

Metrology and Process Safety for Hydrogen Technologies & Applications

772. WE-Heraeus-Seminar

10 Oct - 13 Oct 2022

Physikzentrum

Bad Honnef/Germany

**WILHELM UND ELSE
HERAEUS-STIFTUNG**



Program

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Program

Sunday, 9 October 2022

17:00 – 20:00	Registration	
18:30 – 19:30	<i>BUFFET SUPPER</i>	
19:30	Joachim Ullrich	Inaugural Lecture: Role and challenges in metrology and process safety in the energy transition

Monday, 10 October 2022

07:30	<i>BREAKFAST</i>	
08:20 – 08:30	Scientific Organizers	Welcome
08:30 – 09:30	Robert Schlögl	Hydrogen a key element to a sustainable energy system
09:30 – 10:30	Richard Hanke-Rauschenbach	Hydrogen production by means of proton exchange membrane water electrolysis: An overview
10:30 – 11:00	<i>COFFEE BREAK</i>	
11:00 – 12:00	Aline Leon	High-temperature steam electrolysis using solid oxide cells
12:00 – 12:05	Conference photo (in front of the venue, main entrance)	
12:05	<i>LUNCH</i>	
13:30 – 16:00	Poster Flash Presentation I & Poster Session I	

Program

Monday, 10 October 2022

16:00 – 16:30 *COFFEE BREAK*

16:30 – 17:30 Ulrike Krewer

**Model-assisted analysis and
improvement of fuel cells and
electrolysis: from surface to cell**

17:30 – 18:30 Robert Braun

**Emerging Electrochemical Energy
Systems for Flexible Energy Storage
and Hydrogen Production**

18:30 *HERAEUS DINNER at the Physikzentrum
(cold & warm buffet, with complimentary drinks)*

20:00 **Networking**

Program

Tuesday, 11 October 2022

07:30	<i>BREAKFAST</i>	
08:30 – 09:30	Laurent Selle	Flashback and other risks mitigation in hydrogenfueled gas turbines and boilers
09:30 – 10:30	Thomas Jordan	Safety of cryogenic hydrogen
10:30 – 11:00	<i>COFFEE BREAK</i>	
11:00 – 11:30	<i>Robert Schießl</i>	<i>Hydrogen production by multi-functional energy conversion in piston compressors</i>
11:30 – 12:00	<i>Rainer Kramer</i>	<i>Challenges and perspectives for hydrogen flow metrology</i>
12:00	<i>LUNCH</i>	
13:30 – 16:00	Poster Flash Presentation II & Poster Session II	
16:00 – 16:30	<i>COFFEE BREAK</i>	
16:30 – 17:30	William Green	Thermochemical Conversions for the Energy Transition
17:30 – 18:30	Tina Kasper	Reactivity of mixtures in conversion processes
18:30 – 18:45	Stefan Jorda	About the Wilhelm and Else Heraeus Foundation
18:45	<i>DINNER</i>	
19:45	Panel Discussion moderated by Katharina Kohse-Höinghaus: Peter Wasserscheid Tina Kasper Regis Bauwens Aline Leon William Green	

Posters

POSTERS / Monday, 10 Oct. 2022

Sumit Agarwal & Denghao Zhu	A study on autoignition characteristics of H₂-NH₃-O₂ mixtures with diluents of Ar/N₂ in shock tube for argon power cycle engines
Ahmad Alshwawra	Performance Study of Additively Manufactured Cylinder Liner
Karan Anand	Dynamic modeling of polymer electrolyte membrane (PEM) electrolyzers for flexible operation using artificial neural networks
Jessica Dymke & Stefan Essmann	Ignition properties of ammonia/hydrogen blends
Jacqueline Horstmann	Experimental characterization of turbulent hot jet ignition of ultra-lean hydrogen/air mixtures
Holger Janssen	FCEV-Independent Hydrogen Sampling Methodology and Purity Analysis with IMR Mass Spectrometry
Mengdi Li	Study on the reaction kinetics of ammonia/ethanol oxidation at intermediate temperatures
Arnas Lucassen	Investigation of enhancement of the NH₃ low temperature oxidation by H₂ addition in a plug-flow reactor
Gongping Mao	Development of a reduced chemical kinetic mechanism for HCCI combustion of hydrogen-ammonia mixtures using combined reduction methods
Solmaz Nadiri	Reaction mechanism development for ammonia/methanol blends
Olav Werhahn	Hydrogen metrology in the context of the CIPM MRA

POSTERS / Tuesday, 11 Oct. 2022

Ali Navid	OMEn/Diesel spray injection in an RCCI engine; Combustion analysis in the presence of Hythane
Felix Poschen	Development of a kinetic mechanism for modelling oxymethylene ether combustion and pollutant formation
Leopold Seifert	Effect of dynamic pressure measurement and its influence on understanding reaction kinetics of Hydrogen/Methane mixtures
Sudhi Shashidharan	Experimental characterization of turbulent hot jet ignition of ultra-lean hydrogen/air mixtures
Prashant Shrotriya	An Iterative Methodology for REDIM Reduced Chemistry Generation with Focusing on Partially-Premixed Type of Combustion
Patrick Treffehn	On the Role of Water in Gas-Phase Reactions of Isocyanic Acid under SCR conditions
Johannes Wenz	An Experimental and Theoretical Study of the Unimolecular and Bimolecular Reactions of Dimethyl Car-bonate
Chunwei Wu	Experimental and numerical studies on lean flammability limits of methane/hydrogen/air turbulent flames
Chunkan Yu	Hydrogen as co-fuel in the combustion of low & zero carbon fuel
Simon Drost	Effects of hydrogen addition to auto-ignition properties of methane/air mixtures

Abstracts of Talks

(in alphabetical order)

Hydrogen explosion hazards in industry and efforts to quantify and mitigate these risks

C.R.L. Bauwens and S.B. Dorofeev

FM Global, Research Division, Norwood, USA

The use of hydrogen as an alternative energy carrier is rapidly spreading across a wide range of industries. As a result, new hazards are being created at locations that traditionally did not present explosion hazards. To adequately address these needs, new models and research is needed to properly assess the unique hazards hydrogen can create and to develop appropriate mitigation techniques.

This presentation describes a series of studies performed by FM Global to better characterize the large-scale behavior of hydrogen-air explosions. These studies include work characterizing the rate of spherical flame acceleration of hydrogen at large scale, its interaction with turbulence, and how the scale of the explosion significantly affects the effective reactivity of the flame [1]. Experimental and numerical studies examining the pressures that develop during vented explosions [2]. A simple computation study examining the consequences of a hydrogen release during indoor dispensing and filling operations [3]. And the development of models to estimate the detonable fraction of large-scale hydrogen jet releases and the expected overpressures that are generated [4].

Throughout these studies we will show how the unique properties of hydrogen significantly affects the explosion dynamics in these scenarios and how specialized models and research specifically focused on hydrogen is needed to appropriately characterize its behavior. Finally, the presentation will conclude with some thoughts on the direction of future research into hydrogen being performed at FM Global and the areas that are currently present the most significant emerging hazards.

References

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Emerging Electrochemical Energy Systems for Flexible Energy Storage and Hydrogen Production

Robert J. Braun

Rowlinson Professor of Mechanical Engineering
Department of Mechanical Engineering
Energy & Materials Program
Colorado School of Mines
Golden, Colorado

Abstract

This presentation will highlight research accomplishments related to emerging solid oxide cell and protonic ceramic electrolyzer technologies, which are increasingly being targeted as attractive distributed energy solutions. Movement towards predominately low-carbon energy systems requires renewable resources and could be accelerated by integration with high temperature electrochemical technologies. Currently, substantial penetration of wind and solar resources into the electric power grid is challenged by their intermittency and the timing of generation which can place huge ramping requirements on central utility plants. This talk will discuss advances being made in flexible distributed energy resources that can serve as electrical energy storage and hydrogen production systems. In particular, full-scale hybrid fuel cell/engine system development progress targeting 70% electric efficiency, reversible fuel cell energy storage systems, and Power-to-X energy production based on high temperature electrochemical cells will be highlighted. Reversible solid oxide cells (ReSOCs) are capable of providing high efficiency and cost-effective electrical energy storage. These systems operate sequentially between fuel-producing electrolysis and power-producing fuel-cell modes with storage of reactants and products in tanks for smaller-scale (kW) applications and between grid and natural gas infrastructures for larger scale (MW) systems. Physics-based modeling and simulation of these novel energy systems is a central element to our work, supporting and guiding technology development. The developed models are used to accelerate the design and development of flexible, hybrid electrochemical systems, for both grid-scale energy storage and as a Power-to-Gas platform that can address issues with high renewables penetration. Performance characteristics, scale-up and demonstration activities, and techno-economic outlook of these ceramic electrochemical energy conversion technologies are summarized.

Future challenges of hydrogen utilization for energy conversion

A. Comandini and N. Chaumeix

ICARE - CNRS, 1c Avenue de la Recherche Scientifique, 45071 Orléans, France

The need to reduce our carbon footprint, to rapidly deploy alternative energies to fossil fuels and to reduce our dependence on them has driven the recent debate on the future of energy conversion, including the consideration of hydrogen both as a fuel and an energy carrier. In this effort towards cleaner and more sustainable economies, France has decided to divide its greenhouse gas emissions by four by 2050 compared to the 1990 emission level. The decarbonization of energy consumption in France will have to be achieved keeping in mind that this low-carbon society will require a safe and affordable energy distribution and storage. Hydrogen's attractiveness lies in its versatility; it can be used in a wide range of applications such as power generation, energy storage, and transportation. The latter is overshadowed, however, by its high susceptibility to explosions. In the event of an accidental leak, hydrogen, mixed with air, will ignite very easily given its combustion properties.

As liquid hydrogen is denser than gaseous hydrogen, it will replace the latter in the storage for future applications. These new uses necessarily lead to a re-evaluation of the risks linked to the environment changes. Indeed, different needs must be addressed including (i) a better understanding of the evaporation, dispersion, and ignition of liquid and gaseous H₂, (ii) a need for innovative instrumentations (fast visualizations, non-intrusive H₂ probes, and total radiative flux measurements), (iii) validation of the simplified and detailed numerical tools against laboratory well-controlled experiments, and (iv) a numerical extrapolation to industrial large scales.

The presentation will focus on the current knowledge and tools available to tackle the future challenges of hydrogen utilization from stationary energy production to transportation.

Hydrogen-based fuels for advanced aviation combustion

Friedrich Dinkelacker, Leibniz Universität Hannover

Abstract

The utilization of hydrogen for propulsion is one of the intensively discussed targets for future sustainable aviation. One potential option is based on hydrogen fuel-cell electric aviation, the other on the direct combustion of hydrogen, which from the ecological side has nearly the same positive characteristics, but is much easier to realize. Some actual research questions for direct hydrogen combustion will be discussed.

However, both concepts need hydrogen as energy carrier with challenging storage requirements. In so far, larger energy carrier molecules, being possibly liquid, and being made out of green hydrogen and renewably produced electricity, are possibly more realistic for application in aviation. One option would be based on ammonia (NH_3) utilization, which can be understood as hydrogen carrier. Here, however, other drawbacks prevent the application in aviation.

Current environmental action is focused on the utilization of sustainable aviation fuels (SAF), for instance in the way, that aviation fuel might be produced with sustainably produced (green) electricity together with CO_2 from biomass or from carbon capture - so being one type of so called eFuel. This would reduce the direct CO_2 emission. However, the non- CO_2 contributions would remain.

In our work, an new path is investigated, where with advanced sustainable eFuels also the non- CO_2 emission, especially the soot particulates and also the nitrogen oxide emissions would be addressed. This research vision is based on the hypothesis, that with suitable advanced aviation eFuels the ultra clean lean prevaporized premixed (LPP) combustion concept would be applicable, which has been proposed 30 years ago for aviation but has failed for kerosene. It would allow a dry ultra-low NO_x and particulate free combustion mode. First research steps are discussed to find good sustainably produced eFuels for the special utilization with the LPP combustion concept. The properties of such advanced eFuels need to be fully different from current kerosene substitute fuels.

The different approaches for sustainable aviation will be compared.

Goldmann A., Sauter W., Oettinger M., Kluge T., Schröder U., Seume J., Friedrichs J., Dinkelacker F., *A Study on Electrofuels in Aviation*, *Energies*, 2, 392, 2018.

Goldmann, A., Dinkelacker, F., *Experimental Investigation and Modeling of Boundary Layer Flashback for Non-Swirling Premixed Hydrogen/Ammonia/Air Flames*, *Comb. Flame* 226, 362-379, 2021.

Nadiri, S., Zimmermann, P., Sane, L., Fernandes, R., Dinkelacker, F., Shu, B., *Kinetic modeling study on the combustion characterization of synthetic C3 and C4 alcohols for lean premixed prevaporized combustion*, *Energies*, 2021, 14, 5473.

Thermochemical Conversions for the Energy Transition

William H. Green

Massachusetts Institute of Technology, Department of Chemical Engineering,
Cambridge, USA

Hydrogen is expected to be a pillar of the energy transition away from fossil fuels. This energy transition needs to happen soon to reduce the harm from rapid climate change. However, it is not yet clear how best to produce and transport/distribute all the needed low-greenhouse hydrogen, nor how it should/will be used in different applications. Solutions are needed which work in all parts of the world, for people with vastly different incomes, and which ensure (or at least do not reduce) energy security. The lack of clarity about which options are most beneficial to society (and potentially most profitable and most sustainable) leads to hesitancy in making major investments, and sometimes to reluctance to institute policies that would allow or encourage deployment. Development of technical consensus within the engineering community that a certain option is either very promising or very unlikely to succeed can be quite helpful in developing a societal consensus. In this talk we discuss some of the pros and cons of particular thermochemical routes for producing hydrogen, and related routes for producing low-greenhouse fuels and energy carriers, highlighting some of the unresolved questions. Many of the options require addressing safety and/or metrology issues before they could be deployed on a large scale.

Hydrogen production by means of proton exchange membrane water electrolysis: An overview

R. Hanke-Rauschenbach and B. Bensmann

Leibniz University Hannover, Institute for Electric Power Systems, Hannover, Germany

The development of proton exchange membrane water electrolysis (PEM-WE) for hydrogen production to satisfy the industrial demand regarding scale, performance and lifetime is a challenging task. The objectives with the highest priority are the reduction of the power-specific cost and increases in efficiency, reliability, and durability.

Within this talk we give an overview on this important hydrogen production technology and present some of our own research papers in this context.

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Reactivity of mixtures in conversion processes

T. Kasper

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33098 Paderborn, Germany

The goal of curbing climate change requires a reduction in greenhouse gas emissions and forces the transition to CO₂-neutral technologies in the electricity, mobility, industry and building sectors. Combustion for energy and heat conversion is an advanced and reliable technology, which can help mitigate the risks of this transition. One short- to mid-term strategy is to defossilize the fuel used in combustion processes, e.g., by using hydrogen, or synthetic and biomass-derived carbon-containing fuels. Consequently, the reduction of pollutants and the improvement of the efficiency of combustion processes remains an important task. Predictive process simulation of fuel conversion of hydrogen/hydrocarbon mixtures can overcome empiric process optimization and requires a detailed understanding of the reaction pathways and chemical kinetics. A related problem is the production of higher value chemicals from synthetic or natural gas in gas phase chemical conversion processes. These processes can in principle be more efficient than current synthesis routes but have not been investigated in detail.

The work presented here, addresses both types of processes. Results of how methane can be activated by additives to undergo partial oxidation at moderate temperatures and pressures to yield products such as methanol or synthesis gas will be shown. The underlying kinetic processes will be explored, and the experiments used to derive these data will be introduced.

The kinetics of the interaction of hydrogen with hydrocarbon fuels are investigated at a fundamental level in low pressure laminar flames. These experiments, the associated diagnostic techniques, and their results are presented here.

In both processes the same transient intermediates control the reactivity of the system and the fuel. These important reaction pathways will be explained.

Challenges and perspectives for hydrogen flow metrology

Rainer Kramer, Physikalisch Technische Bundesanstalt

Abstract

hydrogen flow rate, traceability to SI, Reynolds number dependency, Venturi nozzle, orifice meter, rotary meter, diaphragm gas meter, laminar-flow element, Coriolis meter

Hydrogen is used for industrial applications since more than 100 years. For instance, hydrogen is used in the steel industry for tempering processes and for hot galvanizing of steel plates. Hydrogen is also an important base substance in the chemicals industry. This has led to the construction and usage of hydrogen pipeline networks in the Rhein area and in Saxony-Anhalt, hence there is already some experience with metering techniques for hydrogen flows. The increasing usage of hydrogen for mobility, insertion of hydrogen in the natural gas grid and its storage triggered a large number of projects, which concern also the flow rate measurement and the traceability to SI-units.

The department of gases at PTB uses different fundamental facilities to trace back flow rate measurements to the SI units for length and time. This includes a bell prover and some piston provers of different sizes. In order to achieve the traceability of flow measurements of hydrogen, fundamental facilities are usable, provided the explosion safety can be guaranteed by the instrumentation and the available test rooms. For flow rates up to $Q = 500$ l/h, mercury sealed piston provers are used for the calibration of nozzles, laminar flow elements and other devices. The results of piston provers are nearly independent from the kind of gas because their moving parts are not expected to cause gas-dependent leak flows.

A further approach is to realize the traceability by air calibration of meters and to investigate the need for corrections. In case of wet gas meters, a direct application of air-calibrated meters may be the basis for hydrogen measurements. For this purpose, the influence of the solubility of different gases in the sealing liquid was considered. By using wet gas meters, Venturi nozzles, rotary meters and laminar-flow elements have been calibrated for usage as working standards. The results for different gases, including hydrogen, will be presented.

In order to guarantee the correct billing of gas consumers in case of hydrogen insertion in existing natural gas grids, diaphragm gas meters were investigated in respect to their error curves, if used with air, N_2 , CH_4 , H_2 , and mixtures of CH_4 and H_2 . It was found that diaphragm gas meters are not influenced systematically by the kind of gas. In case of rotary meters, a clear dependency of the error curves by the kind of gas is to be observed. In the middle part of the Reynolds number range an overlap of the error curves is found. For lower flow rates (low Reynolds numbers) the error curves do not overlap. The cause is, among others, the influence of mechanical friction in the bearings.

A possibility for hydrogen flow rate determination is also the usage of orifice meters and critical nozzles. By knowing the mechanical dimensions, a calculation of flow rates on the basis of the state of gas equation led already to uncertainties of less than 1 %. In a project, air measurements will be compared with hydrogen measurements. For this purpose, an orifice meter was realized as a DN 50 test run. In this test run, meters with other measuring principles shall be tested, in particular Coriolis meters and ultrasonic meters. The technical restrictions of these meter techniques shall be discussed.

Model-assisted analysis and improvement of fuel cells and electrolysis: from surface to cell

U. Krewer¹

¹*Karlsruhe Institute of Technology, Institute for Applied Materials – Electrochemical Technologies, Karlsruhe, Germany*

Fuel cells and electrolyzers promise efficient conversion between electrical energy and hydrogen. Knowledge-driven improvement of their performance requires in-depth understanding into the bottlenecks and the interplay of processes causing these bottlenecks. But how to get this insight, and how to predict, what would be better configurations? Here, model-based analysis and optimization is a promising methodology, as it gives insight into not measurable processes or states, and as it allows a virtual design of better catalysts, electrodes, cells or operating conditions.

In this talk, we will show how this works at the example of three cell technologies. For the PEM electrolysis, a deep microkinetic analysis of the processes at and degradation of the oxygen evolution catalyst is given. Dynamic microkinetic modeling is used to analyze the single reactions and their interplay during OER at the electrode surface. [1] The model allows to study the electrocatalytic reaction mechanism including the coverage of emerging surface species for a wide potential, and limiting steps. Interestingly, even degradation effects can be backtraced to changes in specific reaction steps. [2] For oxygen depleting cathodes, the importance of local pH changes on O₂ saturation and electrode performance is revealed. It is shown how slow electrolyte transport can be detected using dynamic potential-step measurements [4,5], and what impedance spectra tell about degree of flooding. [6] For alkaline membrane fuel cells, a cell level analysis is conducted to identify strategies to prevent ambient CO₂ impact on performance. [3] The model reveals the effect of CO₂ carbonation on the concentration profiles in membrane and anode and assesses temperature and current dependence.

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High-temperature steam electrolysis using solid oxide cells

A. Léon¹, A. Micero¹, B. Ludwig¹, C. Benel¹, D. Dritschler¹, J. Schefold¹

¹*Institute for Energy Research (ElFER), Karlsruhe, Germany*

Within the energy transition, hydrogen demand is estimated to increase by 10-fold [1]. As such, multiple resources have to be envisaged based on carbon or without carbon like water. Different processes of electrochemical conversion can be envisaged using water like electrolysis or photo-electrolysis. As concern water electrolysis, three technologies are scaled-up to the gigawatt scale namely proton exchange membrane electrolysis (PEMEL), alkaline electrolysis (AEL) and high-temperature steam electrolysis (HTEL) [2]. This presentation will focus on high-temperature steam electrolysis (HTEL) that uses waste heat from industrial processes, uses less critical material, has the potential to operate reversibly in fuel cell or electrolysis mode as well as to produce syngas in the co-electrolysis process. The performance, durability and flexibility of this technology will be shown when scaling-up from single cell [3] to short-stack (10 cells) [4], stack (30 cells) and module (90 cells) [5]. Long-term operation of cell (above 20,000 hours) and stack (above 4500 hours) as well as ON/OFF switching profiles (above 10,000 cycles) will be shown and discussed in terms of degradation rate. It will be shown that tracing the source of degradation requires a multi modal approach with classical and advanced imaging, scattering and spectroscopy techniques down to nanoscale. As so, 2D nano X-ray fluorescence maps of the cells will be presented to highlight the active as well as the detrimental layers to the electrochemical reaction [6].

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Competence Centre H₂Safety@BAM – Safeguarding the Quality Infrastructure in the Hydrogen Economy

**E. Askar, S. Günzel, K. Holtappels, G. Mair, M. Maiwald,
T. Orellana-Perez, O. Sobol, C. Tiebe**

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Hydrogen is a central component of the energy transition [1] and the European Green Deal [2] for a climate-neutral Europe [3]. To achieve the goals defined for 2050, the EU and the German government have developed a framework for action and are making long-term investments in research, development, and the rapid implementation of innovative hydrogen technologies.

With the Competence Centre "H₂Safety@BAM", BAM is creating the safety-related prerequisites for the successful implementation of hydrogen technologies at national as well as European level.

To this end, BAM conducts research, testing and consulting in a holistic and interdisciplinary manner under one roof – in the Competence Centre H₂Safety@BAM. The activities of the competence centre focus on ensuring the safety of infrastructures, plants, and processes as well as innovative hydrogen transport and storage systems based on digital quality testing and the experimental testing of components and systems. It thus creates the prerequisites for the implementation and adaptation of legal framework conditions as well as for standardization. Closely related to this are investigations into the properties and compatibility of metallic materials and polymers as well as friction systems for the safe operation of components, plants, processes, and systems. This interdisciplinary and holistic approach is complemented by the development of gas analytics and suitable sensors, online measurements of gas properties in process control, test scenarios under real conditions as well as impact assessments of accidents and risk assessments and risk management systems derived from them. With its portfolio of tasks and competences, BAM builds trust in the safety and reliability of technical system solutions for hydrogen.

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Hydrogen production by multi-functional energy conversion in piston compressors

S. Drost, R. Schießl, U. Maas

Institut für Technische Thermodynamik, Karlsruhe Institute of Technology - KIT

In response to the demand for flexible energy supply and storage technologies, novel coupled energy and material conversion technologies are considered. One such process type stimulates chemical conversion by gas compression in piston-engine type reactors to create valuable and highly energetic substances from cheap energy and material. In this paper, results from Rapid Compression Expansion Machine (RCEM) experiments and simulations on hydrogen production by two candidate conversion processes are presented; these processes are:



The results exhibit how the processes are dominated by the combination of high activation energies of the underlying elementary reaction steps and the strong endothermicity. The former demands high temperatures to allow reactions to commence. The latter causes negative thermal feedback because endothermal reactions tend to lower the temperature, and thus impose a self-inhibiting effect on the conversion.

The efficiency of several methods for raising the conversion and yield of hydrogen is assessed by combined experimental and simulation studies. These include the addition of Argon as a low-heat capacity diluent, as well as the addition of oxygen as a source of temperature-raising exothermal reactions. The influence of pre-compression conditions (temperature and pressure) on the conversion is also studied, as well as the effect of operation parameters like compression ratio, the duration of the compression-expansion process, and the repetition of compression-expansion strokes.

The required input of compression work per mass of produced pure hydrogen for the proposed processes is compared to the corresponding work for water electrolysis. The studies exemplify how a detailed view of chemical kinetics, physical processes and their coupling helps to assess and improve the potential of new concepts for chemical energy conversion.

Hydrogen a Key Element to Sustainable Energy Systems

Robert Schlögl

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Sustainable energy systems will be based upon electrons from solar power. A fraction of those will be used directly within electrical grids. As capacity factors and abundance of RES will not suffice to cover the average demand, a significant fraction will have to be stored, transported and traded in a global supply system for derived (“liquified sunshine”) solar energy.

Elemental hydrogen is the first form of chemically stored energy. In regional (Europe) transport and (underground) storage this compressed (or possibly liquified?) hydrogen can be used for all applications such as industry, process heat, power generation. Large amounts (thousands of TWh) need global exchange and bulk storage as derivatives like ammonia, methanol, methane and possibly other forms.

At present the evolution of this hydrogen-based energy carrier system is evolving in the world but with limited participation of Europe. Technologies are ready for first generation roll-out. Europe has a world-class industry for this value chain, it is lacking agility to meet the scale of demand. What is still missing is the demonstrated value chain from generation to usage with robust regulatory and economic boundary conditions. The uncertainty about the creation and operation of the essential infrastructure in the off-taker countries is a severe obstacle in rapid evolution of the solution.

Faster scalable technologies and process simplifications through system design and adapted materials are challenges for science and technology. Verifiable quality definitions and standardisations of properties, leak detection and other safety measures and certification of material and devices are missing essential elements to create business cases and economic stability that is transparent and sufficient for the assessment of the systemic efficiency of hydrogen and its derivatives in energy systems.

Flashback and other risks mitigation in hydrogen-fueled gas turbines and boilers

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Hydrogen is a peculiar fuel in the sense that its combustion properties are very different to that of classical hydrocarbon fuels. Specifically, its large burning velocity and wide flammability limits enhance the risk of flashback or increased heat loads for applications where the fuel and oxidizer are partially premixed. Dynamic phenomena such as hard ignition or combustion instabilities may also be affected by the switch to hydrogen. These issues should be identified and mitigated at the design stage to avoid a costly trial and error optimization process.

This presentation will focus on flashback but address these other risks in two target applications. First for gas turbines, a dual-swirl low-NO_x burner has been developed at IMFT [1] with the intent to completely avoid flashback while ensuring low emission levels and minimal heat loads to the burner head. Both experiments and numerical simulations of this configuration will be presented, illustrating the wide range of flame shapes that can be obtained with this versatile design. The second application is that of boilers for residential heating. Two existing designs were tested experimentally and their flashback and blowoff limits versus hydrogen content in the fuel is investigated [2]. Some fundamental aspects of the flashback mechanisms in laminar flames will also be discussed.

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Strength of knowledge in risk assessments for hydrogen systems in industry and society

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Hydrogen is expected to play an important role in the global energy transition. Existing technologies can convert energy from renewable and non-renewable sources to hydrogen, hydrogen can be stored and transported in compressed, liquid or chemical form, and fuel cells, engines or turbines can convert hydrogen to electrical or mechanical energy and heat on demand. At the same time, hydrogen is arguably the most reactive and easily ignitable of all energy carriers ever considered for widespread use in industry and society. This implies that it is not straightforward to achieve and demonstrate the required level of safety for hydrogen systems. Widespread deployment of hydrogen technologies in society will require massive investments, and the prospect of severe accidents represents a significant risk to all stakeholders. There have been several accidents involving hydrogen in recent years, and the stakes with respect to the potential for severe losses will increase as the use of hydrogen shifts from controlled environments in industrial facilities to the public domain, and transport applications extend from passenger cars and buses to trains, ferries and airplanes.

The purpose of a risk assessment is to increase the knowledge about a system, and to support decisions that may entail difficult economic, ethical or political deliberations. There is increasing awareness and recognition of the importance of reflecting knowledge and expressing uncertainty in the understanding, analysis, assessment, management and communication of risk, and various researchers have proposed methods for assessing the strength of knowledge (SoK) in risk assessments. The talk will focus on one aspect of the SoK in risk assessments for systems where hydrogen explosions represent a significant hazard: the understanding of physical phenomena and the ability of models and modellers to predict the consequences of accidental explosions in industry and society. Results from experimental campaigns and model predictions will be used to explore the inherent limitations in the predictive capabilities of model systems for fuel-air explosions in complex geometries, including the implications of weak knowledge from an ethical as well as a practical perspective. The suggestions for further work emphasise the importance of conducting further large-scale explosion experiments in test facilities that capture the complexity and spatial scale of the actual systems found in industry or society, in conjunction with blind-prediction benchmark studies for developers and users of consequence models.

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Chemical hydrogen storage - towards a hydrogen-free hydrogen economy

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Global logistics of renewable energy equivalents will create additional driving force towards a future hydrogen economy. However, the special nature of H₂ requires dedicated infrastructures and this has prevented so far its massive introduction to the energy sector.

Recent scientific and technological progress in handling hydrogen in chemically bound form supports the technological vision that a future hydrogen economy may work without handling large amounts of elemental hydrogen using the existing infrastructure for fuels. Liquid Organic Hydrogen Carrier (LOHC) systems are composed of pairs of hydrogen-lean and hydrogen-rich organic compounds that store hydrogen by repeated, catalytic hydrogenation and dehydrogenation cycles.[1] CO₂-based LOHC systems add interesting features to the more traditional systems based on aromatic/heteroaromatic compounds and their perhydro counterparts.

The contribution will highlight fundamental and applied aspects of LOHC hydrogenation and dehydrogenation catalysis and the related processes. It will focus on the development of optimized catalytic materials for LOHC hydrogenation/dehydrogenation,[2,3] and on operational stability aspects gained from demonstration units.[4,5] Application scenarios for stationary energy storage systems, hydrogen logistics and mobile applications will be discussed.

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Abstracts of Posters

(in alphabetical order)

A study on autoignition characteristics of H₂-NH₃-O₂ mixtures with diluents of Ar/N₂ in shock tube for argon power cycle engines

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Hydrogen-fueled Argon Power Cycle engine is a novel concept for high efficiency and zero emissions, which replaces air with argon/oxygen mixtures as working fluid. However, one challenge is severe backfire caused by elevated temperature resulting from the high specific heat ratio of Argon. The autoignition features of H₂ are crucial for understanding the combustion of fresh charge during the intake stroke in the engine combustion chamber and the intake manifold. Therefore, measurements of the ignition delay times of H₂-O₂ mixtures have been conducted in a shock tube at 0.1 MPa, 900 ~ 2000 K, with equivalence ratios of 1.0, 0.5, and 0.25, dilution ratios of 79% and 90%. Both argon and nitrogen were chosen as diluents to make a comparison. As a fuel with a long ignition delay time, NH₃ was also blended into H₂ to validate its probability to inhibit the backfire in the engine. Experimental results show that the ignition delay time of H₂ is insensitive to the equivalence ratio and dilution ratio. Besides, at the same temperature (<1110 K), the replacement of Ar by N₂ shortens the ignition delay time slightly. This phenomenon proves that the intensified backfire in the Argon Power Cycle engine is caused by the higher temperature rather than by the chemical features of Argon. In addition, the blending of NH₃ into H₂ lengthens the ignition delay time. This effect is significant when the NH₃ ratio reaches 80%. For instance, when the ignition delay time is near 100 μs, the corresponding temperature is respectively 1882 K, 1325 K, 1140 K, and 1132 K, when the ammonia ratio is 100%, 80%, 40%, and 0%. This result suggests that the blending of NH₃ might be a feasible method to control the backfire in Argon Power Cycle engines.

Keywords: hydrogen, ammonia, shock tube, ignition delay time, argon power cycle

Performance Study of Additively Manufactured Cylinder Liner

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One of the most important topics nowadays is the use of liquid or gaseous sustainable fuels such as hydrogen and biofuel in ICE. Improving the efficiency of ICE is a crucial factor for achieving a sustainable ICE and maximizing the benefit of conversion to sustainable fuels in this type of engine. To address this issue researchers are required to reduce friction which is one of the most important aspects of improving the efficiency of internal combustion engines. One of the most important parts of an engine that contributes to friction is the piston ring cylinder liner (PRCL) coupling. Controlling the linear deformation enhances the engine's performance and, as a result, contributes positively to its performance. It is possible to improve the performance of piston ring-cylinder liner coupling by implementing new and advanced manufacturing techniques. In this work, a validated finite element model was used to simulate the performance when advanced manufactured materials were adapted. The deformation of the cylinder liner due to thermal and mechanical loads is simulated with five different additive manufactured materials (Inconel 625, Inconel 718, 17-4PH stainless steel, AlSi10Mg, Ti6Al4V). Simulated roundness and straightness errors, as well as maximum deformation, are compared with conventional grey cast iron liner deformation. Some additive manufactured materials, especially Ti6Al4V, show a significant reduction in deformation compared to grey cast iron, both in bore and circumferential deformation. Results show that Ti6Al4V can reduce maximum liner deformation by 36%. In addition, the roundness has improved by 36%. The straightness error when Ti6Al4V was used has also improved by 44% on one side, with an average of 20% over the four sides. Numerical results indicate that additive manufactured materials have the potential to reduce friction within the piston-liner arrangement of internal combustion engines.

Dynamic modeling of polymer electrolyte membrane (PEM) electrolyzers for flexible operation using artificial neural networks

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Hydrogen is a promising energy carrier to decarbonize multiple sectors, e.g., chemical industry and mobility. One way to decarbonize the sectors is using green hydrogen that is produced via water electrolysis and renewable electricity. Due to the fluctuating nature of renewable electricity, the water electrolyzer needs to be operated flexibly which requires advanced control strategies to ensure that safety constraints, e.g., temperature constraints, are met during flexible operation [1]. Advanced control strategies such as model predictive control require fast and accurate models. Since rigorous nonlinear dynamic models are computationally expensive, we investigate the performance of artificial neural networks as surrogate models. Artificial neural networks pose a promising option since, firstly, once trained, they can be significantly faster than rigorous nonlinear dynamic models and secondly, the models can be retrained during online operation, further increasing their accuracy and robustness [2].

In this work, we investigate the performance of different recurrent neural network architectures (RNN) such as Jordan and long short-term memory to capture the dynamic and steady-state behavior of a PEM electrolyzer. To this end, we model a PEM electrolyzer as a differential algebraic equation system, perform multiple simulations using randomized system inputs and train and test the RNN architectures using the simulated data. We compare the results to the simulation model, which serves as a benchmark.

All trained networks accurately capture both the steady-state and dynamic behaviour. All RNN-architectures outperform the benchmark by more than 900%, regarding the computational time. Our results show that the prediction of the temperature dynamics poses the most significant challenge due to the thermal inertia of the PEM electrolyzer. We conclude that recurrent neural networks are a promising surrogate model for PEM electrolyzers.

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Effects of hydrogen addition to auto-ignition properties of methane/air mixtures

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Substituting a part of the methane (CH_4) or natural gas used in combustion devices by hydrogen (H_2) is considered as a major step towards lower carbon dioxide emissions. Quantitative knowledge on this effect is a key for assessing how the safety of devices burning H_2 /natural gas is altered relative to operation with pure natural gas.

Rapid Compression Machine experiments are performed to study the ignition enhancing effect obtained when H_2 is blended to CH_4 /air mixtures under stoichiometric conditions. Four different CH_4/H_2 blends (90/10; 80/20; 50/50 and 0/100 CH_4/H_2 , molar) are studied in a pressure range from 6 to 15 bar and a temperature range from 930 to 1160 K (post-compression conditions). The experimental findings are compared to numerical results obtained by homogeneous reactor simulations performed with our in-house code HOMREA. Simulation studies are performed with two different reaction mechanisms (AramcoMech 3.0 and UCB Chen), in order to assess how well predictions from a strongly reduced reaction mechanism (UCB Chen) match the predictions from a more detailed reaction scheme (AramcoMech 3.0), and the experiment.

The results extend the ignition delay (IDT) time database for CH_4/H_2 fuel blends. Both, increasing the compression pressure and/or increasing the H_2 amount in the fuel, enhances the ignition under the investigated conditions. The reaction mechanisms are able to predict the experimental results. The effect of adding H_2 to CH_4 is investigated in detail by analyzing the results of the simulations (sensitivity analyses and path flow analyses). Sensitivity analyses for different CH_4/H_2 fuel blends are performed. Here, the influence of H_2 on IDT is investigated, showing especially at high CH_4/H_2 ratios, that the addition of H_2 has a strong influence on the underlying chemical kinetics. At a ratio below approx. 80/20 CH_4/H_2 , the IDT is still reduced by adding more H_2 , however, the effect of H_2 addition is smaller compared to higher CH_4/H_2 ratios.

Ignition properties of ammonia/hydrogen blends

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Ammonia is an attractive green fuel since it does not contain carbon atoms, thus enabling decarbonization of the mobility sector in the same way as hydrogen as a fuel. Further, ammonia has been used for many years and hence, knowledge regarding safety and infrastructure is well-developed. As opposed to hydrogen, ammonia is not easily ignitable and pure ammonia/air mixtures burn slowly. Therefore, blending hydrogen with ammonia seems appealing to obtain the desired ignition and burning properties for use in thermochemical conversion systems. While numerical simulations suggest that even small amounts of hydrogen will significantly lower the ignition energy and increase the flame speed [1], experimental data is yet scarce [2, 3]. This work presents the current state of knowledge and an experimental approach to study the ignition of ammonia/hydrogen blends in detail.

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Experimental characterization of turbulent hot jet ignition of ultra-lean hydrogen/air mixtures

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The ignition of a combustible/air mixtures by a hot gas jet is a topic of interest as an advanced ignition system for automotive applications, but also concerning flame arresters and flameproof enclosures. This turbulent hot jet ignition (THJI) is considered to be a promising ignition strategy concerning the challenges encountered with lean combustion (e. g. lean-burn limit). The combustion of lean and ultra-lean mixtures gains in importance here, since the low combustion temperatures result in very low NO_x emissions. In this work, the ignition of different lean hydrogen/air mixtures at atmospheric pressure and temperature was investigated. A stoichiometric mixture inside the pre-chamber was ignited by an electrical spark. After ignition a turbulent hot jet passed the orifice and entered the main chamber to ignite a lean mixture with $\lambda > 3$ (< 12.3 vol. % H₂).

For the basic characterization of the ignition process inside the main chamber a high-speed schlieren system (50 000 frames per second) was used, which delivers information about the subsequent flame propagation. Two piezo-resistive pressure sensors gave information about the explosion pressure and pressure rise inside both chambers. To provide additional information about the ignition timing, ignition location and ignition delay time high-speed laser induced fluorescence on hydroxyl radicals (OH-LIF) is currently being integrated.

First experiments show reproducible ignitions, pressures and pressure curves which verifies the suitability of the setup for quantitative reproducible investigations. The recorded images prove sufficient resolution and contrast of the schlieren setup to visualize cold and hot gas jets as well as the ignition inside the main chamber.

FCEV-Independent Hydrogen Sampling Methodology and Purity Analysis with IMR Mass Spectrometry

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Contaminations in hydrogen have a strong impact on the long-term stability and thereby performance of proton exchange membrane (PEM) based fuel cells for the application in fuel cell electric vehicles (FCEV). While these influences have been intensively studied [1], particularly the purity of the hydrogen provided at public hydrogen refueling stations (HRS) is rarely analyzed. We have taken samples of hydrogen at HRS with a specially designed mobile refueling module enabling the FCEV-independent sampling at 70 MPa. With a method specifically developed in this study [2], we seek to ensure that other sources of contamination can be excluded during the probe sampling. With analysis techniques able to determine concentrations of contaminants down to the parts per billion (ppb) level the hydrogen samples are investigated in the laboratory. While single routes of contamination, such as the synthesis route, have been individually studied in detail elsewhere, the provision of hydrogen with different storage processes, as well as transport and compression at the HRS are considered in these investigations as a holistic system. In the first approach series, HRS supplied by on-site electrolysis showed high purity as expected, in general, but also noteworthy contamination above the threshold of the international standard ISO 14687 [3] in the form of water (19.23 ± 4.24 ppm), carbon dioxide (2.90 ± 0.09 ppm), and nitrogen (761.68 ± 22.72 ppm). With this study, it can be stated whether the dispensed hydrogen meets the high-quality requirements of fuel cells for mobile applications.

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Study on the reaction kinetics of ammonia/ethanol oxidation at intermediate temperatures

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Ammonia (NH₃) is recognized as a sustainable hydrogen energy carrier for mobile and remote applications due to its high volumetric hydrogen density. Nevertheless, the low reactivity and narrow flammability significantly inhibit its practical application. In this work, ethanol (C₂H₅OH) is employed as an additive in the fuel to investigate its influence on the reactivity of ammonia. Auto-ignition properties of ammonia/ethanol fuel blends close to engine operating conditions were investigated by Rapid Compression Machine (RCM) measurements. Additional speciation measurements were performed with a jet-stirred reactor (JSR) coupled with Molecular Beam Mass Spectrometry (MBMS) to get deeper insights into the ongoing chemistry. The experiments reveal that ethanol can drastically promote the reactivity of ammonia. A new chemical kinetic mechanism for NH₃/C₂H₅OH mixtures has been developed and validated against the experimental data. The sensitivity and reaction pathway analysis indicated that the addition of ethanol to ammonia fuel blends provides the additional interaction between ammonia and ethanol and thus enriches the O/H radical pool further promoting the auto-ignition process.

Development of a reduced chemical kinetic mechanism for HCCI combustion of hydrogen-ammonia mixtures using combined reduction methods

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The detailed chemical kinetic mechanisms of ammonia-hydrogen mixtures, which contains 151 species and 1397 reactions, were progressively simplified by the combined reduction methods of Directed Relation Graph with Error Propagation (DRGEP), Directed Relation Graph with Path Flux Analysis (DRGPFA) and Full Species Sensitivity Analysis (FSSA) under the conditions of Homogeneous Charge Compression-Ignition (HCCI) and different relative tolerances (5%, 10%, 15%). Three simplified mechanisms were obtained, containing 21 species and 123 reactions, 20 species and 106 reactions, and 18 species and 79 reactions, respectively. The ignition delay time, laminar flame velocity, in-cylinder pressure, and heat release rate were calculated for different ratios of hydrogen-ammonia fuel mixtures by coupling the combustion model with the simplified and detailed mechanisms. The results show that the mechanism containing 18 species and 78 elementary reactions is probably the best simplified mechanism compared to the other two simplified mechanisms because of its relatively smaller scale and higher accuracy.

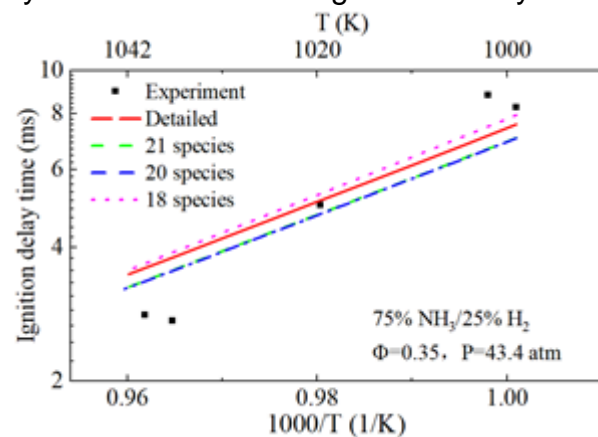


Fig.1 Comparison of ignition delay times predicted by simplified, detailed mechanisms and experimental values

References

Reaction mechanism development for ammonia/methanol blends

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Ammonia (NH₃) as a carbon-free nitrogen-based hydrogen carrier fuel has attracted research interest in the past few years. Despite many advantages of ammonia, namely, higher energy capacity, easier to be liquified, stored and transported, and safer, ammonia as fuel still has several downsides, such as low combustion intensities, slow laminar burning velocity, and narrow flammability range. Numerous studies have focused on overcoming these challenges, such as blending ammonia with combustion promoters. Among them, the ammonia and methanol blends are of particular interest due to methanol's low carbon footprint, high reactivity, and low toxicity. In combustion science, the detailed kinetic mechanisms containing elementary reactions are effectively employed to study the complex chemistry of the combustion of different fuels and survey the concentration profiles of all produced stable species and radicals. Therefore, performing a simulation using such a kinetic mechanism could be beneficial for the environment and the industry. The objectives of this study are focused on exploring the current capabilities of Reaction Mechanism Generator (RMG) software to automatically generate a model for ignition of NH₃/CH₃OH fuel blend at elevated pressures. Beyond the experimental results for the IDT of NH₃/CH₃OH from literature [1,2], the autoignition of NH₃/CH₃OH mixtures has been investigated in a high-pressure shock tube (HPST) at high temperatures to provide additional experimental points for a wide range of temperatures that is beneficial for the model validation. The detailed mechanism satisfactorily predicted the combined set of IDTs of ammonia/methanol blends. Further analysis with the kinetic model showed that the reactions involving C- and N- containing species are found to be significant for the autoignition of different NH₃/CH₃OH mixtures.

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OME_n/Diesel spray injection in an RCCI engine; Combustion analysis in the presence of Hythane

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Compressed natural gas (CNG) is considered as an alternative vehicle fuel because of its positive features in economy and environment. However, it has a low flame speed. Adding hydrogen to CNG (Hythane) allows the mixture to burn with a higher flame speed and in relevant leaner conditions, and is already done in the gas grids of some countries. On the other side, engine emissions, especially soot, can be declined by using polyoxymethylene dimethyl ethers (OMEs) in dual fuel engines due to the lack of C-C bonds. With cetane numbers of 63 for OME₂ up to 90 for OME₄, OME₂₋₄ can be used as a high reactivity fuel.

Reactivity controlled compression ignition (RCCI) is a dual fuel strategy that uses fuels with different reactivities. In this study, Hythane is used as a low reactivity fuel in order to keep the compression high and diesel or OME_n with high reactivity is used to start the combustion. For this project, Hythane consists 5% of the incoming air mass, and OME_n/diesel is sprayed under fully lean condition. The current study concerns the effect of using OME₂₋₄ on the blend of Hythane in order to analyze pressure, temperature, and emission. Thus, Chemkin software for 0-D and 1-D flame simulations and sensitivity analysis as well as AVL Fire for 2-D and 3-D CFD simulations are utilized. Results explore that increasing the chain length from OME₂ to OME₄ rises the peak of heat release rate earlier and the time for the second combustion phase (diffusion) increases. Simultaneously, NO emission increases because of high temperature and due to the lack of C-C bonds in OME_n fuel, for OME_n configurations soot declines drastically.

Development of a kinetic mechanism for modelling oxymethylene ether combustion and pollutant formation

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As fossil fuels are depleting, so-called e-fuels produced from sustainable electric energy sources are expected to gain influence as drop-in fuels or substitutes for conventional diesel or gasoline fuels. Because emission regulations become more and more strict, pollutant formation in the combustion of these alternative fuels is an important issue.

Oxymethylene ethers, $\text{H}_3\text{CO}(\text{CH}_2\text{O})_n\text{CH}_3$ (OME_n) with $n \geq 1$, are known for their low soot emissions that makes them promising drop-in fuels [1]. In order to understand and model the combustion of these compounds and the formation of pollutants like NO_x and oxygenated hydrocarbons, a detailed reaction mechanism with reliable kinetic data is needed.

In our contribution, we present and discuss a kinetic reaction mechanism that was developed for modeling the combustion of n-heptane and oxymethylene ethers up to OME_6 . This joint mechanism comprises sub-mechanisms for hydrocarbon oxidation and explicitly considers NO_x formation. The sub-mechanisms are set on top of a base mechanism recently proposed for smaller oxymethylene ethers [2].

In addition, measurements on a single cylinder research engine at different operating points and strategies with OME_{3-6} blends with diesel fuel are presented. By using the developed reaction mechanism, the influence of e-fuels on the formation of nitrogen oxides in the combustion engine will be investigated more closely.

Major aspects of the mechanism development, the choice of the kinetic parameters, and the comparison with the engine results will be presented and discussed.

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Effect of dynamic pressure measurement and its influence on understanding reaction kinetics of Hydrogen/Methane mixtures

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The current state-of-the-art hydrogen blending to natural gas mixtures in many applications is limited to less than 50%, and more research is needed to improve the design of these reactors. The design of these reactors can be simplified using simulation models and detailed chemical kinetic mechanisms that allow the prediction of key parameters for these reactors. However, these vital parameters must be investigated in fundamental reactors to serve as validation targets for kinetic mechanism development.

One such parameter is the auto-ignition characteristics of hydrogen and its mixtures with methane. The auto-ignition of hydrogen is considerably investigated in the literature in various reactors, and multiple research groups have established detailed kinetic mechanisms. Rapid compression machines (RCM) and shock tubes are typically used to study various fuels' auto-ignition characteristics. In the RCM, the dynamic pressure measurement serves as a key diagnostic for the definition of ignition delay time and aids in estimating the compressed temperature. These two parameters describe the reactivity of the fuel for a particular mixture condition.

This work uses four different sensors from the literature to measure the reactor's dynamic pressure. Although many reference studies on the choice of pressure measurement have been mentioned in the literature, a wide range of pressure sensors are still being used in RCMs. This comparative dynamic pressure measurement will provide an overall uncertainty of the estimated temperature. Preliminary experiments show a noticeable difference between the pressure sensors used, affecting the simulations used for mechanism validations. An experimental matrix comprising of hydrogen and methane at various conditions is used in this work to evaluate these effects and the uncertainties related to the measurand. Different established mechanisms from the literature are used to simulate the experiments from this work and further understand its oxidation pathways.

Diffusive thermal instabilities in Hydrogen and Methane-Hydrogen mixtures

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The usage of hydrogen as a direct fuel in traditional combustion-based processes has always been considered as a means of reducing the ecological impact of combustion. Efforts are constantly made to measure fundamental combustion properties of hydrogen and mixtures of hydrogen with hydrocarbons to better understand the kinetics and also improve their usability. In flat freely propagating flames, onset of thermo-diffusive instabilities is seen in rich mixtures as qualitatively described by the Sivashinsky criterion [1]. Such instabilities are also observed in burner stabilized flame configurations at low flow rates. The origin of these diffusive thermal instabilities is the imbalance that occurs between the heat transport and the rate limiting reactions. The coupling between the reaction and transport processes causes a feedback mechanism that results in oscillations of the reaction wave. The usage of detailed reaction mechanisms to predict the onset of such instabilities has shown that the phenomenon is highly sensitive to the kinetics of reaction mechanism used [2].

By characterizing these unstable combustion regimes using hydrogen and also mixtures of methane-hydrogen, a method to verify the validity of mechanisms in such regimes can be developed. The structure of the pulsating solutions observed along with the relaxation regime is useful to explain the divergence of simulations from experimentally observed results and also to validate available combustion models. Performing a sensitivity analysis for both the stable and unstable regimes gives further insight into the role of elementary reactions responsible for the onset of these instabilities while providing ways to improve detailed reaction mechanisms.

Considering the computationally expensive nature of such calculations, it is also advantageous to develop reduced models that are capable of capturing this phenomenon. Such reduction methods will also be presented, discussed, and validated.

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An Iterative Methodology for REDIM Reduced Chemistry Generation with Focusing on Partially-Premixed Type of Combustion

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Partially-premixed combustion is ubiquitous in the practical combustion systems such as gas turbines, diesel engines and gasoline direct injection engines. It is of significant practical interest to develop combustion models that can accurately predict the important characteristics of partially-premixed flames (PPF) in particular for hydrogen based fuels. PPF include the characteristics of both the premixed and non-premixed type of flames. Since the governing physics of both premixed and non-premixed type of flames differs from each other, it becomes challenging to develop combustion models for PPF.

Detailed reaction mechanisms can be used to simulate the PPF. However, more or less detailed reaction mechanisms are used only as reference solutions because of massive computational cost associated with these mechanisms. One alternative to such computationally expensive methods is to use tabulated chemistry based approaches which implements the effects of detailed chemical kinetics at a reduced computational cost [1]. Nevertheless, development of the PPF combustion models using tabulated chemistry based approaches faces some inherent limitations of these approaches. Usually, in tabulated chemistry based approaches, one needs a-priori knowledge about the type of combustion. This is because if the tabulated chemistry is generated by considering premixed flames, it neglects the effects of interaction between iso-equivalence-ratio surfaces or non-premixed flame based tabulated chemistry does not include the effects of propagating premixed flames.

Hence, development of an approach which is valid between these limits (premixed and non-premixed combustion) represents a challenging task. The reaction–diffusion manifold (REDIM) method [2], as an another more general tabulated chemistry approach, can be used to cope with this problem. The REDIM can include PPF effects via gradients provided during solving the REDIM evolution equation. An iterative approach to generate REDIM table focusing on the PPF will be presented and discussed, which can be easily applied to different combustion systems relevant in hydrogen based fuel.

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On the Role of Water in Gas-Phase Reactions of Isocyanic Acid under SCR conditions

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Hydrogen combustion engines could be a good alternative for classic fuel engines due to lower air pollution. There are no carbon-based pollutants like CO₂ in the exhaust gas. Nevertheless, like a diesel engine, it produces NO_x emissions, which are a significant problem for human health and the environment. To minimize these NO_x emissions, the urea-based selective catalytic reduction (urea-SCR) is an efficient and widely used exhaust gas aftertreatment strategy. The reducing agent is ammonia that is obtained in situ by thermal decomposition of urea and subsequent (mainly catalytic) hydrolysis of isocyanic acid. It is known that under technical conditions, competing reactions of HNCO with urea and its condensation products biuret and triuret can lead to the formation of solid byproducts like cyanuric acid that can block the exhaust gas system. To successfully model and optimize the technical process, including the avoidance of unwanted byproducts, an adequate reaction mechanism with corresponding kinetic data is needed.

In our contribution, we present theoretical and experimental investigations of gas-phase reactions of the main intermediate HNCO. On the basis of quantum chemical calculations [1, 2], kinetic-mechanistic aspects of byproduct formation by reactions of HNCO with urea, biuret, and triuret in presence and absence of water were investigated. Moreover, the thermal decomposition and hydrolysis of isocyanic acid were studied experimentally, and the impact of O₂ and NO₂ on these reactions were examined. These measurements were carried out in a heated flow reactor with molecular beam sampling and mass-spectrometric detection at temperatures between 295 and 773 K and pressures ranging from 10 to 30 mbar, i.e. at conditions that resemble those in the exhaust gas aftertreatment system. From the results, it can be concluded that homogeneous gas-phase reactions of closed-shell species containing N, C, O, and H are kinetically unimportant under typical urea-SCR conditions.

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An Experimental and Theoretical Study of the unimolecular and Bimolecular Reactions of Dimethyl Carbonate

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Due to the self-accelerating carbon dioxide-based climate change and the role of conventional fuels in it, the need for alternative fuels is constantly growing. A promising candidate is dimethyl carbonate (DMC). Due to the absence of C-C bonds, a significantly reduced soot formation can be found. In order to establish DMC as a sustainable fuel, its combustion and pyrolysis behavior has to be understood, and described by an adequate reaction mechanism.

In our study, we used shock-tube experiments to analyze the unimolecular decomposition of DMC, as well as its bimolecular reactions with H atoms. Two shock tubes with different detection techniques, namely hydrogen atom resonance absorption spectrometry and time-of-flight mass spectrometry, were used. While a current literature mechanism [1] proved sufficient to reproduce most of our experimental data, there were inconsistencies with some of our TOF-MS profiles. It is the aim of this contribution to resolve these inconsistencies and improve the mechanistic understanding of DMC pyrolysis and combustion.

We used highly accurate quantum chemical methods as well as statistical rate theory to analyze the DMC pyrolysis. The energetics of the unimolecular reactions were characterized at CCSD(F12*)(T*)/cc-pVQZ-F12//B2PLYP-D3/def2-TZVPP and W1BD level of theory. The bimolecular reactions were described by using an analogous approach but employing in the coupled cluster calculations a triple-zeta basis set instead of the quadruple-zeta basis set. The kinetics were modeled with multi-channel master equations by using microcanonical rate coefficients from RRKM theory and a simplified statistical adiabatic channel model. In addition, high-pressure limiting rate coefficients were calculated by canonical transition state theory with one-dimensional WKB-IRC tunneling correction. The combined findings of the experiments and modeling calculations were used to propose a comprehensive mechanism for the early steps of DMC pyrolysis.

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Hydrogen metrology in the context of the CIPM MRA

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The CIPM Mutual Recognition Arrangement (CIPM MRA) is the framework through which National Metrology Institutes demonstrate the international equivalence of their measurement standards and the calibration and measurement certificates they issue [1]. The CIPM MRA provides one of the most profound frameworks for internationally recognized metrological traceability to the international system of units (SI). CIPM MRA activities comprise the organization and evaluation of key and supplementary comparisons and the publication of calibration and measurement capabilities (CMCs) in the BIPM key comparison database (KCDB) [2,3]. In this contribution we showcase up to date CIPM MRA activities related to hydrogen as a future option of energy source diversification such as identified relevant metrology areas, relevant key comparisons and CMCs published in the KCDB.

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Experimental and numerical studies on lean flammability limits of methane/hydrogen/air turbulent flames

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Fuel-lean combustion of methane (CH₄) is an attractive technology because of its potential for high efficiency and low emissions. However, fuel-lean methane flames are prone to instability and extinction. Addition of hydrogen can significantly improve flammability, and thereby allow combustion systems to operate more efficiently and in a wider range of conditions, compared to operation with neat methane.

We determine the flammability limits of turbulent CH₄/air and CH₄/H₂/air flames to investigate the effect of H₂ addition on lean methane combustion. The study combines experiments in a fan-stirred turbulent combustion bomb and numerical simulations of the transient evolution of flames emerging from an ignition source and developing either into a self-sustained propagating flame or extinguishing.

In a first set of studies, the dependence of the lean flammability limit on turbulence intensity and equivalence ratio was determined for CH₄/air. In the experiments, the results show an overlap between the regions of successful and failing ignition, rather than a sharp limit. The lean flammability limit shifts towards higher fuel/air equivalence ratios (closer to stoichiometric) with increasing turbulence, in both experiments and simulations. Moreover, above a certain turbulence level, the methane/air mixture cannot be ignited at all, even for stoichiometric mixtures.

The study was repeated with 90%/10% methane/hydrogen fuel, instead of neat methane. Results show that the overlap region in experiments is thinner than for pure methane fuel. Compared to combustion with neat CH₄, the lean flammability limit shifts towards lower fuel/air equivalence ratios. The turbulence level above which even stoichiometric mixtures cannot be ignited, increases with the addition of hydrogen.

In conclusion, at the same initial temperature, pressure and equivalence ratio, the addition of hydrogen to lean methane/air mixtures significantly increases the domain of flammability, yields a more stable flame, and allows ignition at higher turbulence intensities.

Hydrogen as co-fuel in the combustion of low & zero carbon fuel

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The hydrogen is considered as clean fuel because it is free of carbon. However, due to its high explosive property and fast chemical reaction rate, its safety issue must be considered. The low carbon fuels (e.g. natural gas, propane etc.) and zero carbon fuels (e.g. ammonia) are regarded as potential fuels to produce powers during their combustion processes and, meanwhile, reduce carbon dioxide emissions. However, these low and zero carbon fuels are usually related to low combustion efficiency: long ignition delay times (IDT), high spark ignition energy (SIE), low laminar burning velocity (LBV) and low extinction strain rate (ESR). The most common strategy is to treat hydrogen as co-fuel, which would significantly enhance the combustion efficiency while keeping the emission at a low level. For example, for the hydrogen-enriched ammonia gas mixture, the LBV and EST increase significantly while the minimum energy for a successful spark ignition decreases noticeable. This confirms that the combustion efficiency could be improved largely and the required energy for a successful spark ignition becomes smaller. Furthermore, experimental measurements show that the addition of hydrogen in ammonia gas mixture would largely shorten the IDT while the corresponding thermal NO_x emission remains almost unchanged. Therefore, the hydrogen can be considered as promising co-fuel to be used in the main low and zero carbon fuel while the highly explosive property of hydrogen is minimized. This poster will show some examples of the LBV and ESR for the application of hydrogen in low carbon fuel (e.g. CH₄) and zero carbon fuel (e.g. NH₃), and the corresponding flame structures will be discussed. Specific emphasize will focus on showing the combustion properties together with the corresponding emissions (e.g. CO, CO₂, NO_x).