the gas-phase oxidation chemistry of these compounds and analyzing our knowledge on the formation and consumption chemistry of these compounds. In the present presentation, some selected examples concerning the chemistry of CE high-temperature degradation with enlightening the specific experimental and modeling features of the involved reactions are presented and discussed.

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# Development of a detailed surface reaction mechanism using thermodynamic analysis to investigate steam reforming of methane over nickel catalyst

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The reforming of light hydrocarbons to produce synthesis gas, H<sub>2</sub>, and CO, is an important intermediate in the chemical industry for manufacturing valuable basic chemicals as well as synthetic fuels and has gained much attention in recent years [1]. The reforming of methane with either steam or steam/CO<sub>2</sub> mixture is particularly efficient for producing synthesis gas from greenhouse gases. In industry, the steam reforming of methane is getting renewed attention due to a widespread interest in operating with an increasing CO<sub>2</sub> amount in the feed. Steam reforming is preferably performed using a nickel catalyst as nickel is the conventional catalyst in the industry due to its fast turnover rates, good availability, and low costs.

To reach a profound understanding of the catalytic reforming of methane over nickel, it is needed to better comprehend the elementary steps involved in the reaction mechanism at a molecular level. Several techniques have been used to study the reforming of methane, and different reaction mechanisms and corresponding kinetic models have been proposed [2]. Despite all the experimental and theoretical investigations, the detailed path for the conversion of methane to syngas remains a controversial issue. The majority of open literature discusses the kinetic models for steam- or CO<sub>2</sub>-reforming in the gas phase. Although a variety of detailed multi-step surface reaction mechanisms have been published, for instance in [2,3] and the references therein, there are not any mechanisms available in literature that provides kinetically consistent reaction mechanism. The available surface reaction mechanisms only consider thermodynamic consistency.

In the present study, a one-dimensional (1D) model [4] is utilized to develop a detailed surface reaction mechanism for modeling the steam reforming of methane over a nickel-based catalyst. The 1D tool is computationally -effective due to the reduction in dimensionality, in contrast to the experimental investigations that are not always feasible, or the 2D/3D simulations, which are computationally expensive, especially when we include the full reaction mechanism. The model is based on a series of perfectly stirred reactors (PSR) which is applicable to the simulation of all standard after-treatment catalytic processes of combustion exhaust gas and other chemical processes involving heterogeneous catalysis such as the Sabatier process [5,6].

The conversion of methane and steam into a mixture of H<sub>2</sub>, CO and CO<sub>2</sub> can be examined as a combination of several reactions. We have considered two surface reaction mechanisms from the literature [2,3]. The multi-step reaction mechanism from [2] consists of 52 and from [3] 42 elementary-step reactions which are thermodynamically consistent. Based on these mech-

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anisms, a kinetically consistent mechanism has been developed that consists of 21 reversible reactions achieved with the help of thermodynamic analysis. The method is presented for ensuring kinetic consistency and this, in turn, brings thermochemistry of species in play while developing a surface reaction mechanism. The applicability of the mechanism is tested by comparing the results from [2,3] for several chemical reaction terms, such as, selectivity, conversion and H<sub>2</sub>/CO ratio.

Figure 1 below shows the conversion of methane and water as a function of temperature while keeping all the other parameters fixed as steam-to-carbon ratio (S/C) 2.77, pressure (P) 1 atm, mass flow rate 593 mL/min, and 75% Argon dilution. The closed symbols represent the experimental data from [3]. Further simulations are performed for varying inlet gas compositions and operating temperatures. The detailed mechanism developed in the given investigation is able to accurately capture steam reforming of methane over the nickel catalyst for various profiles.

*Keywords:* Nickel-based catalyst, One-dimensional modeling, Methane, Steam reforming, Detailed reaction mechanism

Figure 1: Methane and water conversion as a function of temperature while keeping all the other parameters fixed as S/C=2.77, P=1 atm, mass flow rate 593 mL/min and 75% Argon dilution. Closed symbols are experimental data from [3].

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# A combined experimental and kinetic modeling study on the low-temperature oxidation of oxymethylene ether-2 (OME-2)

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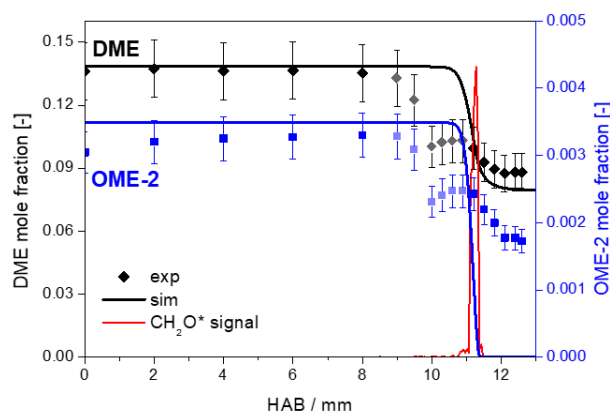


Fig. 1. Mole fraction profile of the fuels as a function of the height above the burner (HAB) obtained from stagnation plate burner experiments.  $\phi = 0.5$ ,  $\alpha = 50 \text{ s}^{-1}$ ,  $x_{O_3} = 1.6\%$ , 2.5%OME-2/97.5%DME

The present research focuses on the combined experimental and kinetic modeling work on the low-temperature oxidation of oxymethylene ether-2 (OME-2). Oxymethylene ethers (OMEs) are a promising family of molecules whose structure consists of alternating carbon and oxygen atoms and which exhibit excellent fuel characteristics. These molecules can be produced in a carbon-neutral manner by means of captured CO<sub>2</sub> and renewable energy. Furthermore, blending OMEs with conventional diesel reduces the particulate matter emissions compared to fossil fuels, because of the absence of carbon-carbon bonds, and reduces the trade-off between soot and nitrogen oxides. This results in less harmful emissions and contributes to a more sustainable transport sector as aimed by the Paris climate agreement objectives. To promote the use of these classes of molecules as sustainable fuel alternatives, it is important to fully understand the low-temperature oxidation chemistry of OMEs. The development of detailed microkinetic models for small OMEs, here OME-2, provides this fundamental insight and enables extrapolation towards larger OMEs.

Great progress has been made in the construction of reliable kinetic models for pyrolysis and combustion of (oxygenated) hydrocarbons. The resulting models typically contain hundreds of species, and several thousands of associated reactions. The manual generation of a microkinetic model would thereby be a tedious, error-prone and often incomplete process. To prevent

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this, automatic kinetic model generation routines have been developed, such as the in-house developed code Genesys [1], to systematically develop kinetic models. In this work, a new microkinetic model for the combustion of OME-2 has been constructed with Genesys based on first principles. This model is an extension of an earlier developed model [2] to better describe the low-temperature chemistry by also including the addition of hydroperoxyl alkyl radicals to molecular oxygen. Within Genesys, the possible reactions are generally defined in terms of reaction families, e.g., addition of a primary alkyl radical to molecular oxygen to form a peroxy radical. Reaction families from earlier studies on smaller oxymethylene ethers such as dimethoxymethane [3] have been considered and used for this new OME-2 model. The Genesys model is then merged with an older OME-2 model to include accurate chemistry for smaller (oxygenated) hydrocarbons.

A prerequisite for the construction of reliable kinetic models is the availability of accurate thermodynamic and kinetic parameters for species and reactions, respectively. Ideally, these parameters are obtained from experiments or high-level quantum chemical calculations. In this work, thermodynamic and kinetic parameters have been obtained from quantum chemical calculations at the CBS-QB3 level of theory for important low-temperature reaction pathways of OME-2. Potential energy surfaces have been constructed to gain insight in the important decomposition pathways and compare them with typical alkane reaction pathways. The results of these quantum chemical calculations will be extrapolated to be valid for longer-chain OMEs by regression of new group additive values and kinetic rate rules.

To help validate the developed kinetic model, especially in the lowest temperature region of the combustion regime, the chemical structure of stabilized DME/OME-2 cool flames have been determined in a stagnation plate burner. To do so, ozone was seeded in DME/OME-2/O<sub>2</sub> mixtures to facilitate radical generation and the initiation of reactivity. A variety of diagnostics, including in-line mass spectrometry and gas chromatography have been used to accurately measure the mole fraction profiles of the reactants, intermediates and products. Additionally, a rapid compression machine was used to measure ignition delay times under oxygen-rich conditions (equivalence ratio of 0.5) [2] that were also used as validation data.

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