BOOK OF ABSTRACTS

International Conference on Measurements of Energy

ICME 2025

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23-25 June 2025
Orléans, France

CAPRYSSES

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IMEKO
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Technical Committee TC20 Measurements of Energy and Related Quantities

ICME 2025

International Conference on Measurements of Energy

23–25 June 2025 Orléans

		Monday 23/6
12:00		**Registration**
13:00		**Welcome address**
13:15	Chair: Bo Shu	**Noud Maes** Experimental study of hydrogen injections in an Argon Power Cycle
13:40		**Liguang Li** A Novel Hydrogen Energy Storage System: On-site Hydrogen and Oxygen Production from Excess Renewable Power followed by Power Regeneration Employing an Argon Power Cycle
14:05		**Robert Dibble** The Long-Awaited Hydrogen-Fueled Argon Engine with Greater Efficiency Than Fuel Cells, >65% with a path to >70%, May Debut at the End of the World
14:30		**Nicolas Villenave** Infrared-Based Determination of Bunsen-Burner Wall Temperature for Hydrogen/Air Laminar Flames
14:55		**Coffee Break (posters)**
15:15	Chair: Roy Hermanns	**Nils Hansen (online)** Understanding Chemical Transformations in a Closed Carbon Cycle
15:40		**Yanan Huo** Experimental and numerical kinetic study of OME2 and OME3 combustion in low-pressure laminar flames
16:05		**Perla Trad** Cool flame propagation velocities of DEE: determination in an ozone-seeded stagnation plate burner configuration
16:30		**Jens Brunzendorf** Remote Sensing of Hydrogen Flames Under Daylight Conditions
16:55		**Seif Zitouni / Joachim Beeckman** On the accuracy of laminar flame speeds and Markstein lengths measured from spherically expanding ammonia/air flames
18:00		**Welcome cocktail (Hôtel Groslot)**

		Tuesday 24/6
08:30		**Registration**
09:00	Chair: Véronique Dias	**Pascale Desgroux** The challenge of measuring NO in hydrogen and ammonia flames to better understand the NO formation pathways
09:25		**Guillaume Dayma** An experimental theoretical and modeling study of the pyrolysis and oxidation of neo-pentanol using CO time-histroy measurements behind reflected shock waves
09:50		**Olav Werhahn** Nitrous oxide emissions - monitoring a critical aspect of the energy source diversification
10:15		**Christophe SARRAF** Development of Primary Standards for High-Frequency Dynamic Pressure Calibration
10:40		**Coffee Break (posters)**
11:00	Chair: Guillaume Dayma	**Philippe Dagaut** On the characterization of highly oxidized products from cool flames in a continuously-stirred tank reactor
11:25		**Kai Moshammer** Molecular-Beam Mass Spectrometry under the Lens: Uncertainties in Measuring Species Concentrations
12:00		**Zhandong Wang (online)** Ozone-assisted low-temperature oxidation of C1-C4 alcohols
12:25		**Scott Goldsborough** Towards quantitative model comparisons against measurements from RCMs and JSRs
12:50		**Lunch (on site)**
14:10	Chair: Zeynep Serinyel	**Scott Goldsborough** RCM Workshop 3rd Characterization Initiative: Resolving complications of multi-stage ignition
14:35		**Leopold Seifert** Preliminary results from the 3rd RCM characterization initiative: Dimethylether investigations at PTB RCM facility
15:00		**Rana Shebly** Dimethyl Ether Auto-ignition Delay Measurements in a Rapid Compression Machine
15:25		**Florian Hurault** Uncertainties on Initial conditions and IDT measurements in a Rapid Compression Machine
15:50		**Coffee Break (posters)**
16:10	Chair: Christine Rousselle	**Seong-Young Lee** Resolving Mixture Stratification in Hydrogen SCC Using Calibrated LIBS and Acetone PLIF Measurements
16:35		**Vivek Chougale** Impact of Radiation and Water Vapor on Fundamental Properties of Lean Laminar Hydrogen/Air Flames
17:00		**Fabien Halter** Metals as Future Carbon-Free Energy Carriers
17:40	Moderator: D. Fabeck	**WIMER Session** **Women in Metrology and Energy Research** Panelists: Christine Rousselle, Lijuan Wang, Véronique Dias, Caiying Sun, Madlen Chao
18:40		**Dinner (Jardin de l'Evêché)**

		Wednesday 25/6
09:00	Chair: Kai Moshammer-Ruwe	**Caiying Sun** Measurement of CO2 gas-liquid two-phase gas volume fraction using capacitive sensors
09:25		**Lijuan Wang** Vibration Frequency Measurement of Wind Turbine Blades through Moiré Pattern Analysis
09:50		**Jeerasak Pitakarnnop** Development of a National Facility for Traceable Aerodynamic Testing in Thailand: Advancing National Metrology, Energy and Aerospace Applications through 15 kPa Differential Pressure Standard
10:15		**Bo Shu** Simultaneous dynamic NO, H2O, and temperature measurement using an intrapulse laser with MHz time resolution in a shock tube
10:40		**Coffee Break (posters)**
11:00	Chair: Jenz Brunzendorf	**Maedeh Askarzadehardestani** Impact of Different Charge and Discharge Profiles on the Aging Behavior of Second-Life Lithium-Ion Batteries: An EIS-Based Approach
11:25		**Torben Jennert** Assessing the safety of lithium-ion batteries using electrochemical impedance spectroscopy: indicators, challenges and measurement techniques
11:50		**Freyja Galina Daragan** Pressure measurement during thermal runaway of lithium-ion batteries: Comparison of piezoelectric and piezoresistive pressure sensors
12:15		**Nattapong Chuewangkam** Development of a National Shock Tube Facility for Combustion Energy Calibration: Enabling Thailand Advancements in Aerospace Applications and Metrological Infrastructure
12:40		**End of conference remarks**

Experimental study of hydrogen injections in an Argon Power Cycle

Max Peters, Yu Wang, Noud Maes*, Nico Dam, Jeroen van Oijen

Eindhoven University of Technology, Eindhoven, Netherlands

Abstract: Within the Eindhoven University of Technology Zero Emission Laboratory, hydrogen injections have been studied extensively in a range of optically accessible experimental facilities. Targeting an argon power cycle to increase the thermal efficiency because of the increased specific heat ratio, hydrogen jets are characterized in both nitrogen and argon ambient environments. Force measurements were conducted to quantify the momentum of the injected gas, characterizing the flow losses in the used injection equipment. Schlieren is used to quantify the impact of ambient gas and nozzle pressure ratio on jet penetration in a high-pressure constant-volume vessel, while quantitative mixing measurements are performed using planar Rayleigh scattering and planar laser-induced fluorescence with tracer seeding of the ambient gas. Finally, hydrogen jet combustion is studied over a range of high-temperature (900-1400 K), high pressure (4 MPa) nitrogen-oxygen and argon-oxygen ambient (0-21vol% O2) conditions. The reacting jets are studied in another constant-volume pre-burn vessel using high-speed pressure analysis, high-speed schlieren imaging, and high-speed OH* chemiluminescence visualization. At temperatures exceeding 1000 K, auto-ignition is observed, but complete combustion requires temperatures of at least 1100 K. Reduced oxygen percentages are considered beneficial for further increasing the ratio of specific heats, leading to a higher observed pressure rise in the used facility. Current efforts within the Zero Emission Laboratory involve the application of the argon power cycle in a single-cylinder diesel engine.

About the presenter: Noud Maes is an Assistant Professor working for the Power & Flow group in the department of Mechanical Engineering at the Eindhoven University of Technology. His key areas of expertise include high-pressure sprays, internal combustion engines, future fuel technology, combustion, high-speed (optical) diagnostics, and laser-based measurement techniques. He studied Mechanical engineering at the Eindhoven University of Technology and obtained his PhD in 2019 at the same university on the topic of high-pressure, high-temperature fuel sprays. During his PhD, he worked as a visiting researcher at the French Institute of Petroleum (IFPEn) in Rueil-Malmaison and later at the Combustion Research Facility (CRF) of Sandia National Laboratories in Livermore, California, USA. In 2019, he started a post-doc position at Sandia's CRF in Livermore, and since 2020 he holds his current position at the Eindhoven University of Technology

Keywords: hydrogen jets, hydrogen ignition, high-speed schlieren imaging, Rayleigh scattering, Laser Induced Fluorescence, high-speed chemiluminescence imaging

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A Novel Hydrogen Energy Storage System: On-site Hydrogen and Oxygen Production from Excess Renewable Power followed by Power Regeneration Employing an Argon Power Cycle Hydrogen-fueled Engine with a Net Indicated Thermal Efficiency to 70%

Chenxu WANG[1], Jun DENG[1], Robert DIBBLE[2], Liguang LI[1*]

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Introduction: In the context of developing and storing renewable power, hydrogen energy storage systems (HESSs) show excellent application prospects. However, HESS has been discouraged by low round trip efficiencies (RTE) with hydrogen-to-electricity generating efficiency being a key bottleneck; general below 50% when using hydrogen fuel cells (HFCs) or hydrogen-fueled internal combustion engines (HICEs). By using Argon as the working fluids, Argon Power Cycle (APC) HICEs have achieved a net indicated thermal efficiency (NITE) of nearly 70%. The APC HICE offers high efficiency at a high power, zero carbon emissions, and zero pollutions, and can be quickly put into service with few modifications to existing engines. The capital cost of APC HICE is close to conventional HICE using air and is significantly lower than HFC. This work proposes a novel HESS based on APC HICE that utilizes excess renewable power to produce hydrogen and oxygen and then regenerate power using APC HICE. The RTE of the HESS is over 44% and may be increased to 55% with future improvements in hydrogen generating efficiency and water electrolysis efficiency. The proposed HESS is a global solution that reduces the waste of excess power generated from solar, wind power and other fluctuating sustainable power.

Methodology: The use of APC HICE as a power generator is an excellent solution to improve the RTE of HESS. The APC HICE is a novel power cycle concept, which uses argon as the working fluid and supplies oxygen as the oxidizing agent. Due to the high specific heat ratio of argon, the APC HICE has a higher thermal efficiency than conventional HICE using air. The advantages and challenges of applying different hydrogen power devices (including APC HICE, HICE, and hydrogen fuel cell) in HESS are investigated to provide a reference for selecting the best power generation device. In addition, the RTE and capital cost of HESS using different power generation devices are calculated in detail.

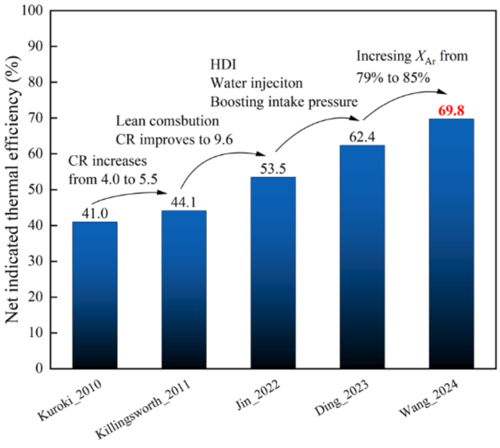

Fig.1 Efficiency improvement path in APC HICE

Experimental Evaluation: Fundamental experiments have been carried out on the APC HICE test bench, achieving a net indicated thermal efficiency to 70%. The strategies include high compression ratio, high pressure intake, water injection, high argon/oxygen ratio. Figure 1 shows the path of efficiency improvement in the APC HICE.

Keywords: hydrogen energy storage, argon power cycle, hydrogen internal combustion engine, high efficiency.

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The Long-Awaited Hydrogen-Fueled Argon Engine with Greater Efficiency Than Fuel Cells, >65% with a path to >70%, May Debut at the End of the World

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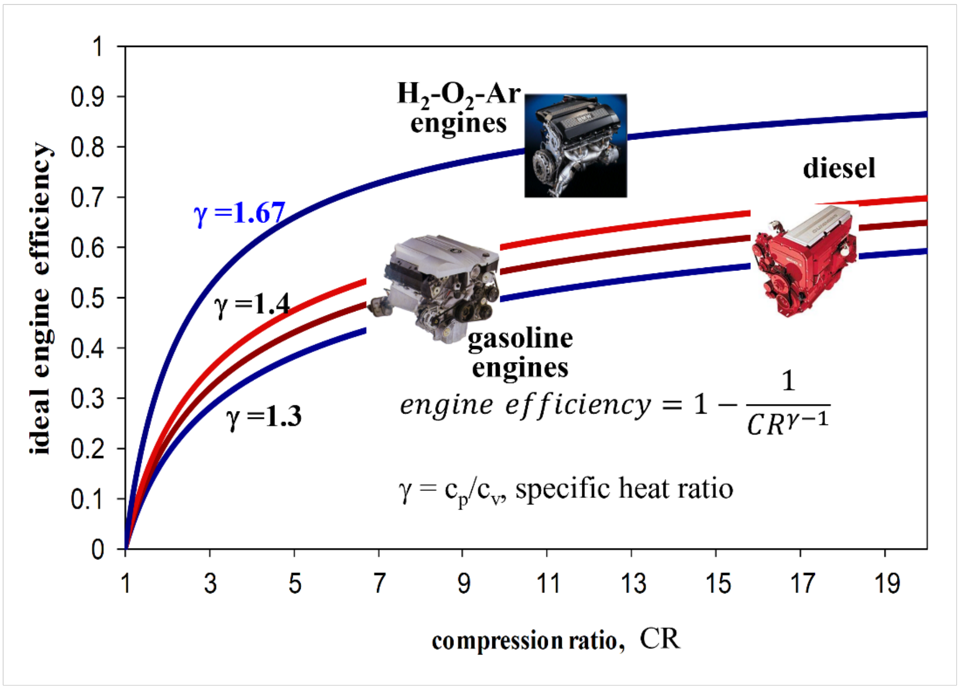
[1]*University of California, Berkeley, USA,* [2]*Tongji University, Shanghai, China*

Introduction: The talk will cover several subjects; a few photos of me at KAUST in 2008, when KAUST was 1 meter high. A discussion of the evolution of the Argon Power Cycle, aka "Dibble Cycle" since, also 2008, with a view, finally, of energy storage for Data Centers in windswept Patagonia. The latest experiments show efficiency at >65% with an easy view to >70% (Argon may find it's place, as a working fluid in some very large Heat Pumps). "As Time Allows" I will venture a few comments on a career in Combustion.



Keywords: argon power cycle; internal combustion engine; thermal efficiency

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Infrared-Based Determination of Bunsen-Burner Wall Temperature for Hydrogen/Air Laminar Flames

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Introduction: The decarbonization of practical combustion systems is increasingly supported by the use of hydrogen as a green e-fuel, particularly in the context of power-to-gas strategies. While the geometry and operating conditions of Bunsen-type burners have been extensively studied, the temperature distribution along burner walls remains poorly documented. This parameter plays a key role in flame stabilization phenomena such as flashback and autoignition, and in defining accurate boundary conditions for computational fluid dynamics (CFD) simulations. General temperature measurements often rely on contact-based methods (e.g., K-type thermocouples) or optical pyrometry techniques (e.g. double-wavelength pyrometer). To complete these approaches, this study introduces a non-intrusive methodology using an infrared camera to assess the surface temperature of burner walls.

Methodology: To complete these approaches, this study introduces a non-intrusive methodology using an infrared camera to assess the surface temperature of burner walls. The method is applied to a laminar, premixed, conical hydrogen-air flames across a wide range of equivalence ratios
($0.6 \leq \phi \leq 1.4$) under ambient conditions (T_u = 298 K, p_u =1 bar). Notably, attention is given to the influence burnt gases – particularly water vapor – which can affect infrared measurements by contributing additional emission and absorption along the optical path. Temperature measurements were performed on both inner and outer burner surfaces, with and without the presence of a coflow.

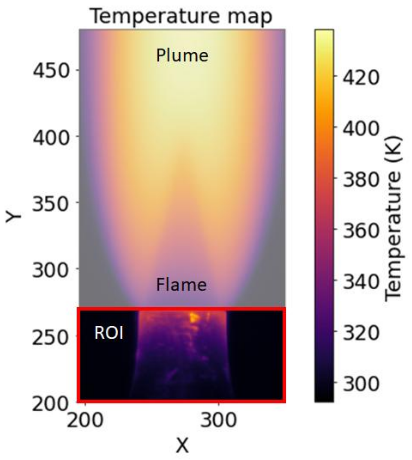

Fig.1 Temperature map for ϕ = 1.0 without coflow.

Experimental Evaluation: Results show a clear increase in wall temperature with equivalence ratio, peaking near ϕ = 1.1, consistent with the peak of the adiabatic flame temperature. At fixed equivalence ratio (ϕ = 1.0), the presence of the coflow skirt significantly increases the outer wall temperature, primarily due to reduced convective heat losses and enhanced thermal preheating of the surrounding surfaces. Conversely, increasing the coflow velocity leads to a decrease in wall temperature, marking a transition from natural to forced convection regimes. Finally, these wall temperature measurements also offer a pathway to estimate the temperature of the fresh gas mixture at the burner exit, providing valuable information for boundary condition specification. Overall, this work establishes a robust and practical methodology for wall temperature characterization, with direct relevance to the retrofitting of low-carbon combustion systems.

Keywords: Hydrogen; Bunsen-burner; Infrared thermal imaging; Temperature

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Understanding Chemical Transformations in a Closed Carbon Cycle

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Introduction: A closed carbon cycle relies on converting carbon-based resources into useful products. By integrating innovative chemical techniques, a closed carbon cycle fosters a circular system where carbon-containing species continuously move through various transformations. This presentation will highlight how basic research can support a transition into such a closed carbon cycle.

Methodology: We have applied mass spectrometric approaches to provide basic insights into chemical kinetics of reaction networks of complex environments and applications, including catalytic and plasma-assisted chemical transformations.

Experimental Evaluation: This presentation focuses on reaction networks found in catalytic heterogenous chemical transformations and on non-equilibrium plasmas that can initiate chemical conversion through the generation of charged species, radicals, and excited state species. We will highlight the chemistry of processes such as the catalytic oxidative coupling of methane, the Fischer-Tropsch process, and plasma-assisted processes such as chemical looping combustion, methane dry reforming, and CO_2 hydrogenation.

Keywords: chemical transformations, CO_2 recycle, plasma, catalysis, mass spectrometry

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Experimental and numerical kinetic study of OME_2 and OME_3 combustion in low-pressure laminar flames

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Introduction: The urgency of reducing greenhouse gas emissions and achieving a circular carbon economy has motivated research on renewable energy. For long-distance transportation and extended storage, electricity can be converted into liquid and gaseous fuels, referred to as e-fuel, benefiting from their high energy density. Oxymethylene ethers (OMEs) are considered a promising component in the ongoing energy transition and one of the significant candidates for e-fuels. Understanding the oxidation kinetics of OMEs remains a prerequisite to optimizing their combustion. However, the investigation of longer-chain species (OME_n, n>1) is limited to a few recent studies. A numerical and experimental study has been performed by Cai et al. on the ignition delay times of OME_{2-4} in a shock tube. Sun et al. explored the combustion chemistry of OME_3 in a stoichiometric flat flame. Recently, Gaiser et al. studied flat flames of OME_{0-3} at an equivalence ratio of 1.7, utilising molecular-beam mass spectrometry (MBMS), and the mechanism of Kathrotia et al.. The UCL mechanism with OME_1 was established and validated by Dias et al. in premixed laminar flames with equivalence ratios of 0.24 and 1.72.

Methodology: Our work aims to investigate the low-pressure combustion chemistry of OME_2 and OME_3 in laminar premixed flames under equivalence ratio conditions being 0.8 and 1.0, by carrying out experimental studies with MBMS and kinetic modeling.

Experimental Evaluation: The stoichiometric and fuel-lean neat OME_2 and OME_3 flames were stabilized at 50 mbar on a mobile Spalding-Botha burner. Species and radicals were measured and identified with MBMS to determine the flames' structure. The temperature profiles of both flames have been measured for the purpose of the kinetic modelling. The mechanism from Kathrotia et al., has been used for comparison with the experimental results of the OME_2 and OME_3 flames. Based on these comparisons, the UCL mechanism has been extended by analogy with OME_2 and OME_3 kinetics from other works. The numerical modeling have been performed by using OpenSMOKE++. The experimental results from the OME_2 and OME_3 flames show good agreement for the main species and some intermediates. With the measurements of the flames and interpretation from the new UCL mechanisms, the dominant consumption pathways of OME_2 and OME_3 flames are determined, showing that the OME_1 chemistry is found to be crucial for the consumption pathways of OME_2 and OME_3 flames. The effects of chain length on the reaction pathways of two fuels are elucidated by comparing the formation of intermediates and the consumption pathway of the fuels.

Keywords: oxymethylene ethers (OMEs); molecular-beam mass spectrometry; laminar flames; flat flames.

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Remote Sensing of Hydrogen Flames Under Daylight Conditions

Jens Brunzendorf *

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Introduction: Hydrogen is increasingly recognized as a cornerstone of sustainable energy systems, playing a pivotal role in the global transition toward decarbonization. However, hydrogen is highly diffusive and can easily escape through minute openings. Even small leaks can lead to serious consequences due to hydrogen's unique properties, as it has an extremely wide flammability range in air, the lowest minimum ignition energy and the smallest safe gap of all gases. This combination makes hydrogen particularly prone to ignition. Small burning hydrogen leaks at industrial installations pose significant safety hazards. Remote sensing of hydrogen flames over distances of many meters requires optical methods. Yet hydrogen flames are the least luminous of all fuels. Remote sensing can either be based on infrared emissions of the hydrogen flame and/or its OH* chemiluminescence in the UV range. Both methods are evaluated in this work side-by-side under outdoor conditions.

Methodology: Professional state of the art UV and MIR cameras are operated side by side and the resulting images are compared. The UV camera contains a GSENSE 400BSI sensor and an OD8 OH* filter with 10 nm FWHM. A commercial FLIR T640 serves as MIR camera. The hydrogen flame to be investigated is placed outdoors in direct sunlight between industrial pipes. Pure hydrogen is burned at the tip of a 6 mm Swagelok pipe with a flow rate from 2 l/min up to 100 l/min (Fig. 1, left image). The resulting hydrogen flame lengths and heights are measured via OH* chemiluminescence from a distance of 2.5 m (Fig. 1, center images). The measured flame lengths vary from 1.6 cm (2 l/min H_2) up to 26.5 cm (100 l/min H_2). Finally, the flames are observed with both cameras from a distance of 40 m, which is considered to be a representative distance for remote sensing (Fig. 1, right image).

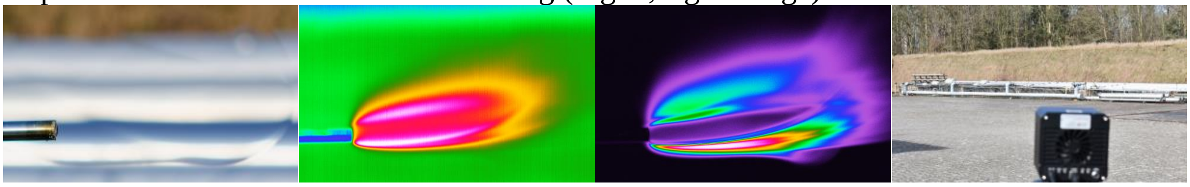

Fig.1 (from left to right): 1.-3.: H_2 flame @ 2.5 m distance (8 l/min H_2): 1. Visual image, 2. OH* mean image (colour-encoded grayscale image), 3. OH* standard deviation, 4. Final Setup @ distance 40 m with H_2 flame.

Results: The detection limit of hydrogen flames in outdoor conditions from a distance of 40 m was less than 2 l/min. Such flames are less than 2 cm long and high. In direct sunlight, the hydrogen flames are discernible in the MIR, though barely perceptible in the mean UV image, despite the narrow-band OD8 filter. This is due to the solar UV reflections on the pipes, which almost outshine the OH* flame signal. However, the presence of the flame is unmistakable in the UV standard deviation image. It should be noted that the ambient conditions were conducive for MIR measurements: cool outside temperature (+10°C), absence of incandescent lights and heat sources. The influence of solar radiation on the UV measurement can be minimized by considering the standard deviation instead of the mean value.

Keywords: hydrogen flame, chemiluminescence, remote sensing, spectroscopy, UV imaging, IR imaging, leakage detection, explosion protection, hazard prevention.

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Cool flame propagation velocities of DEE: determination in an ozone-seeded stagnation plate burner configuration

Perla Trad[1], Pierre Bragança[2], Guillaume Vanhove[1], Christophe Cuvier[2], Thomas Panaget[3], Bertrand Lecordier[4], Amaury Lahccen[1], Sébastien Batut[1], Valentine Bizet[1], and Laure Pillier[1]

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Introduction: Flame propagation velocity is a fundamental parameter in combustion, enabling the validation of detailed kinetic mechanisms. For cool flames, measurement of propagation velocity is limited to microgravity and subatmospheric conditions. Recently, the measurement of cool flame propagation velocities was achieved and validated in a stagnation plate burner for ozone-seeded DME cool flames using PIV (Panaget *et al.*, Fuel 2024). Based on this previous work, we present here the first measurement of ozone-seeded DEE cool flame propagation velocities.

Methodology: A stagnation plate burner with a coaxial nozzle converging geometry is used to stabilize flat laminar cool flames. A reactive DEE/O_2/O_3 mixture is introduced through the inner nozzle (d_i = 10 mm). The stainless-steel plate is heated to 700 K and placed at 13 mm parallel to the burner exit. A co-flow of nitrogen is introduced through the outer nozzle (d_i = 20 mm) to protect the flame from outside perturbations. Both flows are seeded with silicone oil particles (T = 50°C, d_p = 0.8 µm) for PIV measurements. A dual cavity Nd:YAG flashlamp pumped Innolas Splitlight compact 400 laser (150 mJ/pulse; 532 nm) and a series of spherical and cylindrical lenses are used to create a laser sheet (580 µm) that passes between the burner exit and the plate and illuminates the seeded particles in the flow. A LaVision Scmos camera is placed parallel to the laser sheet and captures a particle displacement of 10 pixels between each laser pulse (Δt = 250 µs).

Experimental Evaluation: Four flame conditions were investigated, with equivalence ratios ϕ ranging from 0.3 to 0.5 and O_3 mole fractions in the reactive mixture $x_{O_3}(\%)$ ranging from 1.4 to 1.6%. For each flame condition the total gas velocity at the exit of the burner u_{in} was varied from 0.8 to 1.1 $m.s^{-1}$. For each ϕ - $x_{O_3}(\%)$ - u_{in} condition, 4000 double frame PIV images are captured and averaged to obtain the mean velocity profiles. The axial velocity profiles are then extracted from the PIV data and averaged on a radial width of ± 0.5 mm around the centre of the burner. From these profiles, two parameters are inferred: the reference velocity $S_{u,ref}$, corresponding to the first minimum of the axial velocity, and the strain of the flame K, corresponding to the absolute value of the axial velocity slope 2 mm before the flame front. A series of (K, $S_{u,ref}$) values is obtained for every ϕ - $x_{O_3}(\%)$ flame condition. A numerically assisted non-linear extrapolation method is used to determine the unstrained cool flame propagation velocity S_u^0. The performance of different kinetic mechanisms was evaluated by comparison to the experimental PIV data. The model of Serinyel et al. (Serinyel *et al.*, Combust. Flame. 2018) accurately predicts the velocity profiles while the model of Tran et al. (Tran *et al.*, Proc. Combust. Inst. 2018) underestimates the minimum velocities.

Keywords: Cool flame; Diethyl Ether; Propagation velocity; Low Temperature Combustion; Particle image velocimetry; Ozone assisted combustion

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On the accuracy of laminar flame speeds and Markstein lengths measured from spherically expanding ammonia/air flames

Seif Zitouni[1,2], Roman Glaznev [3], Joachim Beeckmann[3], Christine Mounaïm-Rousselle [1,4], Nabiha Chaumeix[2], Fabien Halter&[1,2]

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Introduction: The unstretched laminar flame speed (LFS) refers to the velocity at which a planar, unstretched, adiabatic flame front moves relative to the unburned gas. It is a key property of a combustible mixture, as it governs the fuel burning rate and plays a critical role in flame stabilization within practical combustion systems. Accurate determination of LFS is essential, as LFS is a key parameter to develop, validate and improve kinetic mechanism models. Several experimental methods, involving stationary flames—such as conical, counter-flow, or flat flames—as well as spherically expanding flames (SEF) have all some advantages and drawbacks. Although SEF experiments have been performed for over a century, the LFS values remain affected by the set-up, the imaging technique and the post-processing; especially in the case of emerging zero-carbon fuels like ammonia and hydrogen. These fuels exhibit fundamental flame characteristics (e.g., flame thickness, response to stretch, and thermo-diffusive behaviour) that differ significantly from traditional hydrocarbon fuels. This study focuses specifically on ammonia/air flames at atmospheric pressure, with the poor quality of ammonia as a fuel requires high ignition energy, while the low LFS are notably influenced by buoyancy and radiative heat losses.

Methodology: Laminar flame speed measurements were conducted using 3 different spherical vessels with inner diameters of 100 mm, 200 mm, and 563 mm, located at RWTH (University of Aachen, Germany), PRISME (University of Orléans, France), and CNRS-ICARE (Orléans, France), respectively. Each vessel is equipped with optical accesses, providing optical radii of 25 mm, 35 mm, and 100 mm, correspondingly. After introducing the combustible mixture into the vessel and ensuring the mixture is quiescent, ignition is initiated at the centre using two tungsten electrodes. Flame propagation was recorded using a standard Schlieren setup.

Experimental Evaluation: Several sources of uncertainties—such as ignition effects, buoyancy, radiation, confinement, mixture preparation, radius data range, non-linear stretch behaviour, and extrapolation models—are examined. Their contributions to the discrepancies in laminar flame speed values are evaluated using one-dimensional simulations of both stationary unstretched flames and transient spherically propagating flames. Additionally, the variation in the influence of these uncertainties with changes in initial pressure, temperature, and gravity is also discussed.

Keywords: Laminar flame speed; Markstein length; Spherically expanding flames; Ammonia combustion.

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The challenge of measuring NO in hydrogen and ammonia flames to better understand the NO formation pathways

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The chemical processes of NO formation in flames are complex and fuel-dependent. In addition to the thermal NO, non-thermal NNH and N_2O pathways of NO formation are important in H_2 flames, while the most part of NO formed in ammonia flames comes from the NH_3 oxidation (fuel-NO).

To better understand these pathways, in situ measurements of reactive species like NO are needed under a large range of flame conditions. To explore the above-mentioned pathways in H_2 and NH_3 flames, dedicated flames produce NO with a mole fraction ranging from a few tens of ppb to a few percent. This wide range of NO to be explored requires specific adaptations of the experimental set-up based on laser-induced fluorescence (LIF), in order to achieve the best sensitivity in H_2 flames, and to avoid problems linked to the absorption of laser radiation in NH_3 flames. The presentation will focus on LIF methodology for NO measurements in H_2 and NH_3 flames, stabilized in a low-pressure chamber. The calibration procedure, based on the standard addition method, will be detailed and quenching correction will be discussed. An illustration of the chemical routes will be given.

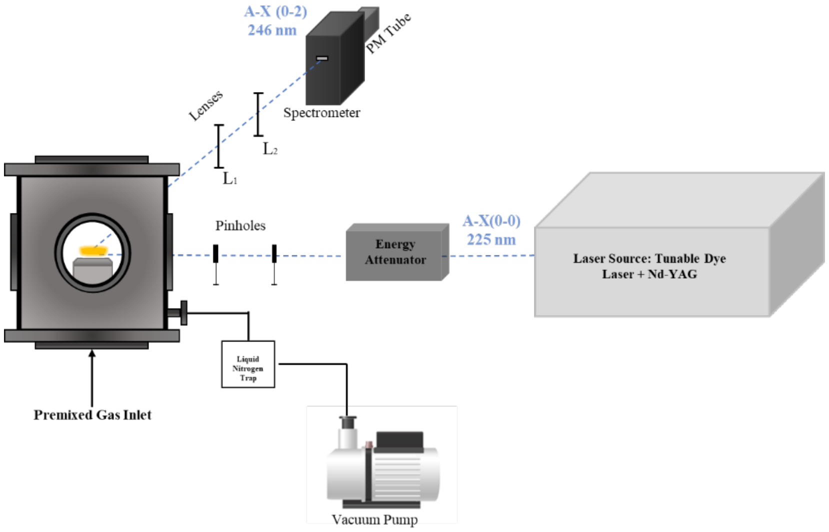

Fig. 1 Experimental set-up

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Oxidation and pyrolysis of neo-pentanol behind reflected shocks: CO time-histories and ignition delay times

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Introduction: The pyrolysis and oxidation of neopentanol (2,2-Dimethylpropan-1-ol) were investigated in this work, providing new targets for detailed kinetic modeling of a peculiar alcohol that cannot undergo dehydration. This work is part of an ongoing effort to better understand the influence of branching and alcohol function position on the reactivity of C_5 alcohols. The new data consists of shock-tube CO time-history profiles obtained near atmospheric pressure and measured behind reflected shock waves using laser absorption diagnostics near 4.6 µm, and ignition delay times measured in a shock-tube at 20 and 40 bar.

Methodology: Pyrolysis experiments were conducted with mixtures of neopentanol highly diluted in Ar/He (99.75%). Oxidation was studied in two different shock tubes: (i) at 1 bar, CO time-history profiles were measured at three different equivalence ratios, $\varphi = 0.5$, 1, and 2, using highly diluted mixtures of neopentanol/O_2/Ar/He, and (ii) at high-pressure, pressure traces were recorded to determine ignition delay times for lean and stoichiometric mixtures with an initial mole fraction of neopentanol of 1% (diluted in Ar). A rich mixture ($\varphi = 2$) was also investigated at 40 bar, but no clear ignition was observed. Under these high-temperature conditions, accounting for the pressure dependency of the rate constants of unimolecular initiation reactions is of paramount importance. A theoretical work has been carried out at a high level of theory in order to evaluate the rate constants of these pathways in a range of pressures. These theoretical results were incorporated into a detailed kinetic mechanism previously developed for 2-pentanol [1] in order to predict CO formation and ignition delay times. As already observed in a previous study [2], this theoretical work confirms roaming reactions have limited impact on the reactivity of neopentanol.

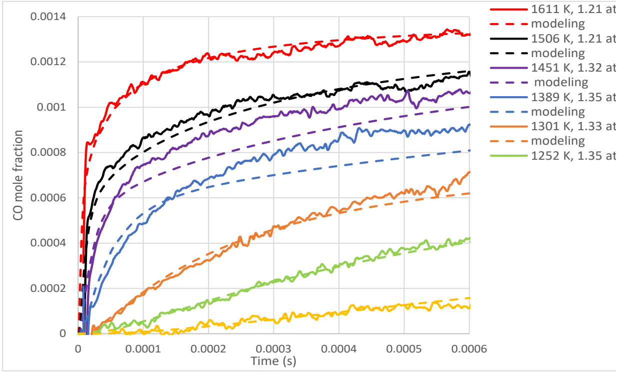

Figure 1 – CO time-history profiles obtained under pyrolytic conditions with 0.25% of neopentanol.

Keywords: shock tube, laser absorption spectroscopy,

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Nitrous oxide emissions - monitoring a critical aspect of the energy source diversification

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Introduction: In the context of hydrogen, N_2O will become crucial to monitor and urgently avoid an excess of emissions following the emerging ammonia use as hydrogen-based fuel. This work describes the current situation with respect to measurements of N_2O in terms of its metrological traceability. We report on the outlined development of new N_2O gas standards and compare them to the needs in emissions monitoring applications and greenhouse gas measurements.

Methodology: We investigated the present situation on available gas standards applicable to calibrate continuous emission measurements (CEMs) of N_2O as an emission from hydrogen's derivative ammonia (NH_3) used as fuel. While real-world data on N_2O emissions of maritime ammonia engine tests is not available, a maximum emission factor of 0.06 g N_2O per kWh (0.158 g N_2 per kg NH_3 consumed) is targeted by the industry. This performance value would guarantee a negligible effect on green ammonia trade and consumption as a fuel. The Key Comparison Database of the International Bureau of Weights and Measures reveals only eight institutes worldwide who can offer N_2O standards, needed for accurate measurements aiming at metrological traceability. Of them, each calibration and measurement capability is related to a reference material-based gas mixture, i.e. a certified reference material (CRM).

An alternative concept to CRM-based gas standards is given by optical gas standards (OGS). Yielding gas concentrations that are directly metrological traceable, OGS offer a flexible alternative to CRM-based gas standards, particularly where CRMs are less stable and difficult to be carried to the field, as, e.g., for CEM.

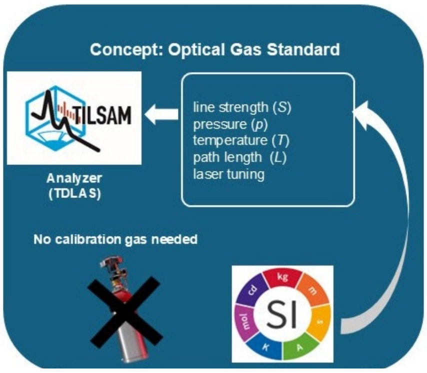

Fig 1: Sketch of an optical gas standard. The analyzer operates according to the TILSAM method.

Experimental Evaluation: Experimental collaborations have been started on nitrous oxide spectroscopy in the 1.65 mm near infrared wavelength range for N_2O emissions and the mid infrared range around 4.5 µm wavelength for background N_2O quantifications. This underlying spectroscopy work is required for the development of new optical N_2O standards as sketched in Fig. 1. In cases a thorough spectroscopic line selection is crucial to customize the optical gas standard for a specific application – or to have it available for general purpose N_2O certification and calibration for example. Metrological characterization and comparisons to available CRM-based N_2O standards are underway.

Development of Primary Standards for High-Frequency Dynamic Pressure Calibration

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Introduction: Accurate measurement of dynamic pressure is essential for the development of industrial energy conversion systems, particularly within the framework of Project MaritimeMET, which aims to assess the emissions of new green fuels. To meet this need, traceable and high-fidelity measurements must be ensured through the development of primary standards and robust calibration techniques, covering pressure amplitudes from 0.1 MPa to 30 MPa and frequencies ranging from 1 Hz to 100 kHz. The performance expected by end users is a relative uncertainty of 1% on the frequency-dependent pressure sensitivity, commonly referred to as dynamic sensitivity.

Methodology: For calibration in gaseous media, primary standards rely on dynamic pressure generators, including Shock Tubes and Fast-Opening Devices. These are designed and operated to produce step-like pressure waveforms that excite the transducer response over a specific frequency range. Within this range, the steps must conform to the assumptions embedded in the uncertainty budget models - that is, they must be quasi-ideal to achieve low primary calibration uncertainty. To that end, systematic effects associated with the generators are identified and either minimized or excluded by restricting the measurement range to conditions compatible with the calibration assumptions. Additionally, the selected transfer standard transducers must exhibit adequate bandwidth to ensure proper traceability. This presentation briefly outlines the design of the step-pressure generators, the metrological models under development for dynamic calibration in compressible gas media, and the selection method for reference transducers.

Keywords: dynamic pressure; primary standards; shock tubes; fast opening devices.

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On the characterization of highly oxidized products from cool flames in a continuously-stirred tank reactor

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Introduction: Terpenes could be used as renewable fuel in the future. However, these chemicals are relatively complex. Therefore, model-fuels could be usedto better understand their oxidation pathways. Methylcyclohexenes were selected for that purpose in this work.

Methodology: In the present study, the oxidation of methylcyclohexene isomers (1-methyl-, 3-methyl-, and 4-methyl-1-cyclohexene) was conducted in a continuously stirred tank reactor at an initial pressure of 10 bar, with excess oxygen (equivalence ratio of 0.5) across a temperature range of 500 to 1150 K. Reaction mixtures were collected using a sonic probe and subsequently analysed offline. The experimental phase of the study involved the utilisation of gas chromatography (GC) and ultra-high pressure liquid chromatography (UHPLC)-Orbitrap mass spectrometry. Gas samples were analysed by gas chromatography (GC). The samples were dissolved in acetonitrile by means of bubbling the gas emanating from the probe. Subsequent analysis was conducted either through direct injection or after UHPLC separation. The incorporation of D_2O into acetonitrile solutions was employed for the purpose of conducting H/D exchange, a process which was utilised to investigate the presence of hydroxyl (OH) or hydroperoxy (OOH) groups within the products of oxidation. The 2,4-dinitrophenylhydrazine reaction was utilised in conjunction with sample solutions in acetonitrile, with the objective of characterising the C=O function in the products of oxidation.

Experimental Evaluation: An extensive data set comprising chemical formulae was analysed. The presence of highly oxygenated compounds, polyunsaturated products, and aromatic products was detected under cool flame conditions. In order to elucidate the outcomes, Van Krevelen plots were employed, and the aromaticity index and aromaticity equivalence index were calculated. As previously documented, the production of benzene has been reported in the context of the oxidation of cyclohexane, cyclohexene, and 1,3-cyclohexadiene. However, the present study has identified the presence of aromatic, polyunsaturated, and polyaromatic hydrocarbons under cool flame conditions. The characterisation of the chemical classes present in the oxidation products was achieved by means of chemometric tools. The present results demonstrate the high complexity of the chemical oxidation pathways and chemical by-products associated with them.

Keywords: methylcyclohexene, oxidation, high-resolution mass spectrometry

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Molecular-Beam Mass Spectrometry under the Lens: Uncertainties in Measuring Species Concentrations

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Quantitative species data for the development and critical examination of combustion mechanisms are crucial for predictive combustion models. Molecular-Beam Mass Spectrometry (MBMS) coupled to various reactors and using different ionization techniques such as electron ionization (EI) and photoionization (PI), is a widely used tool for determining mole fractions of both stable and reactive species in combustion environments. However, the reliability of these measurements depends heavily on how uncertainty is handled throughout the measurement and evaluation process.

To provide precise and accurate data for model development and validation, meticulous attention must be paid to data acquisition and analysis. Uncertainties in MBMS data can arise at multiple stages, including spectral analysis, species identification, and especially during quantification. Key contributors influencing the overall uncertainty include the stability of instrumental parameters, the signal intensity for individual species, and the method used for calibration. Different calibration strategies can yield varying results, and their associated uncertainties significantly impacting the final mole fractions.

A thorough evaluation of these uncertainties, through methods such as sensitivity analysis, enhances understanding of the limitations and reliability of MBMS data. Recognizing and addressing these sources of uncertainty is vital for ensuring that MBMS measurements can serve as robust validation targets in combustion research.

This presentation will provide an overview of selected sources of error in the data evaluation procedure of MBMS data and illustrate their impact on model validation and development. Strategies for mitigating these uncertainties will be discussed, along with an assessment of the reliability of species-specific mole fraction profiles.

Keywords: Molecular-beam mass spectrometry; Uncertainty analysis, Combustion experiments

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Towards quantitative model comparisons against measurements from RCMs and JSRs

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Introduction: Measurements using rapid compression machines (RCMs) and jet-stirred reactors (JSRs) are widely employed to investigate fuel pyrolysis and oxidation over a wide range of conditions covering large spans of temperature, sometimes achieving combustor-relevant pressures and fuel loadings. A primary output consists of targets for chemical kinetic model comparison. Modern equipment designs have benefited from decades of empirical measurements and multi-dimensional computations towards achieving well-defined reacting mixtures. However, non-idealities and 'facility effects' can still be present and accounting for these can improve quantitative model comparisons.

In RCMs, reactivity during piston compression, and pressure decay due to heat loss during the test period are typically represented via the 'adiabatic core' framework; this generally assumes that the global physics are similar between reacting and non-reacting scenarios (i.e., with, and without O2 present). Fuels that exhibit multi-stage ignition can complicate this situation as heat loss increases during the test period, while gas can be forced from the primary reacting zone to the circumferentially-machined piston crevice volume(s). Additional physics (e.g., turbulent mixing) may further be generated.

In JSRs, operation is typically dictated by the David and Matras criteria where tracer concentration measurements can experimentally confirm global residence time distributions. This generally assumes sufficient macro- and micro-mixing are achieved by the nozzle jets while wall heat transfer is adequate to maintain thermal constancy. Experimental campaigns can often be conducted at significantly 'off-design' conditions (e.g., shorter/longer residence times, low molecular weight diluents, high fuel concentrations) in order to acquire wider ranges of reactivity data or improve analytical speciation of the gas constituents. This can lead to imperfect micro-mixing and incomplete thermal homogenization.

Methodology: This talk covers two modeling frameworks, respectively, which attempt to account for these non-idealities. A multi-zone formulation is adopted for the RCM simulations where physical effects of gas flow and heat transfer are determined separately from the chemical kinetic calculations, which still assume a reacting core. The coupling feedback due to multi-stage ignition is achieved via additional volumetric compression or increased internal energy, both of which enhance enthalpic flow from the reacting zone and slightly augment conductive heat flow to the chamber walls. A Pairwise Mixing Stirred Reactor model is adopted to describe the micro-mixing processes in JSRs. Here, the reactor consists of discrete particles with a time-varying composition due to flow into the reactor, outflow, random particle-particle exchange and chemical reaction. A global correlation for convective energy transfer with the walls is also applied. Statistical distributions within the reactor result due to finite-time exchange rates and this affects the interpreted reactivity of the system compared to perfectly-mixed conditions.

Keywords: rapid compression machine; muti-stage ignition; jet-stirred reactor; micro-mixing reduced-order model.

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Ozone-assisted low-temperature oxidation of C1-C4 alcohols

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Introduction: Developing sustainable alternative fuels and advanced low-temperature combustion technology represents a promising approach for achieving clean and efficient combustion processes. C1-C4 alcohols, characterized by their abundant availability and ease of preparation, hold significant potential as sustainable alternative fuels. However, their application in low-temperature combustion is hindered by inherent challenges, such as weak low-temperature oxidation reactivity and difficulties in achieving low-temperature ignition. In addition, combustion kinetic models for C1-C4 alcohols lack adequate validation with low-temperature experimental data. Consequently, the low-temperature combustion chemistry of C1-C4 alcohols require further exploration. This study aims to systematically investigate the low-temperature oxidation reaction mechanisms of C1-C4 alcohols through a combination of experimental measurements and kinetic model analysis.

Methodology: This study achieved the low-temperature oxidation (400~800 K) of C1-C4 alcohols in an atmospheric-pressure jet-stirred reactor using an ozone-assisted experimental method. A state-of-the-art diagnostic technique, synchrotron vacuum ultraviolet photoionization mass spectrometry, was utilized to detect the species distribution in the low-temperature oxidation of C1-C4 alcohols. In the experiments, a series of intermediates and final products were identified and quantified, including aldehydes, ketones, organic acids, peroxides, alkanes, alkenes, etc. These detailed species distributions were critical for elucidating the low-temperature oxidation mechanisms of C1-C4 alcohols, validating their oxidation pathways, and updating the corresponding low-temperature oxidation models. Furthermore, kinetic analysis revealed the key reaction pathways in the low-temperature oxidation of C1-C4 alcohols, highlighting the control effect of certain reaction pathways due to the presence of hydroxyl groups on their low-temperature oxidation behavior.

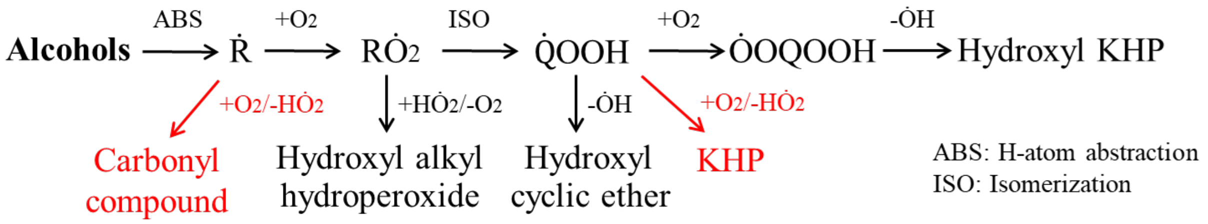

Fig.1 Low-temperature oxidation pathways of alcohols

Keywords: C1-C4 alcohols; low-temperature oxidation; ozone-assisted combustion; kinetic mechanism

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RCM Workshop 3rd Characterization Initiative: Resolving complications of multi-stage ignition

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Introduction: Measurements using rapid compression machines (RCMs) allow low-temperature / negative-temperature-coefficient (NTC) fuel oxidation processes to be investigated at combustor-relevant conditions (e.g., elevated-to-extreme pressure, realistic fuel loadings) in a well-controlled environment. However, non-idealities and ‘facility effects’ must be taken into account towards achieving robust agreement with chemical kinetic models. Reactivity during piston compression, and pressure decay due to heat loss during the test period are typically represented via the ‘adiabatic core’ framework; this generally assumes that the global physics are similar between reacting and non-reacting scenarios (i.e., with, and without O2 present). Fuels that exhibit multi-stage ignition can complicate this situation as heat loss increases during the test period, while gas can be forced from the primary reacting zone to the circumferentially-machined piston crevice volume(s). Additional physics (e.g., turbulent mixing) may further be generated.

Methodology: A multi-institution experimental and modeling campaign is being pursued to: (a) improve quantification of uncertainties for measurements at these conditions; (b) better understand agreement / disagreement between facilities where low-temperature (cool-flame) heat release, NTC behavior, and multi-stage, high-temperature heat release are exhibited; (c) improve reporting and documentation under conditions where reactivity, and especially low-temperature (cool-flame) heat release, can occur during the piston compression stroke, i.e., before the end-of-compression; (d) provide insights into modeling challenges and discrepancies with measurements to develop ‘best practices’ for these; (e) improve the robustness of experimental designs, and measurement / analytical techniques.

Experimental Evaluation: Di-methyl-ether (DME) is selected as a representative fuel, since it is the simplest ether with robust low-temperature NTC behavior at conditions that can be accessed by most facilities, while comprehensive chemical kinetic models for DME are more developed and better resolved than larger, representative hydrocarbons (e.g., n-butane). Initial progress is presented. Experimental results from various facilities are covered in presentations in this session.

Keywords: rapid compression machine; muti-stage ignition; multi-institution collaboration.

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Preliminary results from the 3rd RCM characterization initiative: Dimethylether investigations at PTB RCM facility

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Introduction: The rapid compression machine is used for studying auto-ignition of various fuels in the low-to-intermediate temperature regime (600K to 1100K) and at higher pressures (typ. ≥10 bar). These experimental investigations are typically used for developing and validating detailed kinetic mechanisms for the target fuel, and later, in its reduced form used for understanding the combustion process in various application systems. The RCM characterization initiative is a collective effort from the RCM community to compare the results from different RCM facilities for an agreed condition. The aim being to understand the differences from the various facilities, arrive at individual and overall uncertainties, and standardized methods for simulations. The previous initiative investigated ethanol as a benchmark for a liquid fuel showing Arrhenius reactivity in the RCM measurement regime.

Methodology: In the current initiative, Dimethylether (DME) is chosen as a target fuel that shows a negative temperature coefficient (NTC) behavior in the measurement regime with the aim is to better understand the different facilities, where low-such behavior is exhibited. In this process, the initiative also intends to provide insights into the modeling challenges and come up with a best practice guide in these aspects. In this talk, we plan to present some preliminary results from the RCM at Physikalisch-Technische Bundesanstalt (PTB) at agreed conditions from the initiative, 10 bar compressed pressure, stoichiometric conditions, diluent /oxygen ratio = 10.

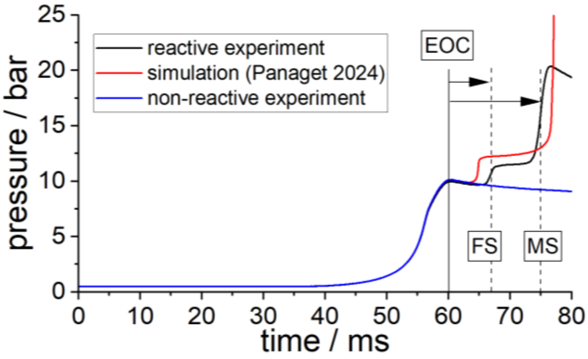

Fig.1: Typical 2-stage auto-ignition behaviour of DME, here recorded at 672 K. Positions marked: FS: first stage, MS: main stage, EOC: end of compression.

Experimental Evaluation: Experimental data of the auto-ignition behaviour of DME has been recorded for the low-to-intermediate temperature regime at 10 bar compressed pressure. Fig.1 illustrates a measurement result and its corresponding simulation by their dynamic pressure traces.

Keywords: rapid compression machine; reaction kinetics; research facility effects; uncertainty evaluation.

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Dimethyl Ether Auto-ignition Delay Measurements in a Rapid Compression Machine

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Introduction: Dimethyl ether (DME) is a clean-burning alternative fuel with high cetane number and low soot formation, making it a strong candidate for use in compression ignition engines and as an ignition enhancer. Its favorable combustion properties and two-stage ignition behaviour, including a pronounced negative temperature coefficient (NTC) region, make it valuable for studying low-temperature combustion. Its symmetry and low carbon number also make it an interesting case study for two-stage ignition physics.

Methodology: In this study, a rapid compression machine (RCM) was employed to measure the ignition delay times (IDT) of dimethyl ether. The RCM used has a geometric compression ratio of 7.28 and was preheated to 75 °C. Experiments were conducted under varying conditions: a fixed dilution ratio of 10:1, compressed pressures (p_c) ranging from 5 to 15 bar, compressed temperatures (T_C) between 600 K and 900 K, and equivalence ratios (φ) of 0.5, 1, and 1.5. The measured IDTs were subsequently used to validate a detailed chemical kinetic model for DME combustion (Panaget et al., 202 1, *J. Phys. Chem. A*).

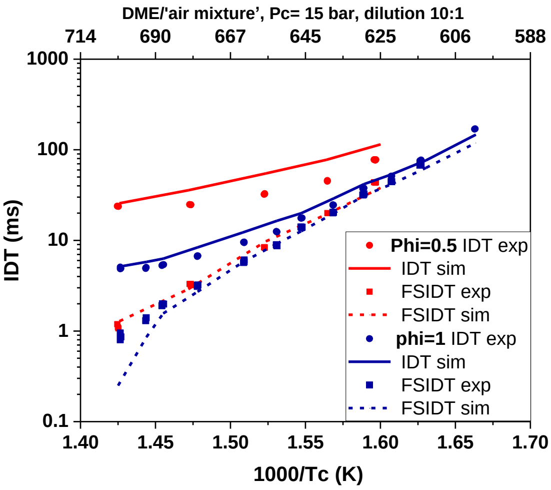

Fig. 1. Evolution of the IDTs of DME at different equivalence ratios (φ = 0.5 and 1) and p_c = 5, 10 and 15. Symbols present experimental results, lines present the simulations done using AM2 model

Experimental Evaluation: Fig. 1 presents the experimental and the predicted evolution of IDT for DME at different equivalence ratios and at p_c = 15 bar. The measured IDTs revealed typical two-stage ignition behavior and a pronounced negative temperature coefficient (NTC) region. These findings provide crucial data for validating and refining chemical kinetic models, improving the accuracy of combustion predictions for DME in compression ignition engines. The model showed excellent agreement for the first-stage ignition events, however, noticeable deviations for the total IDT were observed in the NTC region, possibly originating from piston crevice dynamics, which are not described by the current modelling strategy, indicating the need for further refinement.

Keywords: Dimethyl ether, Combustion, Ignition Delay Time, Rapid Compression Machine.

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Uncertainties on Initial conditions and IDT measurements in a Rapid Compression Machine

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Introduction: Rapid Compression Machines (RCMs) are essential tools for investigating fuel ignition and pollutant formation under conditions representative of modern combustion systems such as internal combustion engines (ICEs) and gas turbines. These machines can provide condition temperature ranges from 600 K to 1200 K and pressures up to 80 bars. A wide variety of fuels can be studied using RCMs, including hydrogen, ammonia, syngas, as well as conventional fuels like methane, propane, alkenes, and aromatics. At the PRISME Laboratory, a RCM was developed to conduct these studies. This study will focus on the evaluation of uncertainties, after describing the set-up and its specificities, to conclude about a comprehensive overview of its capabilities and applications in combustion research.

Methodology: The measure of Ignition Delay Times (IDTs) is very sensitive not only to the initial and thermodynamic conditions of the air/fuel mixture but also to the geometry and materials used in the combustion chamber. The air/fuel mixtures are prepared in an auxiliary tank, where they are continuously mixed and heated to ensure homogeneous gas phase. This mixture is then introduced into the combustion chamber, which is pre-vacuum and set to the desired initial temperature and pressure. Once sealed, the chamber undergoes rapid pneumatic compression, raising the gas to the target end-of-compression conditions, ultimately leading to autoignition after a specific delay defined as the IDT.

Experimental Evaluation: Several factors influence the accurate measurement of Ignition Delay Time (IDT), beginning with mixture preparation and continuing through to ignition. i) Errors in mixture distribution can arise due to the volume of the intake manifold and piping, further affected by the non-linearity of mass flow controllers. These issues can introduce 8–12% error in the final real equivalence ratio of the air/fuel mixture, potentially leading to significantly biased results. ii) To ensure homogeneity, both simulations and experimental tests are conducted to verify uniform mixture composition at the tank outlet. iii) Thermal analyses—both experimental and numerical—have shown that the internal wall and gas temperatures within the combustion chamber are approximately 8–9% lower than the external wall temperature. Procedure and material modifications have been made to reduce thermal losses, particularly at the piston head. iv) Additional simulations were performed to determine the necessary waiting time for achieving a uniformly heated mixture with a minimum gravitational effect that could lead to stratification before compression. v) During the compression phase, the piston produces an acoustic wave inside the combustion chamber which was characterised vi) Finally, thermal simulations were used to define the maximum IDT duration that can be reliably measured before buoyancy-induced stratification of hot and cold gas layers occurs.

Keywords: Rapid Compression Machine, Measurements, Equivalence ratio, Stratification, Surface temperature.

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Resolving Mixture Stratification in Hydrogen SCC Using Calibrated LIBS and Acetone PLIF Measurements

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Introduction: Hydrogen is a promising alternative fuel due to its high efficiency and zero carbon emissions, but it poses challenges such as backfire, pre-ignition, and low power output in engines. Stratified charge combustion (SCC) with direct injection can improve stability and efficiency by creating local rich zones, but its performance depends strongly on the local equivalence ratio. Accurate measurement of this ratio is essential, as it influences flame speed, heat release, and emissions. This study uses laser-induced breakdown spectroscopy (LIBS) to measure local equivalence ratios in hydrogen jets under non-reacting conditions and employs laser plasma ignition to ensure combustion at the same locations. Combustion characteristics are analysed through pressure data and schlieren imaging. Acetone-traced planar laser-induced fluorescence (PLIF) is used to visualize jet mixing, and helium and nitrogen are tested as surrogate gases to safely observe mixture behaviour without combustion.

Methodology: A 1.4 L constant-volume chamber with quartz windows was used to visualize hydrogen jets and combustion. Hydrogen was injected through a hollow-cone injector at 40–100 bar, controlled by a pressure regulator. Injection and ignition were precisely timed using signal and delay generators. Local equivalence ratios were accurately measured using LIBS, where a 532 nm Nd:Yag laser was employed to generate plasma at precise locations, and the resulting atomic emissions from hydrogen and nitrogen were captured and analysed using a high-resolution spectrometer. A Z-type schlieren system captured jet and flame structures and gradient-based image processing quantified jet boundaries and intermittency. PLIF was employed to visualize the mixture formation process, using acetone as a tracer, which was excited by a 266 nm laser sheet shaped through cylindrical lenses to enable precise and detailed imaging of the equivalence ratio field. Split injections with varying ratios were tested and laser firing was varied after injection.

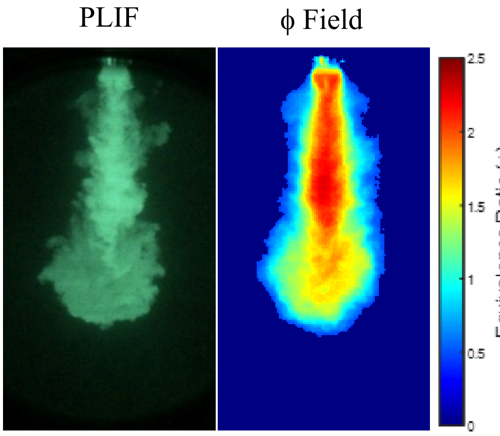

Fig.1 Raw PLIF and Mixture Field

Experimental Evaluation: Hydrogen was used to study stratified combustion and quantify local equivalence ratios. LIBS provided pointwise measurements under nonreactive conditions, allowing for the calibration of emission intensity to quantitative mixture composition; to extend these measurements to spatial mapping, acetone PLIF was employed to visualize the 2D mixture field. This combined approach allowed analysis of hydrogen mixture formation and its impact on combustion. Fig. 1 show the raw PLIF image and corresponding equivalence ratio.

Keywords: hydrogen combustion; stratified charge; equivalence ratio; laser diagnostics; mixture visualization.

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Impact of Radiation and Water Vapor on Fundamental Properties of Lean Laminar Hydrogen/Air Flames

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Introduction: Hydrogen is a promising fuel for decarbonizing the transportation industry, as its combustion produces significantly fewer emissions than conventional hydrocarbon fuels. Water vapor dilution can enhance flame stability and simultaneously reduce nitrogen oxide (NO_x) emissions. While the effect of water vapor dilution on combustion chemistry and transport properties has been extensively studied, thermal radiation effects are often neglected in simulations. This study focuses on the combined impact of water vapor addition and thermal radiation on fundamental combustion properties for lean and ultra-lean hydrogen/air flames.

Methodology: The one-dimensional freely-propagating flame model from Cantera is employed, using the Villenave et al. (2024) kinetic mechanism. Radiative heat losses are considered through the gray gas approximation and by assuming an optically thin medium. This simplified approach captures the first-order effects of thermal radiation in hydrogen/air laminar premixed flames where H_2O is mainly present in burnt gases. Radiation is treated in a simplified way through grey gas approximations or empirical heat loss functions, rather than solving the full radiative transfer equation. The computed laminar flame velocities and burnt Markstein lengths are compared to experimental measurements obtained in a constant volume spherical chamber under the constant pressure hypothesis and using the non-linear model for the extrapolation to zero stretch. The conditions studied are as follows: Water vapor content from 0 to 20% vol. with an initial pressure of 1 bar and initial temperature ranging from 303, 373 and 423 K.

Results and Discussion: Numerical results indicate that the laminar flame speed decreases with an increase in water vapor addition, while thermal radiation has no direct effect. When compared with the experimental results at 0% water vapor addition, the laminar flame speed shows greater divergence from the numerical values at lower equivalence ratios but aligns more closely at higher equivalence ratios. At 10% water vapor addition, the flame speed shows good agreement at lower equivalence ratios but diverges at higher values. In contrast, for 20% water vapor addition, a larger deviation from the simulated results is observed across all equivalence ratios. Concerning flame fundamental properties, simulations shows that the adiabatic flame temperature decreases as water vapor content increases. The effective Lewis number, based on hydrogen and oxygen diffusion, shows no significant difference between radiative and adiabatic conditions. Theoretical burnt Markstein lengths are calculated using two formulations: Bechtold & Matalon, and Chen. Both show a decrease in burnt Markstein length with increasing water vapor content. When radiation effects are considered, the Markstein length decreases further for both formulations. Compared to experimental results, the values diverge the most at 20% water vapor addition. At 0% and 10% of water vapor addition, the values diverge significantly at lower equivalence ratios, but converge towards the numerical values at higher equivalence ratios.

Keywords: Hydrogen combustion; Water vapor dilution; Thermal radiation; Laminar flame speed; Burnt Markstein length

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Metals as Future Carbon-Free Energy Carriers

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Introduction: Micrometric metal particles offer a promising source of sustainable energy. Upon ignition, they generate a significant amount of energy without emitting carbon dioxide. Additionally, this process yields metal oxides that can be regenerated using wind or solar energy. This cyclical system of energy production and recycling enables renewable energy to be stored securely and sustainably, accessible at any needed time or location. This presentation introduces an innovative and promising approach that centers on the high-temperature oxidation of metals. It forms part of a ground breaking technology that has the potential to tackle global warming.

Methodology: In atmospheric air, aluminum particles of sufficient radii burn in a diffusive regime. As aluminum evaporates from the burning droplet, oxidation occurs, resulting in the production of alumina. The presence of this aluminum oxide results in the formation of an oxide cloud, comprising nanometric droplets, which is situated in close proximity to the burning droplet. The comprehensive characterization of this cloud is of paramount importance and can be accomplished with the current experimental apparatus using a backlight and a color camera equipped with a triple band filter.

Fig.1 Typical stability result [Times New Roman 10]

Experimental Evaluation: As a result, the alumina particle size profiles and volume fraction profiles around the burning particle are inferred experimentaly. Furthermore, the optical thickness of the cloud is directly proportional to its emissivity. A deconvolution procedure that accounts for self-absorption can be employed to determine the local cloud emission, which can then be divided by the local emissivity to obtain the local blackbody emission. By utilizing a blackbody calibration for the camera, a temperature profile can be established at all points within the oxide cloud surrounding the particle, thereby facilitating a comprehensive characterization of this cloud.

Keywords: metal particle combustion, three-color pyrometry, nanoparticle size and temperature profiles

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Vibration Frequency Measurement of Wind Turbine Blades through Moiré Pattern Analysis

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Introduction: Accurate vibration measurement of blades is essential for monitoring wind turbines to reduce downtime and ensure operational safety in wind farms. Although imaging-based methods such as digital image correlation and photogrammetry have been applied to achieve non-contact vibration measurement of wind turbine blades, these methods require two or more cameras, complex synchronisation and calibration. This paper proposes a single camera-based approach to measure the flap-wise vibration frequency by analysing the moiré pattern generated by a marker on a blade.

Methodology: The principle of the proposed measurement method is shown in Figure 1. The camera is positioned in front of the wind turbine pointing to the maker on the blade. Each frame goes through spatial analysis to obtain the moiré signal. The moiré signals from all frames then go through temporal analysis to determine the vibration frequency of wind turbine blades. The first frame in the frame sequence is used for initialisation, which detects and analyses the marker's grating pattern and generates a static grating. By superimposing the static grating on each frame, moiré patterns will appear on the image. The moiré signals can be extracted using a bandpass filter. Finally, the instantaneous phases of the moiré signals are calculated by taking the angle of the Hilbert transform on each frame. Then the vibration frequency can be measured by applying frequency analysis on the phase differences between frames.

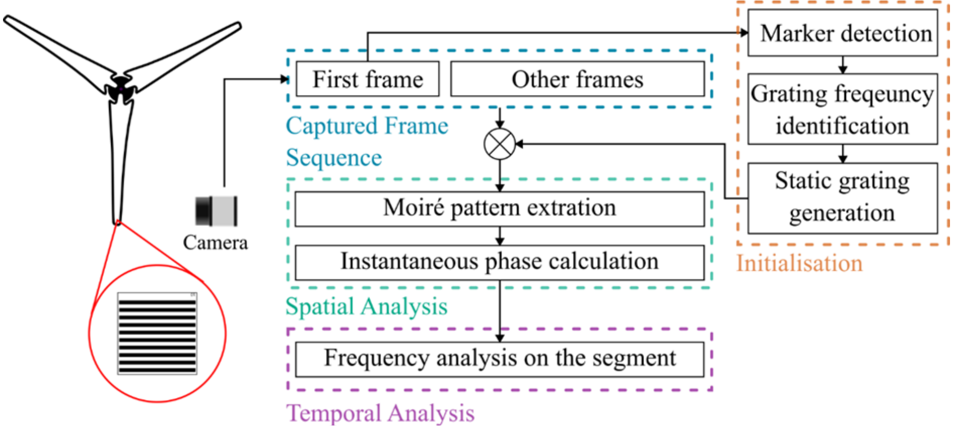

Fig.1 Overview of the proposed method

Experimental Evaluation: Experiments were conducted on a laboratory test rig to assess the proposed measurement method for different camera distances, marker stripe widths, camera pitch and yaw angles and vibration frequencies. The results show that the moiré pattern analysis method is able to accurately determine the vibration frequency up to 30 Hz with a camera frame rate of 60 fps, compared with the reference vibration frequency obtained from a commercial accelerometer.

Keywords: wind turbine blades, flap-wise vibration measurement, Moiré pattern analysis, image processing

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Measurement of CO_2 gas-liquid two-phase gas volume fraction using capacitive sensors

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Introduction: Gas volume fraction（GVF）is one of the key parameters for calculating the mass flowrate of CO_2 gas-liquid two-phase flow, and it is also an important parameter for monitoring the flow state of CO_2 gas-liquid two-phase flow. Multi-electrode capacitance sensors are often utilized for tomography to achieve the flow pattern recognition and visual monitoring in previous studies. However, unlike the flow pattern recognition or phase distribution reconstruction of two-phase flow, reconstructed images are not usually required for the GVF measurement. In order to accurately measure the GVF of gas-liquid two-phase CO_2, a new method based on capacitive array sensors and flow pattern recognition model is developed.

Methodology: In order to obtain capacitance data under different flow patterns and GVF conditions, a four-electrode capacitance sensor array was installed in the horizontal testing section of the CO_2 gas-liquid two-phase flow platform. By analyzing the capacitance signal, extracting the mean and mean square deviation of different electrode pairs to form feature vectors, a CO_2 gas-liquid two-phase flow pattern recognition method based on Fuzzy C-means (FCM) algorithm and feature vectors is constructed. By fitting each set of capacitance data and reference GVF, GVF measurement models are established for different flow patterns, and the goodness of fit is evaluated by calculating the coefficient of determination for each electrode pair. Using the coefficient of determination as the weight, the fitting relationships with coefficients greater than 0.9 are weighted and fused to obtain the GVF fusion measurement model corresponding to each flow pattern.

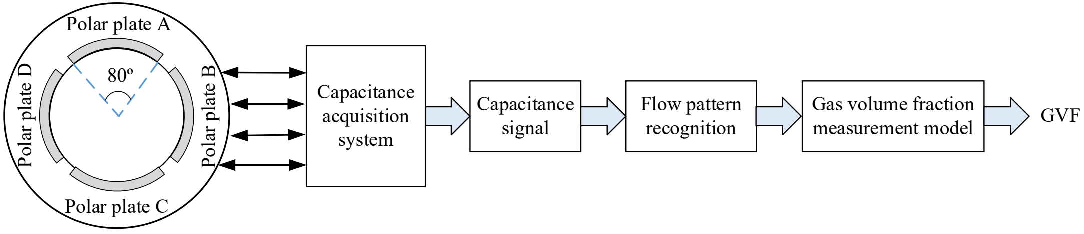
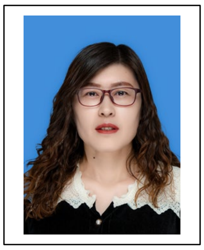


Fig.1 General scheme of GVF measurement for CO_2 gas-liquid two-phase flow

Experimental Evaluation: On the CO_2 gas-liquid two-phase flow platform, with the Coriolis mass flowmeter and high-speed camera as reference devices, the flow pattern identification and GVF measurement model of CO_2 flow are tested and evaluated. Fig.1 illustrates the general scheme of GVF measurement for CO_2 gas-liquid two-phase flow.

Keywords: Gas Volume Fraction (GVF); CO_2 gas-liquid two-phase flow; Capacitive sensors; Flow pattern recognition; Fusion measurement model.



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Development of a National Facility for Traceable Aerodynamic Testing in Thailand: Advancing National Metrology, Energy and Aerospace Applications through 15 kPa Differential Pressure Standard

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Introduction: Thailand’s growing aerospace, energy, and transportation sectors require accurate and traceable flow measurements to support advanced aerodynamic testing and innovation. To address the absence of national traceability in subsonic flow regime, the National Institute of Metrology (Thailand) has established a National Facility for Traceable Subsonic Flow Measurements. At the core of this facility is a 15 kPa force-balanced piston gauge, now serving as the national standard for low differential pressure—an essential parameter for precise subsonic airspeed determination and aerodynamics pressure distribution analysis. This development marks a significant step toward closing the traceability gap in aerodynamic measurements and enables the advancement of both subsonic and supersonic flow applications across critical Thai research and industries.

Methodology: To establish traceable and accurate differential pressure measurements for subsonic aerodynamic testing, the effective area of a 15 kPa force-balanced piston gauge (FPG8601) was characterized through a cross-float comparison with a DHI PG7607 (No. 407 – 5 kPa/kg), a 50 mm diameter traditional piston-cylinder assembly maintained at NIMT. This metrological framework ensures traceability of low differential pressures critical to airspeed determination and aerodynamic pressure distribution analysis using Pitot tubes and surface pressure taps. These traceable measurements support accurate aerodynamic testing, essential for analyzing flow behavior, optimizing aircraft and turbine design, and identifying phenomena such as flow separation and stall, thereby advancing national capabilities in aerospace metrolo

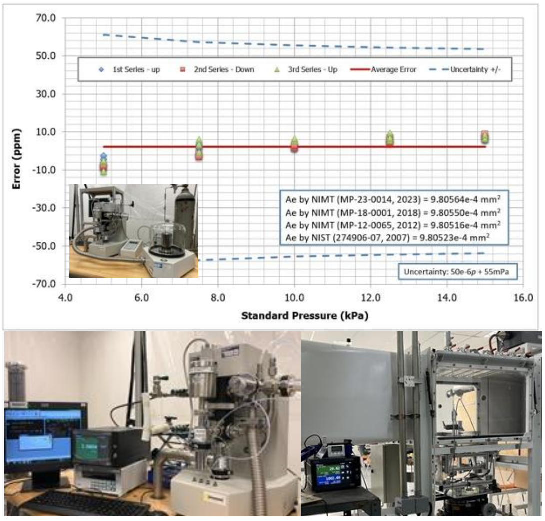

Fig.1 (a) PG-FPG Comparison Results
(b) FPG as a Calibration Standard
(c) Wind Tunnel Testing at Kasetsart Univ.

Experimental Evaluation: The experiments, shown in Fig. 1, includes (a) a cross-float comparison between the PG7607 and FPG8601, confirming the FPG8601’s measurement results as a national standard; (b) its use to calibrate a working standard differential pressure sensor; and (c) application of the calibrated sensor in wind tunnel testing at Kasetsart University, demonstrating reliable traceable aerodynamic measurements.

Keywords: aerodynamics; traceability; differential pressure

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Simultaneous dynamic NO, H_2O, and temperature measurement using an intrapulse laser with MHz time resolution in a shock tube

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This study aims at fast and accurate sensing in dynamic conditions using the intrapulse laser technique. Integrated with a shock tube and three other independent lasers, the intrapulse laser was examined for both fundamental and practical applications across varying temperatures and pressures. The spectral regions selected in this study range from 1914 to 1916 cm^{-1}, including both NO and H_2O absorption peaks, enabling simultaneous measurements of NO and H_2O mole fraction as well as temperature using a two-line thermometry. The intrapulse laser operated at a 900 kHz repetition rate with a 200 ns pulse width, achieving a time resolution comparable to the fixed-wavelength method. The chirp rate of the intrapulse laser is 250-400 MHz, providing a spectral resolution of 0.0156-0.0197 cm^{-1}. To correct the rapid passage effect observed under low-pressure conditions, a novel method of symmetrically flipping half of the unaffected spectrum has been proposed and validated. Specific experiments were designed to validate the capability of the intrapulse laser in accurately quantifying NO, H_2O and temperature. The results show that NO and H_2O measurements from the intrapulse laser aligned well with those from an Interband Cascade Laser (ICL)-NO laser and a Distributed Feedback (DFB)-H_2O laser, respectively. Additionally, the temperatures inferred by the intrapulse laser match well with calculations from one-dimensional shock equations. The average relative differences on NO mole fraction, H_2O mole fraction and temperature are 4.5%, 7.0%, and 5.4%, respectively. In an application case, the intrapulse laser successfully captures the dynamic formation process of NO and H_2O and the associated temperature variations during NH_3 oxidation in the shock tube. The results demonstrate good agreement with simulation results from a chemical mechanism. Thus, the intrapulse laser is a powerful technique that enables simultaneous measurements of multiple species and temperature in dynamic environments, combining the calibration-free advantage of the scanned-wavelength method with the high time resolution of the fixed-wavelength method.

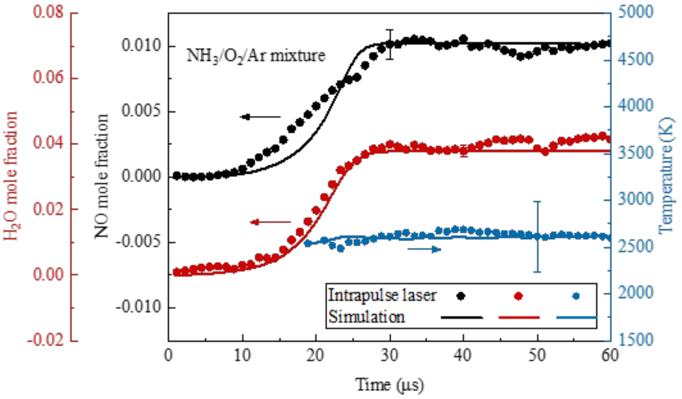

Figure 1: Time-resolved NO, H2O and temperature measured by intrapulse laser in a shock tube

Keywords: intrapulse laser; rapid passage effect; shock tube; dynamic measurement

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Impact of Different Charge and Discharge Profiles on the Aging Behavior of Second-Life Lithium-Ion Batteries: An EIS-Based Approach

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Introduction: Understanding lithium-ion battery degradation under different cycling conditions is crucial for improving their lifespan and performance. State of Health (SoH) as a measure of degradation can be assessed via Electrochemical Impedance Spectroscopy (EIS), a non-invasive tool to probe internal battery dynamics, including ion diffusion, charge transfer, and interface behavior. Accurate SoH estimation is especially relevant as batteries face increasingly demanding applications in electric vehicles, renewable energy systems, and portable electronics. Different charge and discharge rates significantly influence battery degradation, and their effects can be directly observed through EIS. Changes in impedance spectra can reveal how faster or irregular charging stresses the internal components, accelerates aging processes, and affects long-term capacity retention. Yet, the combined impact of varying charge profiles on degradation, especially in second-life applications, remains underexplored. Thus, employing EIS to analyze the aging behavior under different charge/discharge profiles not only advances understanding of the degradation mechanisms but also supports the development of more robust battery management strategies and second-life use cases.

Methodology: Our methodology integrates electrical and thermal diagnostics to monitor degradation mechanisms under defined cycling conditions. EIS is performed on LFP pouch cells with a capacity of 30 Ah. By fitting equivalent circuit models to the spectra, internal resistance components and kinetic processes can be quantitatively assessed and tracked over repeated cycling. Three K-type thermocouples installed at different locations on each cell enabled precise monitoring of thermal behavior throughout the experiments, helping correlate temperature development with electrochemical aging. The test strategy is scenario-based, using manufacturer specifications to define five different charge/discharge current profiles while respecting the thermal limitations of the cells.

Experimental Evaluation: Five cycling scenarios were applied to the commercial LFP pouch cells to study aging under varying current rates, simulating second-life use without active cooling at 25 °C. EIS and capacity tests were performed every 50 cycles. Notably, cells cycled at lower C-rates (e.g., 0.5C–0.5C) reached second-life thresholds (>1000 cycles) significantly later than those exposed to high-rate profiles (e.g., 1C–2C, reaching 60% SoH after ~400 cycles). Early-stage capacity increase was observed, particularly under deep cycling conditions, suggesting activation phenomena. EIS analysis showed progressive impedance growth, especially in the low-frequency region, indicating charge transfer and diffusion limitations. Thermal measurements revealed localized temperature peaks up to 49 °C during charging, particularly near the current collectors, but overall remained within safety margins. These results confirm that cycling intensity strongly influences degradation rate, capacity retention, and internal resistance development.

Keywords: State of Health; Second life lithium-ion batteries; Electrochemical impedance spectroscopy; Aging; Equivalent circuit model; State of Charge

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Assessing the safety of lithium-ion batteries using electrochemical impedance spectroscopy: indicators, challenges and measurement techniques

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Introduction: Lithium-ion batteries have become an integral part of modern energy storage systems. However, with their increasing use in mobile devices, electric vehicles and stationary storage systems, the relevance of battery safety is also growing. The phenomenon of thermal runaway is particularly critical here, as it can have potentially catastrophic consequences. Early detection of safety-critical conditions is therefore essential. Conventional methods such as temperature measurement or mechanical monitoring can only be used to a limited extent in practice, as they can often only be carried out on a few cells and react with a time delay due to thermal inertia.

Methodology: Electrochemical impedance spectroscopy (EIS) is a non-invasive measurement method that can detect changes in the internal resistance and electrochemical properties of battery cells with high sensitivity. This thesis examines the extent to which EIS is suitable for assessing the safety of lithium-ion cells. The focus here is on two approaches: Firstly, potential early indicators of thermal runaway are obtained from the impedance curve over time at different frequencies by derivation. Secondly, the non-linear system response is analysed by determining the distortion factor in order to detect structural changes at an early stage. The investigations are carried out on a laboratory scale.

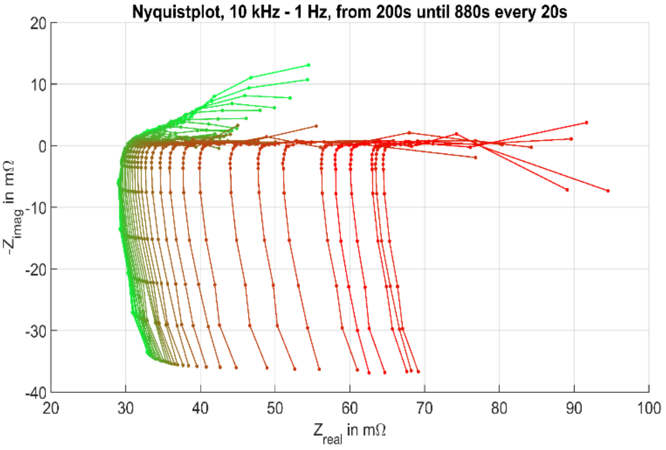

Fig.1: Impedance spectra while heating a lithium-ion-battery

Experimental evaluation: Initial measurements show that changes in the impedance spectra occur before a rise in temperature and therefore represent a possible early warning signal. The results confirm that EIS is a promising method for the early detection of safety-critical conditions and has the potential to effectively supplement conventional monitoring systems in battery systems.

Keywords: lithium-ion batteries; battery safety; condition monitoring; electrochemical impedance spectroscopy; thermal runaway

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Pressure measurement during thermal runaway of lithium-ion batteries: Comparison of piezoelectric and piezoresistive pressure sensors

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Introduction: Although the energy storage technology of lithium-ion batteries (LIBs) has excellent characteristics, it harbors a potential risk due to its ability to undergo thermal runaway (TR). TR is accompanied by a rise in pressure and temperature, as well as possible secondary effects (e.g. explosion). A common mitigation strategy is the housing of LIBs in enclosures with a high pressure resistance (e.g. flameproof enclosures). The maximum pressure that occurs is therefore an important design criterion for such enclosures. Both piezoelectric (PE) and piezoresistive (PR) sensors can be used to measure the pressure. However, it is currently unclear whether one of the two sensor types is better suited for the measurement task. For comparative analysis, TR experiments are carried out in a flameproof enclosure using overheating as the failure mode. In addition to various temperature readings the pressure is recorded using PE and PR sensors.

Methodology: The TR represents a quasi-static process with a high temperature load, unclear pressure wave development and a variable pressure measuring range. PE sensors are characterized by a short response time and high flexibility, which enables them to capture dynamic phenomena. Their distinct acceleration sensitivity is usually a disadvantage in systems, where rapid pressure increases can excite resonance vibrations that result in the distortion of the pressure signal. By using reference sensors installed in blind holes, both signal components can be separated and thus the true pressure signal can be obtained. Further, PE sensors are sensitive to temperature transients, resulting in reduced pressure values (thermal shock). Through protective coatings the onset of thermal shock during fast pressure rises (e.g., gas explosions) can be delayed, allowing the measurement of a correct peak pressure. However, the applicability of this concept to the much slower TR of a LIB, where multiple temperature-generating processes occur, remains to be tested. PR sensors are slower and less flexible, which can be problematic regarding TR dynamics. However, they are neither particularly sensitive to acceleration nor temperature. This type of sensor is therefore especially suitable for analyzing the position dependence of pressure values.

Experimental Evaluation: To evaluate the suitability of PE and PR sensors for pressure measurements during TR, experiments with multiple sensor configurations were performed while varying the gas atmosphere (air, nitrogen, hydrogen air and propane air) inside the enclosure. This allowed the parameters of TR dynamics, temperature input, parasitic oscillations and secondary fire and explosion to be investigated as factors influencing the accuracy of the maximum pressure of both sensor types.

Keywords: thermal runaway; lithium-ion batteries; flameproof enclosure; piezoelectric pressure sensor; piezoresistive pressure sensor; thermal shock; acceleration sensitivity.

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Development of a National Shock Tube Facility for Combustion Energy Calibration: Enabling Thailand Advancements in Aerospace Applications and Metrological Infrastructure

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Introduction: High-speed gas flow measurements in the supersonic regime are essential for advancing aerospace technologies and supporting energy-related applications such as combustion diagnostics and jet engine performance. This study presents the development of Thailand's national facility centred on shock tube technology to establish traceability and support precise dynamic pressure measurements. The shock tube enables the generation of well-characterized shock waves with high repeatability, simulating rapid pressure transients and extreme thermodynamic conditions relevant to aerospace propulsion and detonation processes. In addition to high-frequency pressure transducers, optical diagnostic techniques such as laser-based detectors and Schlieren imaging are employed to capture shock wave propagation and visualize flow disturbances with high temporal and spatial resolution. These complementary methods enhance the accuracy of shock characterization and support advanced studies in compressible gas dynamics.

Methodology: In this study, a shock tube system was employed for dynamic pressure calibration. The apparatus consisted of high-pressure and low-pressure sections, separated by a diaphragm or a fast-opening valve. Upon triggering, a shock wave was generated and propagated through the driven section. Time-resolved pressure signals were recorded using high-frequency pressure transducers positioned along the shock tube. These signals were analyzed to determine shock wave velocity and associated pressure behavior. To validate the measurements and understand compressible flow dynamics, computational fluid dynamics (CFD) simulations were conducted under comparable initial conditions. This methodology enables precise characterization of transient pressure events and supports the establishment of dynamic pressure standards for metrological and aerospace applications.

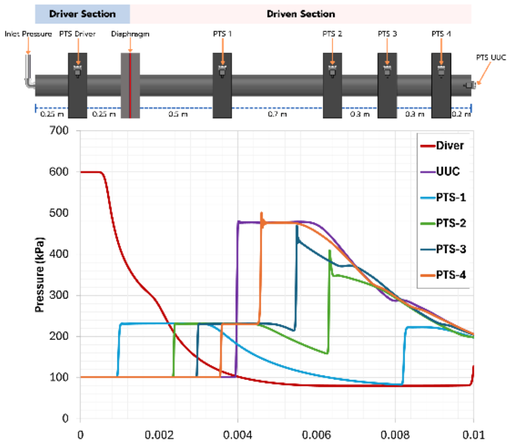

Fig.1 Schematic of the shock tube configuration and the simulated dynamic pressure response

Experimental Evaluation: The experimental setup consists of a shock tube system designed for dynamic pressure evaluation. Fig. 1 illustrates the shock tube system, which incorporates pressure transducer sensors (PTS) mounted at fixed axial positions to capture time-resolved pressure profiles. When the diaphragm ruptures, a shock wave is generated and propagates through the driven section, inducing a sudden pressure rise that is recorded by the PTS.

Keywords: shock tube; combustion energy; supersonic flow; dynamics pressure.

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Laminar Flame Speeds of Methanol and Ethanol at High Pressure and Temperature Conditions: An Experimental and Modeling Approach

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Introduction: Laminar flame speed is one of the fundamental properties characterizing a fuel and is used for the validation of chemical kinetic mechanisms. However, most of the databases available for such a key parameter are still limited in thermodynamic conditions. In the present study, laminar flame speeds were determined experimentally for different methanol/O_2 and ethanol/O_2 diluted mixtures under a wide range of conditions. The aim of this study is to provide new laminar flame speed data for methanol and ethanol, covering high pressures and temperatures previously unexplored. These data of such small alcohols contribute to the base mechanism of kinetic models as validation targets. Therefore, a kinetic mechanism was also developed in this work and was tested on the present experimental results as well as on other literature data to serve as a robust core mechanism in the future.

Methodology: All experiments were carried out in OPTIPRIME, the perfectly spherical combustion chamber with full optical access developed at ICARE laboratory. Initially in liquid phase, the fuel was injected with a syringe, where it was quickly evaporated and directed to the chamber. The oxidizer and diluent were then successively introduced using the partial pressure method. The experiments were subsequently conducted and both pressure and flame radius evolutions were simultaneously recorded to calculate the laminar flame speed using the isochoric method.

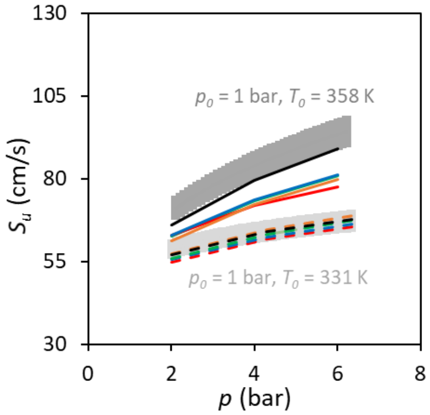

Fig.1 Flame speed evolution as a function of pressure for stoichiometric mixtures of methanol/air (dark gray trace and solid lines) and ethanol/air (light gray trace and dashed lines). Thickened gray traces correspond to experimental results with their associated uncertainty (±5%). Lines correspond to numerical results: Black: present work – Red: HPMech – Blue: POLIMI C1-C3 – Orange: AramcoMech3.0 – Green: NUIGMech1.1.

Experimental and Modeling Evaluation: For the different mixtures studied in this work, the laminar flame speeds were measured and plotted as a function of the pressure, along with the corresponding simulations obtained using the present mechanism. Fig.1 illustrates the results for one of the stoichiometric mixtures tested for each fuel. The performance of this mechanism in predicting the experimental data was compared to that of four distinct kinetic models available in the literature. Sensitivity analyses were then performed in order to identify the reactions controlling the flame speed evolution for methanol and ethanol. Finally, our mechanism was tested on various literature data of both fuels for further validation.

Keywords: laminar flame speed; methanol; ethanol; kinetic model.

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MaritimeMET: Metrology for Green Maritime Shipping - Emission control through traceable measurements and machine learning approaches

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Introduction: In the coming years, the maritime shipping sector seeks to embrace alternative fuels such as green ammonia, hydrogen, synthetic fuels, and Power-to-X (PtX) solutions like methanol and biomethane to reduce their environmental impact. This transition demands the development of engine technologies to adapt to these new fuels and a growing need for accurate and traceable measurement systems to support these advancements and validate their performance. Accurate pressure, temperature, and emission concentration measurements are essential for research and development in this sector and, at the same time, benefit related sectors. Exploiting the advances in machine learning approaches and modelling will significantly help optimize the power units and after-treatment systems.

Methodology:

1. To develop new and improve existing traceable emission measurement methods for online and in-situ measurements of typical gaseous (e.g., NO, NO2, N2O, NH3, CH3OH, CO, CH2O) and PM, black carbon (BC) emissions generated from PtX fuels. The methods and selected commercial low-cost sensors will be validated and applied for dynamical measurements on test engines running on selected fuels. Sources of measurement uncertainties will be identified and quantified.
2. To establish quality-assured dynamic measurements of the in-cylinder dynamic pressure and temperature necessary for assessing and optimizing the quality and efficiency of the energy conversion processes using renewable fuels. This will be achieved by developing primary standards and robust measurement methods covering the 0.1 MPa – 30 MPa pressure range and up to 2500°C in temperature. The frequency ranges of 0.5 kHz – 100 kHz and up to 1 kHz in pressure and temperature, respectively, with an uncertainty of 1 % will be targeted. An inter-laboratory comparison and engine tests will validate the developed standards and methods. The outcome results will be used in the predictive model development.
3. To create predictive models for engine emissions and performance using chemical kinetics and machine learning. Furthermore, virtual sensor concepts are developed based on data-driven and physics-based models to estimate hard-to-measure quantities or substitute costly sensors. Emission measurements (objective 1) and in-cylinder pressure and gas temperature (objective 2) will deliver the required database for model development, a mandatory input to complete these objectives.
4. To facilitate the take up of the technology and measurement infrastructure developed in the project by the measurement supply chain (e.g. accredited laboratories, instrument manufacturers), standards developing organizations (e.g. ISO, CEN/CENELEC) and end users (e.g. marine, power and aviation industries), using effective communication, dissemination and exploitation strategies and via relevant European metrology networks (EMNs).

Keywords: Metrology, Maritime emissions, Traceability, dynamic pressure, dynamic temperature, machine learning models, virtual sensing.

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Metrology to support ammonia use in emerging applications

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Introduction: The European Union through its initiatives (REPowerEU, REFuelEU, and FuelEUmaritime) aims to reduce the EU's net greenhouse gas emissions. Green hydrogen is central to this context, but the demand will be met through import. Ammonia promises to be a suitable hydrogen energy carrier with its extended use in end-case applications (e.g., ammonia cracking, shipping, and power generation). The project aims to ensure that the metrology infrastructure and relevant services are in place to facilitate using ammonia in these emerging applications. The overall objective of the project is to develop a comprehensive metrological framework that supports the deployment of ammonia as an energy carrier across various sectors, including energy, transportation, and industry. This involves establishing reliable measurement techniques and standards throughout the entire ammonia value chain, addressing gaps in current infrastructure, and facilitating the broader adoption of ammonia in both existing and emerging applications.

1. To develop new primary reference materials and gas analysis methods for ammonia as an energy carrier. This will include analysing different groups of impurities (e.g., H2O, CO2, CH4, H2S) arising from various production process value chains. Furthermore, to develop static and dynamic gas reference materials for priority air pollutants (e.g., NH3, N2O) from hydrogen production processes for leakage measurement and emission monitoring during thermo-chemical ammonia conversion processes.
2. To develop calibration and validation procedures for flow meters used for gas and liquid ammonia flow measurement, and custody transfer under field conditions. In addition to investigate the use of surrogate fluids (e.g., water, air, nitrogen) and optical methods (e.g., laser-Doppler-velocimetry) for calibration of ammonia flow meters under laboratory conditions (uncertainty target smaller than 0.3 %) and under field conditions for both gaseous and liquid ammonia.
3. To develop traceable monitoring methods for accurately quantifying ammonia leaks in its value chain and to establish a metrology infrastructure to support ammonia leak detection by developing capabilities to create SI traceable and controlled releases that mimic leaks. In addition, to determine the material compatibility of sensors and instruments (e.g., temperature, pressure, flow) in an ammonia-enriched environment by evaluating performance degradation, ageing, and adsorption/desorption effects. These studies will be extended to evaluate the material's compatibility for long-term storage of ammonia.
4. To develop traceable and validated real-time online stack emission (e.g., NH3, N2O, NO, NO2) and flow monitoring measurements (including uncertainty estimations) with an evaluation of the effects of ammonia impurities on pollutant formation (e.g., SOx, CO, CO2) during the thermo-chemical conversion of ammonia. In addition, to conduct an attributional LCA for ammonia for a set of specific applications (e.g. as a fuel), by providing estimates for 17 mid-point environmental categories and associated key uncertainty (e.g., pollutants, GHG emissions, eco-toxicity).

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The Experimental Flame Speed Measurements of 2,3-Butanediol and the Development of a Novel Kinetic Sub-Mechanism

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Introduction: 2,3-butanediol has recently been proposed to be a potential Mars-specific rocket propellant [1]. Although its biotechnological production on Mars seems viable, its combustion mechanism still remains unexplored. In this regard, the fundamental combustion characteristics, such as flame speeds, ignition delay times and oxidation species profiles of this fuel need to be studied over a wide range of conditions to model its combustion and understand its oxidation chemistry. In this study a kinetic mechanism was developed for the high temperature oxidation of 2,3-butanediol and its flame speeds were measured as a validation target.

Methodology: The flame speeds were measured in a perfectly spherical constant volume vessel (OPTIPRIME, located at ICARE-CNRS) by applying spherically propagating flame methodology. The pressure-time history during the flame propagation is acquired to determine the flame speeds. An increase in pressure is induced by the centrifugal consumption of fresh gases by the flame front and the fresh gases temperature increases as a result of the isentropic compression. Hence, the flame speed is evaluated for a range of pressures and temperatures.

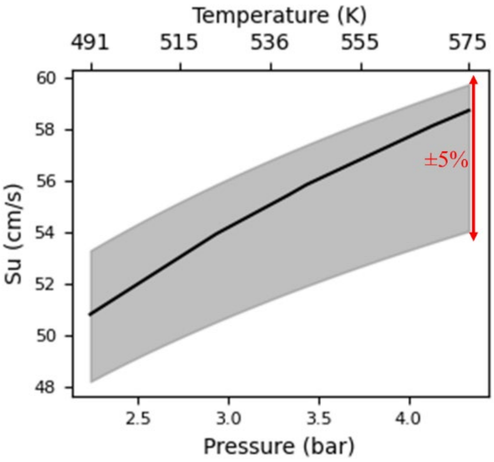

Fig.1 Experimental (uncertainty range in grey) versus predicted flame speeds (in black line) by the novel 2,3-butanediol kinetic mechanism for $\varphi = 0.8/p_0 = 1$ bar.

Experimental Evaluation: The flame speeds of 2,3-butanediol were measured for equivalence ratios between 0.8 and 1.2 at initial pressures of 1 and 2 bar and at initial unburned gas temperature of 403 K. The high-temperature kinetic sub-mechanism developed in this study was found to perform well against the experimental measurements, although some minor deviations were still observed in some cases. Fig.1 shows the results for $\varphi = 0.8$ at $p_0 = 1$ bar. Furthermore, sensitivity analysis was performed for lean, stoichiometric and rich conditions, the results of which revealed that the flame speeds are mainly sensitive to C_0-C_1 kinetics, while no fuel-specific reactions were detected among the top sensitive reactions. Finally, reaction pathway analysis demonstrated that the fuel decomposes almost totally via H-abstraction reactions to its two radicals, particularly by the attack of O, H and OH radicals.

Keywords: 2,3-butanediol; laminar flame speed; kinetic mechanism.

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Experimental and numerical investigation of the use of ammonia in a staged combustion engine

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One of the main obstacles to put a brake on global warming is the dependence on fossil fuels that still accounted for more than 80% of the primary energy worldwide in 2023. Despite the increasing use of electric motors, their limitations in heavy duty transport or off-road machinery requiring more power density will ensure the persistence of internal combustion engines.
In this context, one of the solutions that has been investigated during the past few decades is the development of electro-fuels to replace fossil fuels. Electro-fuels are produced by electrolysis of water using electricity. This reaction will produce hydrogen that in turn can react with, among others, carbon to generate methane or with nitrogen to generate ammonia.

The use of NH_3 in internal combustion engines (for decentralized CHP units, for example) has some interesting advantages compared to other electro-fuels, such as its ease of storage in liquid form and its high energy density at liquid state. However, it still presents some issues that need to be investigated. The main challenge that this work will try to overcome is the high emissions of NO_x during the combustion of NH_3 and NH_3/H_2 blends.

Some previous studies about NH_3 combustion in a gas turbine showed that the emissions of NO_x can be reduced by using a two-staged combustion, with a slightly rich primary combustion. In the engine sector, similar combustion conditions are present in staged combustion engines that are the focus of this work. A staged combustion engine operates with pairs of cylinders coupled in series. A fuel-rich mixture enters the first cylinder where it undergoes a 4-stroke conventional engine cycle. Due to the richness of the mixture injected in the first cylinder, the exhaust products of this cycle contain a considerable amount of combustible species. These products are then mixed with additional air before being inducted into the second cylinder where they undergo another 4-stroke cycle.

Gasoline-powered staged combustion engines have been studied in the late 20th century with the objective of reducing the exhaust emissions while achieving a good fuel economy but have since received less attention. Indeed, to reach the performance of a conventional gasoline-fueled spark ignition engine, the staged combustion engine requires a 40% increase in engine displacement.
Their application with NH_3 has not been studied yet and could be interesting since the working principle of staged combustion engines -characterized by the use of fuel-rich mixtures in the first cylinder and low temperatures- will reduce NO_x emissions.

Therefore, during my thesis, I will start with simulations of the staged combustion of NH_3 and NH_3/H_2 blends These will be performed with Cantera, OpenSmoke++ and GT-Power under several initial conditions and combinations of combustion modes (SI, HCCI). Then, a conventional internal combustion engine will be modified to a staged combustion engine to conduct the experimental part of the work. The emissions of the engine using NH_3 and NH_3/H_2 blends as fuel, as well as output variables such as the indicated mean effective pressure (IMEP), will be experimentally measured to assess whether the use of a staged combustion engine is justified to reduce NO_x emissions from NH_3 combustion.

Keywords: ammonia; staged combustion engine; NO_x; electro-fuel; spark ignition; homogeneous charge compression ignition; combustion.

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