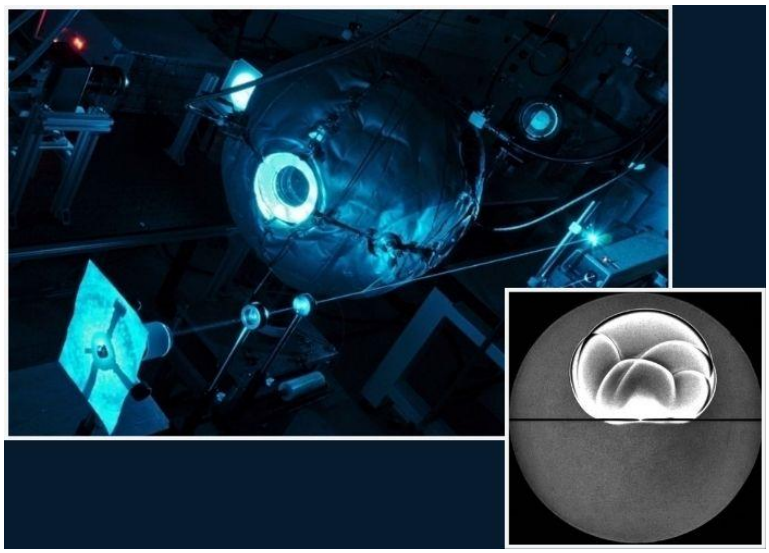
8th International Flame Chemistry Workshop



41st International Symposium on Combustion

July 25th-26th 2026
Doshisha University's, Shinmachi Campus
Kyoto, Japan

Book of Abstracts

Summary

Introduction

Increasing concerns of energy security, climate change and the challenges of the carbon-neutral energy transition drive the design of alternative fuels and their implementation in advanced combustion devices.

The understanding of fundamental aspects of high and low temperature combustion such as ignition, flame chemistry and emissions of new fuels (H_2, NH_3, sustainable aviation fuels, etc.) or under new and advanced combustion conditions (high pressure, plasma assisted, flameless, supercritical combustion, etc.) supports the design of new technologies while expanding technical and scientific knowledge in a key energy sector.

The *International Flame Chemistry Workshop* (FCWS) provides a focused forum to identify key scientific challenges, foster interdisciplinary collaboration, and promote coordinated strategies toward predictive combustion chemistry models. The workshop addresses fundamental and applied aspects of flame chemistry underlying fuels combustion, flame propagation, ignition, pollutant formation, and combustion system performance. Scientists and researchers from academia and industry working in areas such as fuel chemistry, physics, physical and theoretical chemistry, plasma chemistry and physics, mechanical, aerospace and chemical engineering are welcome to join the discussion and to foster collaboration over many fundamental challenges.

Theoretical, modelling and experimental aspects will be discussed in relation to five topics:

1. Sustainable fuels combustion (LFS, IDT, pollutants): H_2, NH_3, SAFs
2. Advanced diagnostics for combustion measurements
3. Plasma combustion: experiments and modelling
4. AI-TST-ME: automation, benchmarking and knowledge transfer
5. Chemical Kinetics Mechanisms: Progress in Accuracy and Details

Building on outcomes from previous editions, discussions at the 8th FCWS will be guided by a recent perspective paper arising from the 7th FCWS (Milan, Italy, 2024), published in *Combustion and Flame*.

This booklet collects abstracts for invited oral contributions in the five topical areas above as well as poster contributions.

Wishing you all a fruitful workshop and an enjoyable time in Kyoto.

The organizing committee

Matteo Pelucchi – Politecnico di Milano, Italy
Bin Yang – Tsinghua University, China
Brandon Rotavera - University of Georgia, USA
Feng Zhang - University of Science and Technology of China, China
Andrea Comandini - CNRS Orléans, France
Liming Cai - Tongji University, China
Stephen Klippenstein – Argonne National Laboratory, USA
Nils Hansen – Sandia National Laboratory, USA

Contacts and information:
FCWS website: https://ifcworkshop.org/
FCWS LinkedIn: https://www.linkedin.com/company/ifcws/

FCWS Special Issue in "Applications in Energy and Combustion Science"

Submission deadline: 31 Jan 2027

The special issue on the *International Flame Chemistry Workshop* (FCWS) welcomes original research and review articles addressing fundamental and applied aspects of combustion chemistry, with particular emphasis on advances discussed at the 8th International Flame Chemistry Workshop (FCWS). Topics of interest include – but are not limited to – one or more of the following topics:

- Sustainable fuels combustion (hydrogen, ammonia, sustainable aviation fuels;
- Advanced diagnostics for combustion measurements;
- Plasma-assisted combustion (experiments and modelling);
- Artificial intelligence, automation, benchmarking, and knowledge transfer in quantum chemical approaches;
- Chemical kinetic models development, including reaction kinetics, thermochemistry, mechanism validation, and predictive modelling.

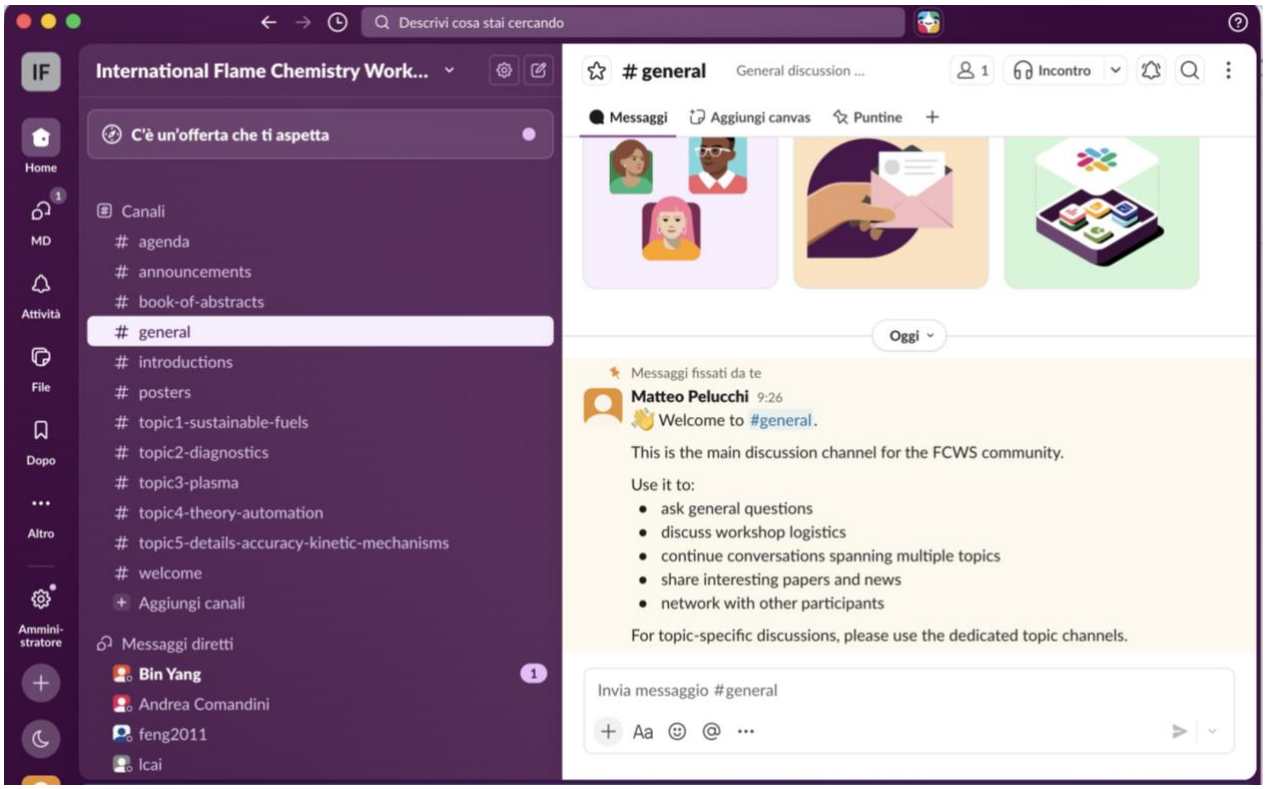
Guest editors: Matteo Pelucchi, Andrea Comandini, Brandon Rotavera, Feng Zhang

FCWS workspace on Slack! Audience Interaction, Q&A, polling

Enhance your FCWS experience by joining the official Slack workspace.

Continue discussions beyond each session, ask additional questions to speakers, participate in live polls, share references and resources, interact with fellow participants, and contribute to future community initiatives. We encourage all attendees to join before the workshop and remain connected afterwards.

International Flame Chemistry Workshop on Slack



Workshop agenda

*Day 1 - **Saturday 25th July***			
	Moderator	**8.00-8.30**	Registration
Joint Session RCM and Flame Chemistry workshops	*Matteo Pelucchi* *Scott Goldsborough*		
		8.30-8.40	Introduction
		8.40-9.05	"*Community-driven Collaboration: Scientific Advances via the RCM Workshop Initiatives*" Scott Goldsborough, Argonne National Laboratory, USA
		9.05-9.20	"*Highlights from the 7th Flame Chemistry Workshop: challenges and objectives in chemical kinetics modeling of combustion and plasma combustion*" Matteo Pelucchi, Politecnico di Milano, Italy
		9.20.9.35	"*Combining Theory, Modeling, and Experiment: An Example from DME Research*" Markus Kohler – German Aerospace Center, Stuttgart, Germany
		9.35-10.00	Open Discussion
		10.00-10.30	Coffee Break and group picture
Opening FCWS	*Matteo Pelucchi* *Bin Yang*	**10.30-10.45**	Welcome, summary and agenda
Topic 1: Sustainable fuels combustion (LFS, IDT, pollutants): H_2, NH_3, SAFs	*Matteo Pelucchi* *Liming Cai*		
		10.45-11.30	"*Theoretical kinetics of reactions between molecular oxygen and nitrogen centered radicals formed during alkylamine oxidation*" Yusuyuki Sakai, Ibaraki University, Japan
			"*Multiscale physics-based, data-driven studies of combustion and emissions of hydrogen and Ammonia"* Mike Burke, Columbia University, USA
			"*Combustion chemistry of SAF and supercritical autoignition of H_2"* Song Cheng, Hong Kong Polytechnic University, Hong Kong
		11.30-12.15	Open Discussion
		12.15-13.30	Lunch
Topic 2: Advanced diagnostics for combustion measurements	*Brandon Rotavera* *Andrea Comandini*		
		13.30-14.15	"*Simultaneous multi-species sensing in shock tubes through variable-pathlength laser absorption*" Ron Hanson, Stanford University, USA
			"*Synchrotron-based diagnostics for chemical kinetic experiments"* Tina Kasper, Paderborn University, Germany
			"*Structured combustion data and databases for kinetic mechanism development and validation*" Tibor Nagy, Research Centre for Natural Sciences, Hungary
		14.15-15.00	Open Discussion
		15.00-15.30	Coffee Break

Topic 3: Plasma combustion: experiments and modelling	*Bin Yang*	**15.30-16.15**	"*Computation of the low-energy electron scattering cross section for NH3 plasma*" Xianwu Jiang, Wuhan University of Technology, China
			"*Laser diagnostics of hydrogen: from quadrupole absorption to Raman scattering*" Wei Ren, The Chinese University of Hong Kong, Hong Kong
			"*Non-Equilibrium Plasmas as an Enabling Technology to Improve Next-Generation Combustion Architectures*" Nicholas Tsolas, Auburn University, USA
		16.15-17.00	Open Discussion
Wrap-up	*Organizers*	**17.00-17.30**	Summary from Day 1
Poster reception		**17.30-19.30**	Poster Session and reception

Day 2 - ***Sunday 26th July***			
	Moderator	**8.00-8.50**	Registration
	Matteo Pelucchi	**8.50-9.00**	Welcome, summary and agenda
Topic 4: AI-TST-ME: automation, benchmarking and knowledge transfer	*Feng Zhang*	**9.00-9.45**	"*Edge migration of aromatic rings by radical reactions—kinetics and directionality: can the outcome of an aromatic edge migration be predicted on the fly?*" Alexander Mebel, Florida International University, USA
			"*Transforming combustion chemistry workflows to handle the big data deluge*" William H. Green, Massachusetts Institute of Technology, USA
			"*Automated kinetic data generation for combustion models using the tabulated model of transition states (TMTS) method*" Baptiste Sirjean, Centre National de la Recherche Scientifique, France
		9.45-10.30	Open Discussion
		10.30-11.00	Coffee Break
Topic 5: Chemical Kinetics Mechanisms: Progress in accuracy and details.	*Brandon Rotavera*	**11.00-11.45**	"*Details in elementary kinetics: setting the foundations for combustion kinetics modeling*" Raghu Sivaramakrishnan, Argonne National Laboratory, USA
			"*Speciation experiments in kinetics: what do we learn from modeling?*" Guillaume Dayma, Centre National de la Recherche Scientifique, France
			"*Developing detailed chemical kinetic mechanisms for fuel combustion*" Henry Curran, University of Galway, Ireland
		11.45-12.30	Open Discussion
		12.30-13.45	Lunch
Discussion and actions	*Matteo Pelucchi* *Bin Yang*	**13.45-15.30**	- Open discussion on challenges - Feasible joint actions and initiatives for Topic 1-5 - Feedback and suggestions from participants - …

Joint Session RCM and Flame Chemistry workshops

Community-driven Collaboration: Scientific Advances via the RCM Workshop Initiatives

S. Scott Goldsborough
Center for Transportation Research, Argonne National Laboratory, Argonne, IL 60439, USA

*Contact: sgoldsborough@anl.gov

Coming soon

Highlights from the 7th Flame Chemistry Workshop: challenges and objectives in chemical kinetics modeling of combustion and plasma combustion

B. Rotavera[1], L. Cai[2], F. Zhang[3], A. Comandini[4], N. Hansen[5], S. J. Klippenstein[6], B. Yang[7], M. Pelucchi[8]

[1]*Department of Chemistry, University of Georgia, 302 East Campus Road, Athens, Georgia 30602, USA*

[2]*School of Automotive Studies, Tongji University, 201804, Shanghai, People Republic of China*

[3]*Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230088, People Republic of China*

[4]*CNRS-INSIS, I.C.A.R.E., 45071, Orléans, France*

[5]*Combustion Research Facility, Sandia National Laboratories, Livermore, CA 94551, USA*

[6]*Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439, USA* [7]*Center for Combustion Energy and Department of Energy and Power Engineering, Tsinghua University, Beijing 100084, People Republic of China*

[8]*CRECK Modeling Laboratory, Department of Chemistry, Materials and Chemical Engineering, Politecnico di Milano, Milan, 20133, Italy*

*Contact: matteo.pelucchi@polimi.it

Continued progress in the development of predictive models for combustion chemistry—including ignition and flame behavior, species evolution, and combustion system performance—relies on overcoming enduring and emerging challenges in experimental measurements, theoretical formulations, and chemical kinetics mechanism construction. As combustion science continues to coincide with advances in sustainable fuels development, plasma technologies, and automated modeling capabilities, the need for coordinated, community-driven strategies is essential. The Flame Chemistry Workshop (FCWS), held biennially before the International Symposium on Combustion, serves as a dedicated platform to identify, consolidate, and address these challenges in a structured and collaborative manner.

This perspective arises from discussions at the 7th FCWS in Milan, Italy (2024), and presents a collective view of the critical barriers currently limiting progress. Across the five technical domains discussed during the 7th FCWS – sustainable fuels combustion, advanced diagnostics for combustion measurements, experiments and modeling in plasma combustion, artificial intelligence and automated methods for theory and mechanisms generation, and chemical kinetic models—a series of persistent and emerging scientific challenges were identified, highlighting the need for deeper integration between three areas: theory, experiments, and modeling. The talk concisely summarizes present challenges that were identified in each of the technical domains in an effort to streamline and coordinate solutions to accelerate progress in combustion science.

Invited contribution

Combining Theory, Modeling, and Experiment: An Example from DME Research

M. Köhler, T. Kathrotia, C. Naumann, S. Jacobs, N. Gaiser, T. Bierkandt, S. Schmitt, P. Oßwald, T. Methling

German Aerospace Center (DLR), Institute of Combustion Technology, Stuttgart, Germany

*Contact: m.koehler@dlr.de

Combustion remains central to global energy supply and drives severe climate and air-quality impacts, making a transition to sustainable, low-carbon fuels and processes essential. In this context, combining detailed molecular-level chemistry, advanced experiments, and multiscale modeling with system-level process and technology design is key to develop clean, efficient combustion systems compatible with carbon-neutral energy scenarios [1]. To address future changes and possibilities in the methodology, dimethyl ether (DME) is chosen here as a showcase for combining theory, modeling, and experiment in the development of sustainable combustion concepts.

DME, often referred to as oxymethylene ether 0 (OME_0, CH_3OCH_3), plays a significant role in fuel research and is particularly intriguing for applications in high-efficiency, low-emission compression-ignition engines or gas turbines. Despite the sheer volume of existing studies and models DME remains a completing target for combustion research. As the simplest ether to exhibit full two-stage ignition with pronounced negative temperature coefficient (NTC) behavior [2], it is an intriguing model molecule for researching low-temperature combustion. The absence of C–C bonds, its 35% oxygen content and high cetane number resulting in more efficient ignition and lower particulate matter emissions makes it an interesting showcase not only from a scientific perspective.

The in-house experimental database combines ignition delay time (IDT) measurements, detailed speciation studies, and laminar flame investigations across a wide range of conditions for DME (OME_0); summary is presented in [3]. The data was obtained by shock-tube experiments (IDT and single-pulse speciation), high-temperature flow-reactor with coupled molecular-beam mass spectrometry and complemented by literature jet-stirred reactor data, and burner-stabilized premixed flames. Single-pulse shock-tube speciation experiments on DME and selected OMEs under pyrolysis and oxidation conditions at pressures around 16 bar resolved key intermediates and product channels at high temperature. Our in-house high-temperature flow-reactor measurements at ambient pressure, using molecular-beam mass spectrometry, delivered detailed concentration profiles for DME, covering fuel depletion, major products, and small oxygenates that constrain both high- and low-temperature pathways. Last, but not least, the systematic oxidation study of DME and OME_x in atmospheric laminar flow reactors coupled to EI-MBMS and i^2PEPICO spectroscopy provides additional, isomer-resolved insight into the intermediate pool. The interaction of DME with nitrogen oxides was characterized using combined flow-reactor molecular-beam mass spectrometry and photoelectron–photoion coincidence (PEPICO) measurements, providing detailed DME/NO_x speciation data that further constrain low- and intermediate-temperature reaction pathways [4]. The detection and differentiation of both *cis*- and *trans*-HONO isomers represents a critical advancement for understanding their distinct roles in the mechanistic pathways and radical pool dynamics of dimethyl ether combustion systems.

Following these studies, implementation into our DLR Concise mechanism followed. The DLR Concise is a semi-detailed, modular reaction model designed to describe the combustion chemistry of a broad spectrum of real fuels via surrogate mixtures within a single, flexible mechanism that is suitable for both transport applications (aviation, ground-based, and maritime) and energy supply systems. Adding oxygenated species as part IV of our methodology extends the comprehensive modeling framework of the DLR Concise to include DME [3]. In the latest extension, the mechanism is expanded from its original jet-fuel focus (DLRConcise2021v1.JF) to DLRConcise2024v2.F by incorporating both high- and low-temperature chemistry for DME and OME_x (x=1–5), as well as adding an optional NO_x sub-mechanism. For DME, the model adopts state-of-the-art high-temperature decomposition and H-abstraction kinetics leading to CH_3OCH_2 and eventually to CH_3 and CH_3O radicals, and includes a detailed low-temperature network of RO2, QOOH, and ketohydroperoxide pathways that generate species such as hydroperoxymethyl formate, methyl formate, and formic acid.

Since dimethyl ether is a well-understood fuel extensively studied by numerous groups and researchers, it could serve as an effective reference fuel for combustion investigations. It has a simple, well-defined molecular structure, lacks carbon–carbon bonds and features an ether functionality. Due to strong community interest, extensive prior work, relatively manageable chemistry, and fewer experimental complications further enhance its suitability and even offer potential links to other research communities. Given this strong scientific basis, DME could be well suited as a reference fuel when tackling combined theory, modeling, and experiment approaches to gain insights into new phenomena and long-lasting questions.

To follow this idea, a combined methodology is presented here. DME is an interesting candidate for investigating multi-stage combustion because it exhibits characteristic low- and high-temperature reactivity while remaining chemically simple enough to analyze the underlying pathways. Multistage combustion plays a central role in modern combustion kinetics because the interplay of low- and high-temperature reactivity strongly influences, how ignition delays and heat-release histories are interpreted. In more detail, investigations of combustion kinetics in shock-tubes reflects an ongoing discussion about whether ignition and speciation data should be interpreted under idealized constant-volume or constant-pressure conditions. Note that real facilities exhibit a thermodynamical evolution that lies between these two limits.

Figure 1 illustrates the impact of the chosen shock-tube modeling approach that is particularly pronounced. The dashed lines indicate the respective model constraints in direct comparison to the experimental data shown as the black line. Using a combination of theory, modeling, and experiment offers a “blended” approach, shown here with the blue line, matching the experimental pressure profile better. The impact is directly shown in the predictions of OH* chemiluminescence as demonstrated below.

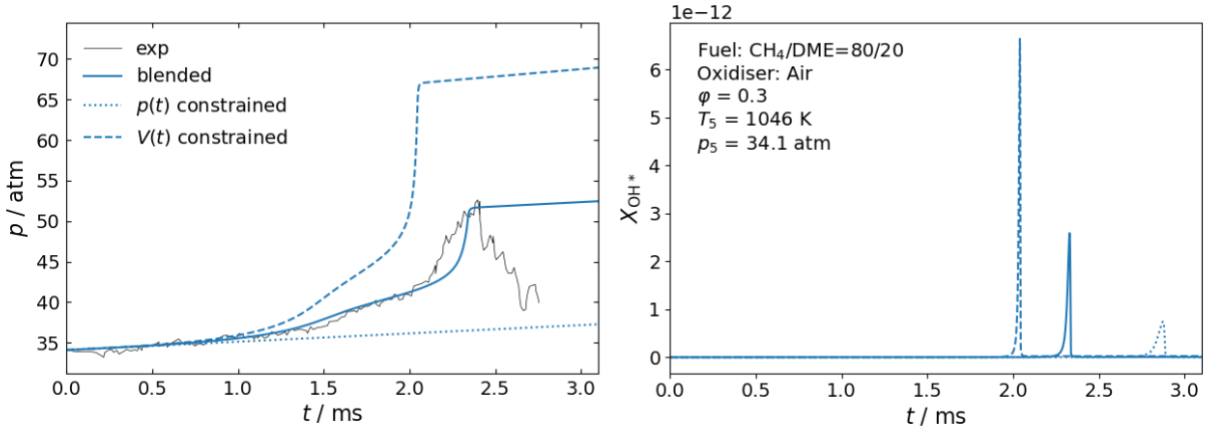


Figure 1: Impact of different shock-tube modeling approaches for a CH_4/DME experiment from Burke et al. [5].

The presentation will demonstrate an approach on the well-understood DME system for analyzing the multistage combustion and shock-tube boundary conditions. By iteratively confronting detailed kinetic models with well-diagnosed experiments and refining the underlying theory, subtle couplings between low- and high-temperature chemistry, transport, and facility effects will be identified and even quantified. This iterative analysis is key to developing more robust, physically consistent models.

These novel insights are an example of the potential of such combined approaches, highlighting how targeted simulations and measurements can jointly reveal previously obscured phenomena and guide the development of more robust, physically consistent models through iterative analysis.

References

[1] Klippenstein, Stephen J., and Kohse-Höinghaus, Katharina. "Combustion in a Sustainable World: From Molecules to Processes" The Journal of Physical Chemistry A 127.17 (2023): 3737-3742.

[2] Wang, Bo, et al. "A Computational Study on the Transient Ignition and NTC Behavior of Non-Premixed Dimethyl Ether/Air Counterflow under Elevated Pressure" Energy&Fuels 34.5 (2020): 6383-6391.

[3] Kathrotia, Trupti, et al. “Combustion kinetics of alternative fuels, Part-IV: Extending reaction mechanism “DLR Concise” to include oxygenates component” Combustion and Flame 271 (2025) 113841.

[4] Pelucchi, Matteo, et al. " On the influence of NO addition to dimethyl ether oxidation in a flow reactor " Combustion and Flame 257.1 (2023): 112464.

[5] Burke, Ultan, et al. “An ignition delay and kinetic modeling study of methane, dimethyl ether, and their mixtures at high pressures.” Combustion and Flame 162 (2015): 215-330.

Speaker Biography

Markus Köhler is head of the department of Chemical Kinetics and Analytics at the Institute of Combustion Technology of the German Aerospace Center (DLR) in Stuttgart, Germany. He studied chemistry at the University of Bielefeld (1999–2005) and obtained his PhD in 2008 in the Kohse-Höinghaus group. After joining DLR in 2009, he worked as a research scientist on the understanding of soot formation, later leading the Mass Spectrometry group (2012–2015) and the Chemical Analytics group (2016–2018), before becoming head of the Chemical Kinetics and Analytics department (2018-today). His work focuses on the chemical kinetics and analytical characterization of synthetic and alternative fuels, linking molecular fuel design and combustion chemistry with real-world emissions. His research aims to enable sustainable and resilient energy and transport systems by providing a mechanistic understanding that supports the development, assessment and optimization of sustainable fuels - from lab to real-world applications.

Topic 1. Sustainable fuels combustion (LFS, IDT, pollutants): H_2, NH_3, SAFs

Invited contributions

Theoretical kinetics of reactions between molecular oxygen and nitrogen-centered radicals formed during alkylamine oxidation

Y. Sakai

Ibaraki University, 4-12-1 Nakanarusawa, Hitachi, Ibaraki, 316-8511, Japan

*Contact: yasuyuki.sakai.qr80@vc.ibaraki.ac.jp

Alkylamines are important nitrogen-containing intermediates that may be formed during the oxidation of ammonia–hydrocarbon co-fuels, biomass-derived fuels, and nitrogen-containing waste materials. During alkylamine oxidation, nitrogen-centered radicals formed through H- abstraction from the amino group can undergo subsequent reactions with molecular oxygen. Previous studies[1,2] have suggested that the reactions of CH3NH and CH3CH2NH with O2 predominantly proceed via O2 addition followed by HO2 elimination to form imines. However, the reaction characteristics of radicals derived from larger alkylamines remain poorly understood. In this study, theoretical kinetic analyses are performed for reactions between molecular oxygen and nitrogen-centered radicals generated during alkylamine oxidation, to develop generalized reaction classes suitable for detailed chemical kinetic modeling.

Figure 1 shows alkylaminyl radicals targeted in this study. The quantum chemical calculations were performed using the Gaussian 16 program[3]. Geometry optimizations and harmonic vibrational frequency analyses for all reactants, products, intermediates, and transition states were carried out at the M06-2X/aug-cc-pVTZ level of theory. Single-point energy calculations were subsequently performed for the optimized structures at the CCSD(T)/aug-cc-pVDZ and CCSD(T)/aug-cc-pVTZ levels, and complete basis set (CBS) energies were estimated. Transition state theory calculations were conducted using the GPOP program[4]. Rate constants were calculated over the temperature range of 600–1200 K, and tunneling corrections were included using the one-dimensional asymmetric Eckart potential approximation.

Fig. 1. Chemical structures of the targeted radicals.

Figure 2 shows the energy diagram for the CH3CH2NH + O2 reaction calculated at the CCSD(T)/CBS//M06-2X/aug-cc-pVTZ level of theory. The considered reaction pathways include O2 addition, concerted HO2 elimination from the ROO radical, 1,3-, 1,4-, and 1,5-hydrogen shift reactions, and H-abstraction reactions from the α- and β-carbon atoms by molecular oxygen. The transition states associated with these reactions are denoted as *O2 add, *eHO2, *13HS, *14HS,

*15HS, *abstα, and *abstβ, respectively. The product complexes formed in the HO2 elimination and H-abstraction pathways are denoted as PC1 and PC2, respectively. In Figure 2, the pathways involving concerted HO2 elimination are shown in red, those involving direct H abstraction are shown in blue, and those involving intramolecular hydrogen shift reactions are shown in green. The rate constants for the CH3CH2NH + O2 and CH3CH2NHO2 reactions (not shown here) indicate that imine formation via O2 addition followed by concerted HO2 elimination is the dominant reaction pathway.

For the reactions of CH3NH, CH3CH2CH2NH, and (CH3)2CHCH2NH with O2, imine formation through O2 addition followed by concerted HO2 elimination was found to be the dominant pathway in all cases. For the (CH3)2CHCH2NH + O2 reaction, concerted HO2 elimination competes with a 1,5-hydrogen shift reaction involving the tertiary C–H site, which is kinetically favorable. Nevertheless, HO2 elimination was found to be faster than the hydrogen shift pathways. These results suggest that the O2 addition reaction and the

subsequent concerted HO_2 elimination should be included as the primary reaction class in kinetic models for the reactions between nitrogen-centered radicals and molecular oxygen.

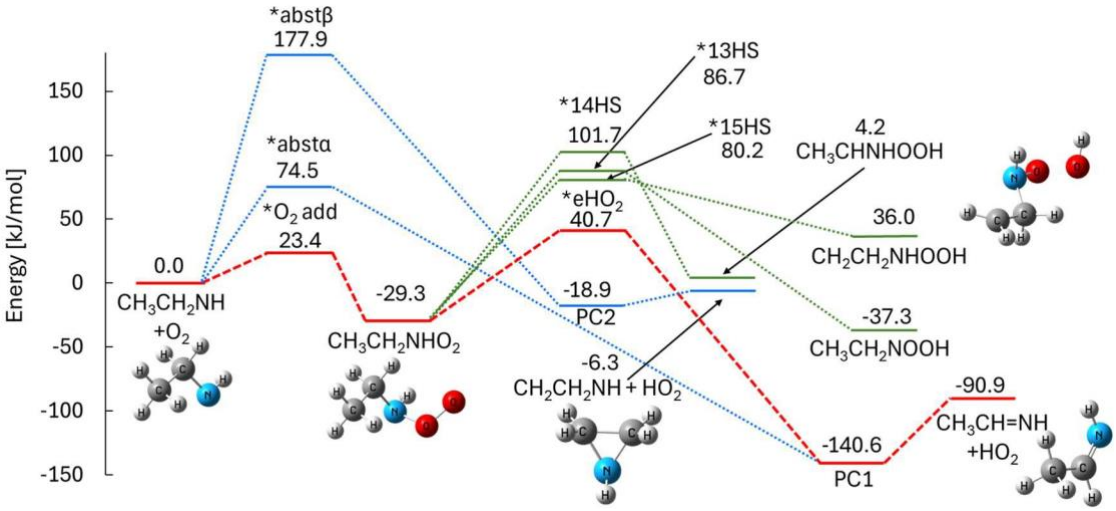


Fig. 2. Energy diagram for the reaction of the ethylaminyl radical $CH_3CH_2NH + O_2$, calculated at the CCSD(T)/CBS//M06-2X/aug-cc-pVTZ level.

References

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[2] Y. Tang and C.J. Nielsen, Atmospheric Environment, 2012, 55, 185–189.

[3] Gaussian 16, Revision C.01, M.J. Frisch et al., Gaussian, Inc., Wallingford CT, 2019. [4] A. Miyoshi, GPOP software, rev. 2022.01.20m4. See http://akrmys.com/gpop/.

Speaker Biography

Dr. Yasuyuki Sakai is a Professor in the Graduate School of Science and Engineering at Ibaraki University, Japan. He received his Ph.D. in Chemical System Engineering from the University of Tokyo in 2008 for his research on the development of detailed chemical kinetic models for gasoline surrogate combustion. He subsequently served as an Assistant Professor, Lecturer, and Associate Professor at the University of Fukui before joining Ibaraki University in 2021. His research interests include thermal engineering, combustion chemistry, and computational chemistry, with a particular focus on fundamental energy and environmental technologies for a carbon-neutral society. His research covers elementary reaction mechanisms of hydrocarbon, ammonia, and hydrogen combustion, the development of detailed chemical kinetic models, and AI-assisted combustion analysis and optimization for internal combustion engines and industrial furnaces. More recently, he has developed a strong interest in the surface reactions of gaseous combustion intermediates on heated metal surfaces, particularly iron, including adsorption, surface diffusion, and bulk diffusion, with applications to hydrogen- and ammonia-fired industrial furnaces. Since last year, he has been conducting quantum chemical studies in this area and is currently working on the development of integrated kinetic models that couple gas-phase and surface reactions.

Multiscale Physics-Based, Data-Driven Studies of Combustion and Emissions of Hydrogen and Ammonia

Michael P. Burke

Department of Mechanical Engineering and Data Science Institute Columbia University, New York, USA

*Contact: mpburke@columbia.edu

Given its role in NO_x emissions of H_2 combustion and global reactivity and emissions of NH_3 combustion, the kinetics of nitrogen-containing species are a key consideration in both of these carbon-free fuels. Characterizing nitrogen kinetics is especially challenging given that so many of the key species can be formed via multiple different pathways (in fractions that are highly sensitive to the thermodynamic conditions) and so many of the key reactions proceed through multiple stabilizable potential energy wells and can form multiple distinct product channels (yielding rate constants and product branching ratios that depend on temperature, T, pressure, P, and mole fractions of each species, $\underline{X}$). These features exacerbate the typical challenges for traditional methods for kinetics studies:

1. Experimental data alone are often insufficient to confirm both the kinetic pathways and relevant parameters describing them.
2. Experiments at typical conditions can fail to differentiate among multiple distinct pathways and can have blind spots to certain pathways.
3. Traditional rate-parameter optimization to match experimental data can mask mechanistic deficiencies and is poorly constrained under extrapolation.

Fortunately, achieving deep integration of theory, experiment, and modeling (as advocated at this workshop two years ago [1]) *via a data-driven framework* aids in overcoming such challenges in that:

1. Ab initio calculations can characterize the kinetic pathways and their parameters, thereby constraining experimental interpretations and enabling physics-based extrapolation.
2. Optimal experimental design can pinpoint experimental conditions that accentuate specific kinetic pathways, differentiate among competing pathways, and maximize information.
3. Uncertainty quantification based on theoretical and experimental data can formally evaluate the consistency of a proposed mechanism with available data.

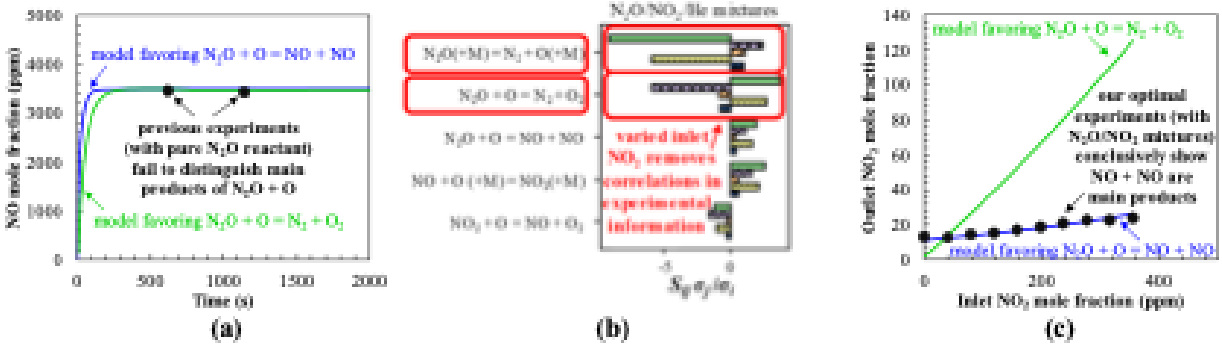

Fig. 1. Utility of a multiscale data-driven approach for unraveling complex kinetics: (a) Time profiles from previous N_2O/diluent experiments can be explained equally well using a model favoring $N_2 + O_2$ as the main products of the $N_2O + O$ reaction and using a multiscale-informed model instead favoring NO + NO (consistent with earlier ab initio calculations) [3]. (b) Optimal experimental design identifies that measuring NO_2 in N_2O/NO_2/diluent mixtures with varied NO_2—which had not been explored in any previous experiments—enables unambiguous determination of the main products of the $N_2O + O$ reaction [4]. (c) Experiments at these pinpointed conditions reveal that the main products of $N_2O + O$ are NO + NO—contrary to the earlier indirect inferences from experimental data (such as those in (a)) [4].

We have been developing and applying a multiscale, physics-based, data-driven approach that combines these elements. In this talk, I will describe how we used various iterations of this approach to derive insights into reactions relevant to N_2O emissions from NH_3 combustion and NO_x emissions from high-pressure H_2 combustion.

Namely, we have found $N_2O + NH_2$ [2] and $N_2O + O$ [3-4] (cf. Fig. 1) to be much slower than previously thought and found HNNO—a species absent from previous kinetic models—to be a major product of $N_2O + H$ [5-6] (cf. Fig. 2).

Altogether, these studies present a very different picture for N_2O consumption at low to intermediate temperatures during NH_3 combustion and introduce a new HNNO-mediated route to NO_x formation during combustion of any hydrogen-containing fuel in air.

We have also recently identified the importance of (previously ignored) pressure and composition [7] dependence of two of the most important reactions in NH_3 combustion—$NH_2 + NO$ and $NH_2 + NO_2$—which also give rise to (previously ignored) chemical species (H_2NNO, H_2NNO_2, and their isomers) [8]. In our view, this kind of potentially important, currently neglected pressure/composition dependence and associated new stabilized species of many more reactions may comprise a much wider gap in kinetic models—such that many more surprises may be in store for mechanistic understanding of NH_3 combustion kinetics. Progress on this front requires more systematic methods of identifying, confirming, and characterizing "missing chemistry" [8-9] to accelerate scientific progress and aid in quantifying engineering risk.

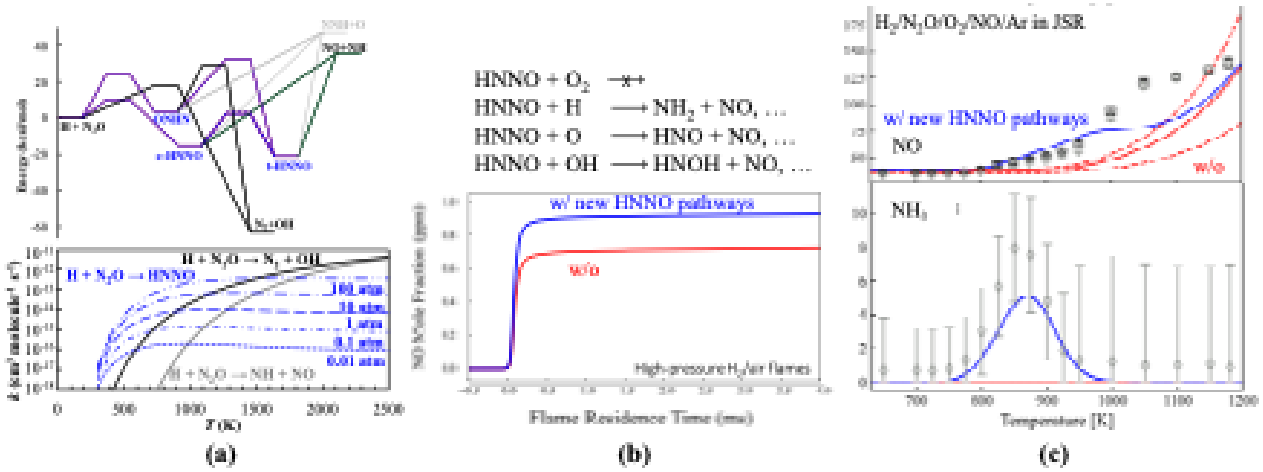

Fig. 2. Utility of a multiscale data-driven approach for confirming the existence of and characterizing hypothesized new kinetic pathways: (a) Ab initio master equation calculations [5] showed that HNNO—a species previously omitted from kinetic models—is a major product of the $H + N_2O$ reaction at intermediate temperatures and pressures and is, in fact, the dominant product up to 1500 K at 10-100 atm. (b) Modeling studies [5-6] with a new reaction set describing HNNO formation and consumption reveals that HNNO reacts primarily with radicals to yield NO_x in high yields in high-pressure H_2/air flames but the previous experimental validation dataset for NO_x formation had a blind spot to it. (c) Experiments [6] at conditions chosen to pinpoint HNNO pathways indeed reveal NO and NH_3 formation below 900 K which cannot be explained by other known pathways and can only be explained via the HNNO mechanism.

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Speaker Biography

Michael P. Burke is an Associate Professor of Mechanical Engineering at Columbia University, where he is also affiliated with the Data Science Institute. Prior to joining Columbia in 2014, Burke earned his Ph.D. in Mechanical and Aerospace Engineering in 2011 at Princeton University, where he was a Wallace Memorial Honorific Fellow, and he worked as a Director's Postdoctoral Fellow in the Chemical Sciences and Engineering Division at Argonne National Laboratory. Burke is a recipient of the National Science Foundation's CAREER award, the Combustion Institute's Research Excellence Award, the Combustion Institute's Hiroshi Tsuji Early Career Researcher Award, and the American Chemical Society's PRF Doctoral New Investigator Award. Burke serves as Secretary of the United States Sections of the Combustion Institute, as Executive Board member and Awards Chair of the Eastern States Section of the Combustion Institute, and on the Editorial Board of Combustion and Flame.

Combustion Chemistry of Sustainable Aviation Fuels and Supercritical Autoignition of Hydrogen

Song Cheng*

Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong SAR, People's Republic of China

*Contact: songryan.cheng@polyu.edu.hk

Keywords: Sustainable aviation fuel (SAF), Supercritical hydrogen autoignition, High-pressure combustion, Real-fluid effects, Real-fluid kinetic modeling

This work will present recent progress in the combustion chemistry of two representative low-carbon fuels, namely sustainable aviation fuels (SAFs) and hydrogen, with emphasis on high-pressure and supercritical combustion conditions relevant to advanced propulsion and power systems. The motivation of this study is that future aviation, rocket, and other high-efficiency engine concepts are expected to operate at increasingly elevated pressures, where both detailed fuel chemistry and non-ideal thermophysical effects become important.

The first part of the workshop will focus on the combustion chemistry of SAF. SAFs are among the most promising low-carbon options for aviation because they can substantially reduce lifecycle carbon emissions while remaining compatible with existing aircraft systems. However, their practical application is challenged by the large compositional diversity arising from different production pathways, such as HEFA, FT, and AtJ, as well as by the need to predict their blending behavior with conventional jet fuels. To address this, the workshop will introduce SAF-MechV1.0 [1,2], the first comprehensive chemical kinetic model developed for all major SAFs and fossil-derived jet fuels within a unified framework, with comprehensive validations conducted (see Fig. 1a and 1b). The discussion will highlight the major fuel classes involved, including *ten n*-paraffins, *twenty iso*-paraffins, *four* cycloalkanes, and *nine* aromatics, and explain the role of consistent rate rules in extending mechanisms across different fuel structures and in capturing nonlinear blending behavior.

The second part of the workshop will report the first measurement of supercritical hydrogen autoignition in the ultra-high-pressure rapid compression machine at the Hong Kong Polytechnic University at compressed pressures up to 160 bar (see Fig. 1c). At these high-pressure conditions, the ideal-gas assumption may become insufficient, and that the calculation of compressed temperature and autoignition simulations would require rigorous treatment of real-fluid effects. This will be demonstrated with the *ab initio*-based real-fluid modeling framework recently established [3-4].

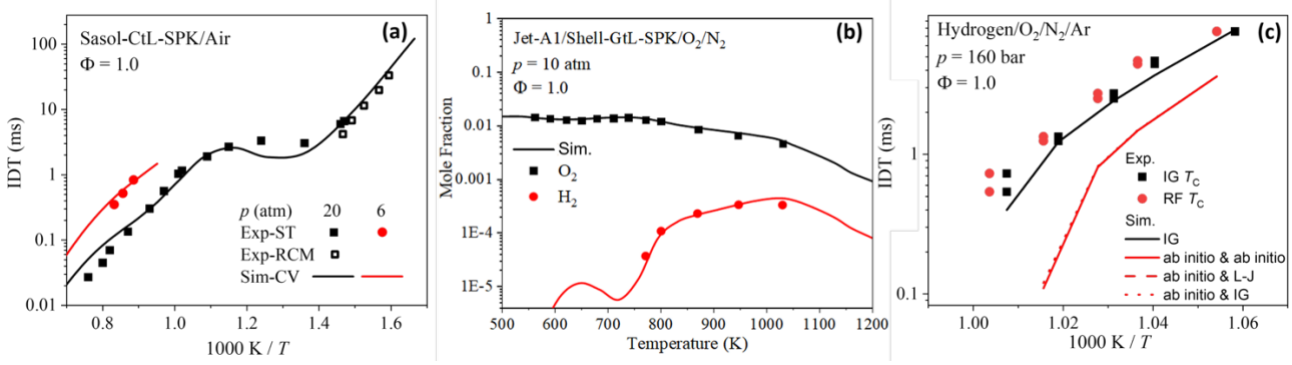

Fig. 1. (a) measured and simulated IDTs for Sasol-CtL-IPK [5–7]; (b) measured and simulated species profiles for Jet-A1/Shell-GtL-SPK oxidation in a JSR [8]; (c) measured (using UHP-RCM) and simulated IDTs for H_2/air mixtures with and without real-fluid effects incorporated.

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Speaker Biography

Prof. Cheng Song received his Ph.D. degree from the Department of Mechanical Engineering of the University of Melbourne. He was appointed a Visiting Researcher in the Department of Mechanical Engineering of the University of California, Berkeley from 2017 to 2018, and a Postdoc in the Energy Systems Division of Argonne National Laboratory from 2019 to 2021. In 2021, Prof. Cheng joined the Department of Mechanical Engineering of the Hong Kong Polytechnic University as an Assistant Professor. Prof. Cheng's current research interests include gas-phase chemical kinetics, trans-/super-critical combustion fundamentals, uncertainty quantification and optimization, and AI-enabled combustion applications.

Topic 2. Advanced diagnostics for combustion measurements

Invited contributions

Simultaneous Multi-Species Sensing in Shock Tubes through Variable-Pathlength Laser Absorption

Ronald K. Hanson
High Temperature Gasdynamics Laboratory, Stanford University
Contact: rkhanson@stanford.edu

Shock tube kinetics experiments are most commonly performed behind reflected shock waves, near the shock tube endwall, where the gas is nominally stagnant and generally free of boundary layer and transport effects. Diagnostic methods include pressure, emission spectroscopy and laser absorption. For purposes of measuring ignition delay time, pressure and emission are generally sufficient, but for work focused on detailed kinetics where the target quantities are species time histories, the preferred method is laser absorption using monochromatic CW laser sources that enable species-specific high temporal resolution. The first use of laser absorption for speciation in shock tube experiments was in the early 1970s, at a time when lasers were first becoming available for scientific inquiry. Over time, the availability of laser sources has grown substantially, allowing access to a wider range of laser wavelengths enabling detection of a growing number of combustion-relevant species. This is an important development in that it has enabled experimentation involving measured time histories of multiple species in a single experiment, allowing more refined evaluation of detailed kinetics models and in many cases the direct determination of reaction rate constants for elementary reactions that may involve multiple channels. At the present time, there are a handful of shock tube laboratories around the world that are able to perform experiments with several simultaneous laser absorption wavelengths (up to about 8 at present). While this is a great improvement in shock tube experimentation over even a decade ago, there are opportunities now to even further advance capabilities for kinetics research. One such idea to advance laser absorption in shock tube experiments will be reported here.

Absorption magnitude in shock tube experiments is characterized by the absorbance, i.e. the negative logarithm of the fractional transmission of light, which is proportional to the product of the absorption coefficient/cm (of the target species) and the optical pathlength L, typically the shock tube diameter D. In experiments applying one laser source, targeting a particular species, the common practice is to identify the optimum absorption wavelength and adjust the experimental conditions to allow a measurable absorbance level of the target species. In experiments aiming to measure multiple species simultaneously, at separate wavelengths selected for detection of the individual target species, there is a problem with single-pass absorption in that it is often impossible to simultaneously obtain sufficient absorbance values for all the species of interest. While it is feasible to magnify the single-pass absorbance through multi-pass arrangements, this magnification is typically limited to a few passes owing to non-ideal effects including intensity losses in windows and beam-steering effects. A solution to this problem can be found with the ring-amplified shock tube (RAST) concept pioneered by Strand et al. at Stanford [1]. This approach makes use of internal reflections in the shock tube from a large number of highly reflective refocusing optical elements (facets) in the ring together with a single inlet window and single outlet window. This arrangement allows easy variation in the optical path length L by changing the angle of incidence at the inlet window so that the light reflects from a specific optical facet on the far wall, undergoing a fixed number of passes across the tube before exiting the outlet window. This approach allows multiple light beams to be introduced simultaneously into the shock tube at different angles, with each angle providing a different path length amplification. A multiplicity of different species, each with a different absorption coefficient, can be measured simultaneously through variation of the inlet angle. In experiments at Stanford, up to 8 different wavelengths (and hence species) are employed to enable detection of an equal number of target species (or quantum states of specific species).

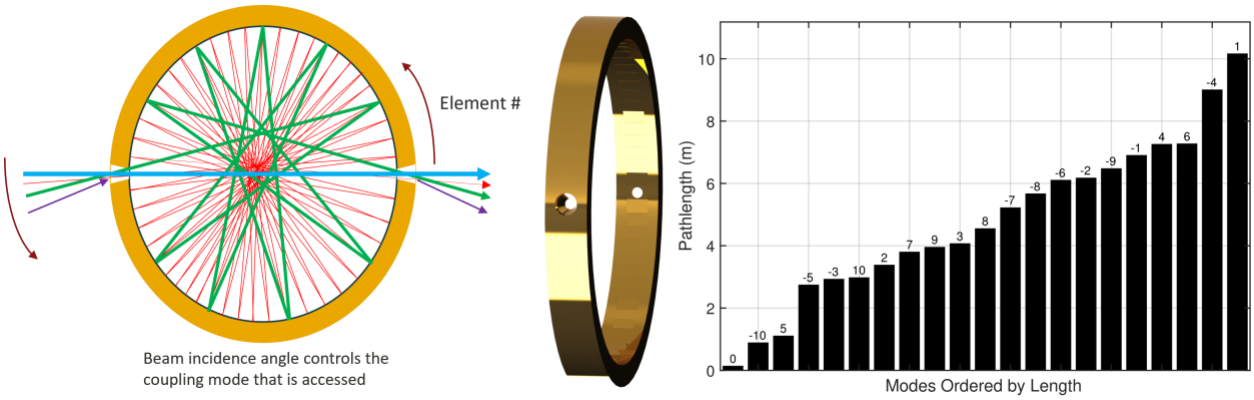

Figure 2, Segmented circular multi-pass ring used for pathlength amplification

The presentation will introduce the measurement concept and provide representative results in reflected shock wave experiments. Relevant references to work with RAST are listed below.

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Speaker Biography

Professor Hanson earned his PhD from Stanford University in Aeronautics and Astronautics and has been affiliated with the Mechanical Engineering Department at Stanford since 1971. He currently holds the Woodard Chair of Mechanical Engineering and served as Department Chair from 1993-2003. His research is concerned with laser diagnostics and sensors, spectroscopy, shock-wave physics, combustion and gas-phase reaction kinetics. He is a Fellow of AIAA, ASME, Optica, the Combustion Institute and the International Shock Wave Institute and a member of the National Academy of Engineering. He has received gold medal awards from the Combustion Institute, the Institute for Dynamics of Explosions and Reactive Systems, and multiple gold medals from the AIAA.

Synchrotron-based diagnostics for chemical kinetic experiments

Tina Kasper[1,*]

[1]*Technical Thermodynamics, Paderborn University, Warburger Str. 100, 33098 Paderborn Germany*

*Contact: tina.kasper@uni-paderborn.de

Complex reacting systems such as combustion, low-temperature oxidation, pyrolysis, and radical-driven molecular growth involve dense networks of transient intermediates and radicals. Different isomers can have very different reactivities and roles in these reaction networks, so that isomer-sensitive detection is often needed to constrain kinetic mechanisms [1,2].

Photoelectron–photoion coincidence spectroscopy (PEPICO) combines photoelectron spectroscopy with mass spectrometry by detecting both charged particles produced in a single photoionization event. A true coincidence correlates an electron and cation originating from the same neutral molecule: the cation time-of-flight provides mass information, and the electron kinetic energy offers spectroscopic information [3]. The correlation of the information results in mass-resolved or mass-selected photoelectron spectra for individual m/z channels, giving structural information that is not available from mass spectrometry alone [2]. Often VUV photons from continuous or high-repetition-rate synchrotron sources are used for single photon ionization because dedicated beamlines provide the broadly tunable light in the energy range of 5 - 20 eV required for near-threshold ionization of typical intermediates in reacting flows.

PEPICO detection has been combined with several kinetic experiments located at different suited beamlines. Initial flame experiments investigated the formation of fuel radicals and branching of the first reactions in fuel consumption after molecular-beam sampling from laminar flat flames at the VUV beamline of the Swiss Light Source (SLS, Villingen, Switzerland) [4,5]. Subsequently, an atmospheric flow reactor [6] and a high-pressure flow reactor were added to the kinetic experiment portfolio [7] and used to explore low-temperature oxidation of OME [8] and nitrogen chemistry at high pressure [9], while a reactor for catalysis is used for example to investigate the pyrolysis of lignin model compounds [10]. At the DESIRS beamline of Soleil synchrotron (Soleil, Paris, France) a jet-stirred reactor (JSR) has been implemented and used to study low-temperature oxidation and pyrolysis [11]. In addition, different flame-sampling setups were used to study flame chemistry in laminar-flat flames stabilized on a matrix burner [12], cool flames using a stagnation plate burner configuration [13], or soot precursors and poly aromatic hydrocarbon (PAH) formation in flames stabilized on a Gülder-type burner sampled by a quartz microprobe [14]. The radical species driving the reactions in many high temperature chemical conversion processes can be produced in radical sources either by pyrolysis [1,2,15,16] or by photolysis [2] and PEPICO spectroscopy is used to investigate which radicals are formed and follow their reactions as a function of time. In side-sampled reactors the outcome of chemical reactions can be investigated. Such a kinetic flow tube reactor was coupled with a new PEPICO spectrometer at the SLS and used in proof-of-principle experiments to measure the rate constant for the CH_2I+O_2 reaction [17] or later to investigate the oxidation chemistry of allyl radicals formed by photolysis.[18] An optimized version of this PEPICO spectrometer has been installed at the Advanced Light Source (ALS, Berkeley, USA) [19].

The main advantage of PEPICO is its ability to provide isomer-sensitive detection in complex mixtures. Beyond identification, PEPICO offers multiplexed data streams that can support quantitative analysis. Coincidence datasets can be represented as mass spectra, electron kinetic-energy distributions, angular distributions, ion velocity components, and kinetic time or distance profiles [20]. In favorable cases, linear combinations of reference photoelectron spectra can be fitted to experimental spectra to estimate isomer mole fractions [20]. When combined with quantum-chemical calculations, Franck–Condon simulations, and kinetic modeling, PEPICO data become a tool for validating and improving reaction mechanisms [1].

Several challenges limit the functionality of PEPICO. The most fundamental is the false-coincidence barrier. False coincidences contribute to background signal, reduce dynamic range, and can obscure weak signals from trace species, radicals, and short-lived intermediates [3]. High dynamic range may be required to observe such species.[3] Advanced spatial coincidence filtering and improved detection schemes can reject nearly all false coincidences, increasing dynamic range by two to three orders of magnitude and

enabling detection, identification, and quantification of minor constituents as demonstrated by the team around Osborn at the SLS and ALS [3,17,19,20].

A second challenge is spectral congestion. Large molecules, flexible oxygenates, hydroperoxides, and PAH-like species can produce overlapping photoelectron bands, hot bands, and complex vibrational progressions. The issues are enhanced if the energy stored in the internal degrees of freedom of the molecules is not reduced during the sampling process from a high temperature source [14,21]. Even when PEPICO improves isomer resolution, some uncertainty may remain if several isomers have similar ionization energies, overlapping spectral features or dissociate instantly upon ionization [1]. In addition, identification of different isomers requires the knowledge of reference spectra. While a large amount of experimental photoelectron spectra and appearance energies is available for different classes of compounds in the literature, identification of reactive intermediates relies almost exclusively on quantum-chemical calculations and Franck–Condon simulations [1,14].

A third challenge is quantification. While PEPICO spectra contain rich structural information, converting spectral intensities into absolute mole fractions requires knowledge of photoionization cross sections, mass discrimination, electron/ion detection efficiencies, fragmentation behavior, and appropriate reference spectra. For fragile intermediates such as hydroperoxides, dissociative ionization and conformer-dependent fragmentation can complicate interpretation. Reactor coupling also introduces practical limitations: sampling must preserve reactive intermediates, minimize wall reactions [21].

Overall, PEPICO has become a uniquely powerful method for studying complex reaction chemistry. Future progress will depend on higher dynamic range instruments, broader reference spectral libraries, improved quantum-chemical simulations for large and flexible molecules, and tighter integration of PEPICO data with automated kinetic modeling.

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Speaker Biography

Tina Kasper is a Professor of Technical Thermodynamics at Paderborn University, Germany. Prior to joining Paderborn University in 2022, Kasper was Professor of Mass Spectrometry in Reactive Flows at the University of Duisburg-Essen from 2011 to 2022. She earned her Dr. rer. nat. in Physical Chemistry from Bielefeld University in 2006, following her Diplom degree in Chemistry from Bielefeld University in 2001. She also held postdoctoral appointments at Sandia National Laboratories in Livermore, USA, and at SRI International in Menlo Park, USA. Kasper's research interests include flame synthesis of nanoparticles, flame chemistry of fuel interactions, gas-phase phosphorus kinetics, cyclic processes including triangular and organic Rankine cycles, household cooling appliances, and the determination of thermophysical properties of substances.

Structured Combustion Data and Databases for Kinetic Mechanism Development and Validation

Tibor Nagy[1,*], Máté Papp[2], Tamás Turányi[2]

[1]*IMEC, HUN-REN Research Centre for Natural Sciences, Budapest, Hungary*
[2]*Institute of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary*

*Contact: nagy.tibor@ttk.hu

1. Introduction

Combustion kinetics has entered a data-rich era. Large collections of experimental measurements—such as ignition delay times, laminar burning velocities, and species concentrations—are increasingly central to mechanism development, optimization, uncertainty quantification, and machine-learning workflows. This dependence on data is particularly strong for emerging fuels such as sustainable aviation fuels, ammonia, hydrogen, and oxygenated e-fuels, whose complex chemistry remains incompletely characterized. Since detailed kinetic models connect elementary chemistry to the design of low-emission combustion devices (Figure 1) [1], their predictive capability depends critically on the quality, consistency, and reproducibility of the underlying experimental data.

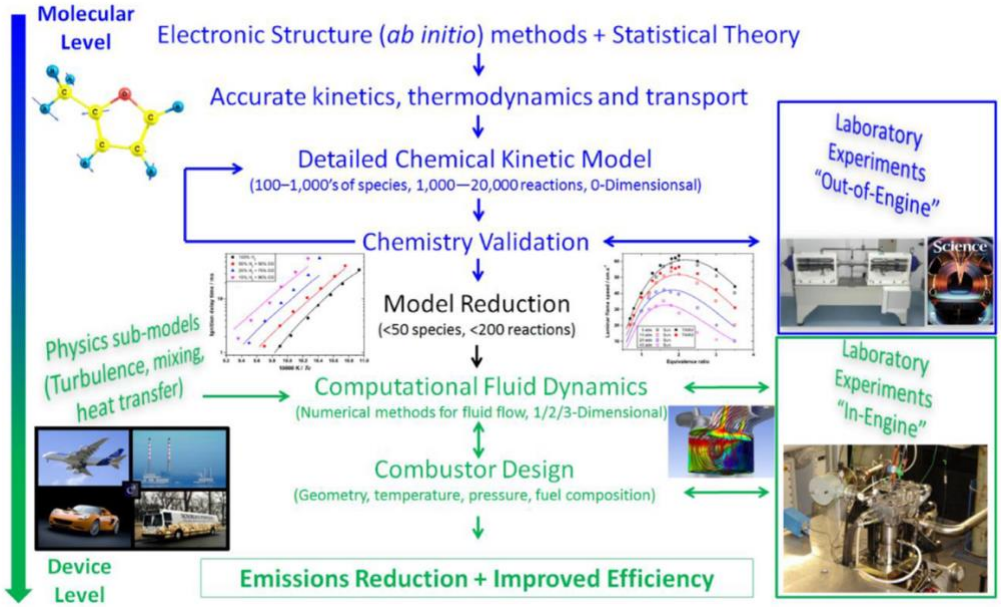

Figure 1: Steps from the elucidation of chemical detail to the design of real combustion devices with increased efficiency and reduced emissions (adapted from Curran [1]).

2. Structured Databases and Data Format Standards

The combustion literature now contains more data for many fuels than can be handled manually. To be useful for kinetic modeling, datasets must satisfy the FAIR principles—Findable, Accessible, Interoperable, and Reusable [2]—and support automated simulation workflows. Structured databases such as ReSpecTh [3], SciExpeM [4], and PrIMe [5], together with standardized formats such as ReSpecTh Kinetic Data [6] and ChemKED [7], provide curated, machine-readable collections of combustion experiments.

Their full potential is realized when they include not only measured values and metadata but also simulation-ready input files containing initial and boundary conditions and solver settings. This enables automated evaluation of kinetic mechanisms using frameworks such as Optima++ [8] coupled with simulation tools including OpenSMOKE++, Cantera, ZeroRK, and FlameMaster.

Achieving interoperability requires standardized reporting practices. Data published only in tables or figures often require manual digitization, which may introduce errors and result in loss of critical metadata. Machine-readable formats such as the ReSpecTh Kinetics Data (RKD) XML format [6] preserve

experimental conditions, diagnostics, provenance, and uncertainty information, therey making FAIR principles operational in combustion kinetics.

3. Data Completeness, Uncertainty, and Consistency Assessment

Reliable combustion data analysis requires sufficiently comprehensive reporting of experimental conditions to enable physically consistent modeling. This includes boundary conditions, correction procedures, and other factors influencing the effective reactor state, such as heat transfer in jet-stirred reactors or volume-history effects in rapid compression machines, as well as the distinction between corrected and uncorrected laminar burning velocities. Such information is essential to ensure that derived quantities are physically meaningful and comparable across different experimental setups [9–12].

Experimental uncertainties are essential for mechanism validation and optimization and should be consistently quantified across all relevant parameters. Particular attention is needed for strongly sensitive observables such as ignition delay times. Uncertainty reporting should distinguish systematic and random contributions, and reproducibility should be supported through replicate measurements [13].

Even well-structured databases require strict curation to assess experimental data for plausibility, consistency, and outliers. To avoid the bias of screening against existing models, we recently developed a statistical method [14] for identifying inconsistent measurements. This approach yields curated, internally consistent datasets with rigorously quantified uncertainties and fitted correlations with prediction bands to be used for model development and validation. Distributed via ReSpecTh with simulation-ready input files, these datasets and correlations are updated as some data turn out to be erroneous or new data are published.

4. Summary

This contribution presents the modeller's perspective on structured combustion data and databases. Emphasis is placed on FAIR, simulation-ready datasets, rigorous uncertainty quantification, and model-free consistency analysis. Improved reporting standards and closer collaboration between experimentalists and modellers can substantially enhance the quality, usability, and long-term impact of combustion measurements.

Acknowledgements

The authors acknowledge financial support from the National Research, Development and Innovation Office of Hungary through grants K147024 (TT), NKKP ADVANCED 150696 (TN), and DKOP-23 (AGS). This work was also carried out within the framework of the CYPHER COST Action (CA22151), "Cyber-Physical systems and digital twins for the decarbonisation of energy-intensive industries," supported by COST.

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Speaker Biography

Tibor Nagy earned master's degrees in chemistry and physics at Eötvös Loránd University and an MChem at the University of Leeds under the supervision of Michael J. Pilling. He completed his PhD in chemistry under Tamás Turányi. As a postdoc, he worked on kinetic modelling with Henry J. Curran and on chemical reaction dynamics and kinetics with Markus Meuwly and György Lendvay. He currently holds a position as a Senior Research Fellow at the HUN-REN Research Centre for Natural Sciences (RCNS) in Budapest, where he guides four PhD students. He is the chair of the Hungarian Academy of Sciences' Reaction Kinetics and Photochemistry Committee. Besides assisting catalysis research at RCNS with computational chemistry, his work focuses on the development of methods and codes for model reduction, uncertainty quantification, and kinetic parameter optimization. He is also a senior member of Tamás Turányi's Chemical Kinetics Laboratory and also collaborates actively with Agustín Valera-Medina and Henry J. Curran.

Topic 3. Plasma combustion: experiments and modelling

Invited contributions

Computation of the low-energy electron scattering cross section for NH_3 plasma

Xianwu Jiang[1,*], Hainan Liu[2], Chi Hong Yuen[3], Viatcheslav Kokoouline[4]

[1] *Department of Physics, Wuhan University of Technology, Wuhan, 430074, P. R. China*
[2] *Department of Basic Courses, Naval University of Engineering, Wuhan, 430033, P. R. China*
[3] *Department of Physics, Kansas State University, Manhattan, KS 66506, USA*
[4] *Department of Physics, University of Central Florida, Orlando, FL 32816, USA*

*Contact: xwjiang@whut.edu.cn

Burning NH_3 as a carbon-free fuel has gained special attention in recent years. Cold plasma technology improves its ignition and combustion and avoids NO_2 emission [1]. The collision of electrons from the NH_3 molecules, along with the fragments NH and NH_2 and the molecular ion NH_3^+ and NH_2^+ in the NH_3 plasma, plays a crucial role in understanding the dynamics behind the plasma-assisted combustion. Obtaining the electron-impact cross sections relevant to NH_3 is thus fundamental to constructing the plasma model. A comprehensive computation of the low-energy electron scattering cross section for NH_3 plasma is performed.

We first evaluated cross sections for rotational excitation, differential, momentum transfer, total elastic, and electronic excitation using the frame of the R-matrix method. The electron-impact dissociation of NH_3 to NH_2+H and NH+H_2 was considered as the molecular dissociative excitations to the correlated dissociation channels. Cross sections for total ionization are estimated by BEB method. The excitation cross section for each vibrational mode of NH_3 which remains controversial was computed by applying the theoretical approach combining the fixed-nuclei R-matrix method, normal mode approximation and the vibrational frame transformation. All the obtained scattering cross section data with uncertainties is shown in Fig. 1.

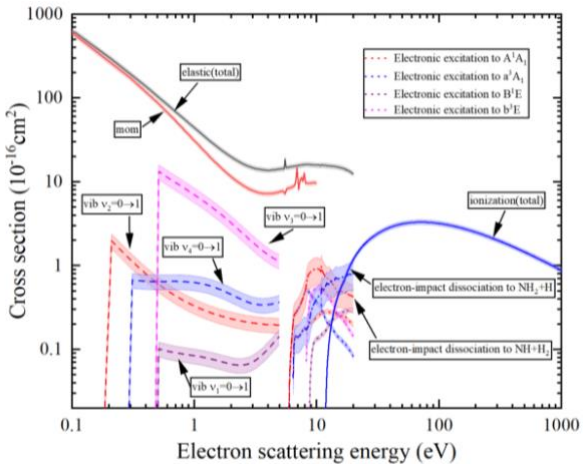

Figure 3: The computed electon-NH_3 collisional cross sections. The uncertainties are specified by the ribbons [2].

With resonance parameters derived from the R-matrix calculations, dissociative electron attachment (DEA) to NH_3 that initiates the cold plasma is considered. Theoretical modeling of this process has been challenging due to the non-adiabatic interplay of electronic motion and multidimensional nuclear dynamics. We apply the theoretical approach developed for polyatomic molecule **Error! Reference source not found.** to investigate the breakup of NH_3 through the NH_3^- 5.5 eV resonance. The potential energy surface of the resonant state is computed to elucidate the DEA mechanism as shown in the left panel of Fig. 2. The cross section of DEA via the 5.5 eV resonance is then calculated for both NH_3 and ND_3. Fig. 2 (right panel) shows the comparison of the DEA cross sections for the NH_3 and ND_3 isotopologues (panel a), and two experiments (panels b and c). The positions of the peaks in both cross sections and the ratio $\sigma_{(NH3)}/\sigma_{(ND3)}$ are in excellent agreement with previous experiments. The developed theoretical model accurately describes the DEA process and could serve as a useful tool for providing DEA cross sections for other molecules to model low-temperature plasma.

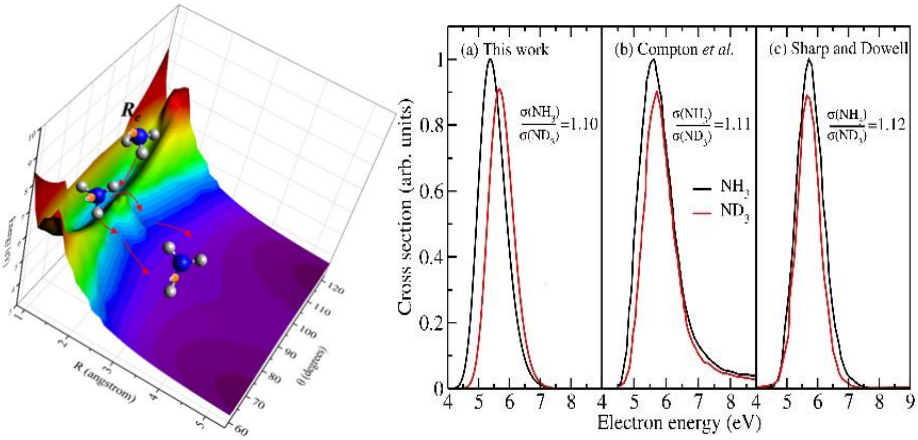

Fig. 2. DEA mechanism (left panel) and cross sections for NH_3 and ND_3 (right panel) [4].

Dissociative recombination (DR) cross sections of ionized species NH_3^+ and NH_2^+ in the NH_3 plasma constitute a data gap in the simulation. We studied the low-energy electron-impact vibrational excitation and DR processes of NH_3^+ in D_{3h} symmetry by the theoretical model combining the fixed-nuclei R-matrix method, normal mode approximation and vibrational frame transformation [5]. Jahn-Teller effect is found to dictate the dominance of the two e′ modes in both processes. Energy range of the treatment is extended to the level of second excited vibrational state (v=2). Thermally-averaged rate coefficients for vibrational excitation and DR processes are given in Fig. 3 for temperatures 0.1-30000 K.

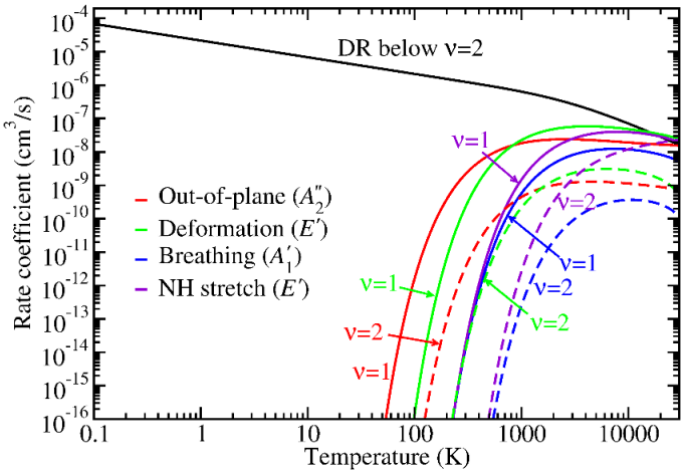

Figure 3: Thermally-averaged rate coefficients for vibrational excitation and DR processes for NH_3^+.

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Speaker Biography

Dr. Xianwu Jiang received his Ph.D. in Physics from Université Paris-Saclay, France, in 2021. He is currently an Associate Professor in the School of Physics and Mechanics at Wuhan University of Technology. He was an exchange researcher at Rollins College, USA, from 11/2019 to 03/2020 and invited visitor scholar at CNR ISTP, Italy from 12/2025-03/2026. His research focuses on theoretical studies and cross-section calculations of low-energy electron collisions with molecules and molecular ions, including vibrational excitation, dissociative recombination (DR), and dissociative electron attachment (DEA), with applications in low-temperature plasma modeling. He has led research projects supported by the National Natural Science Foundation of China and the Natural Science Foundation of Hubei Province. In 2024, he received the Young Researcher Award at the First National Young Scholars Conference on Atomic and Molecular Physics.

Laser diagnostics of hydrogen: from quadrupole absorption to Raman scattering

Wei Ren*

[1]*Department of Mechanical and Automation Engineering, The Chinese University of Hong Kong, New Territories, Hong Kong SAR, China*

*Contact: renwei@cuhk.edu.hk

Accurate, time-resolved quantification of hydrogen (H_2) in reactive flows is critical for low-carbon combustion, hydrogen safety, and optimization of fuel-conversion processes. Laser diagnostics are attractive because they are non-contact, fast, and can be quantitative when anchored to well-characterized molecular transitions. A key challenge is that H_2 is a homonuclear diatomic molecule and therefore lacks a permanent dipole moment. The strong dipole-allowed infrared transitions routinely exploited in laser absorption spectroscopy (LAS) for polar species are absent, and practical H_2 absorption sensing must rely on weak electric-quadrupole ro-vibrational lines. A widely used target is the S(1) quadrupole transition near 2122 nm, which is accessible with commercial semiconductor lasers. Because the line strength is small, sensitivity improvements typically require substantial increases in absorption path length. Direct tunable diode laser absorption spectroscopy (TDLAS) has been demonstrated using an 11.4 m multipass cell, showing that viable H_2 quantification is achievable when long path lengths are combined with careful spectral modeling [1].

Cavity-enhanced spectroscopy provides a more sensitive alternative by using a high-reflectivity optical cavity to increase the effective interaction length by orders of magnitude. Recent studies report sensitive H_2 detection using off-axis integrated cavity output spectroscopy (ICOS) near 2.1 μm [2]. Off-axis injection excites many cavity modes and produces a smoother transmitted baseline, reducing sensitivity to mode matching and improving robustness under practical operating constraints. Together, these advances support H_2 sensors that are simultaneously sensitive, stable, and deployable outside ideal laboratory conditions.

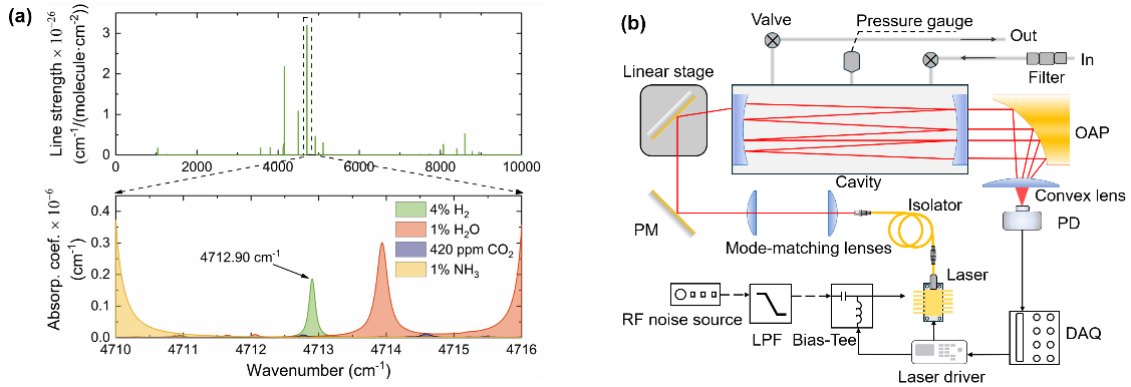

Figure 4: (a) Absorption line selection for H_2 detection. (b) Experimental setup of OA-ICOS H_2 detection system [2].

In contrast to absorption methods, gas-phase Raman spectroscopy detects molecules via frequency shifts associated with rotational and vibrational transitions. Spontaneous Raman scattering is intrinsically weak. Accordingly, recent Raman literature emphasizes strategies to boost signal, including multipass and cavity-enhanced Raman configurations that increase the effective interaction length and enable improved detection limits for H_2 and other species. Stimulated Raman spectroscopy (SRS) offers an important alternative to spontaneous Raman [3]. In SRS, two spatially and temporally overlapped fields (pump and Stokes) drive a Raman transition when the laser frequency difference matches a molecular Raman frequency. Rather than detecting weak, frequency-shifted scattered photons, SRS measures a small intensity change on the excitation beams (i.e., stimulated Raman gain on the Stokes). For hydrogen, SRS is particularly attractive because it retains Raman's selectivity while enabling high-speed, high-SNR measurements.

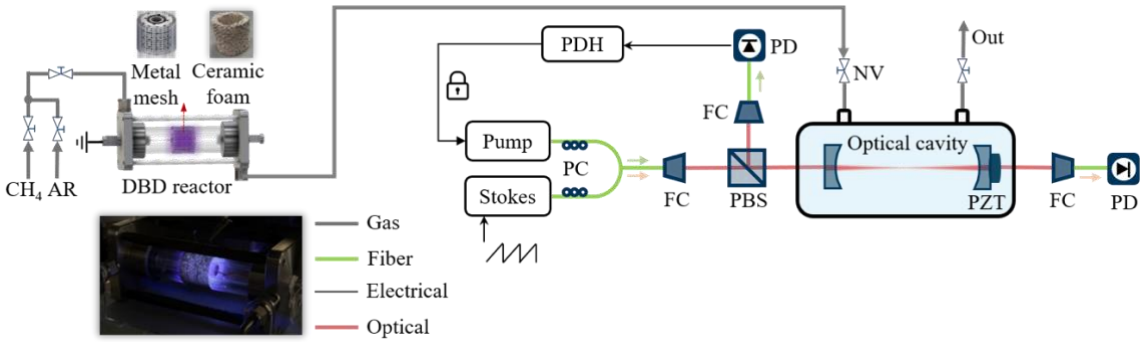

Figure 2: Schematic of the DBD reactor and the laser diagnostic system [4].

Building on these concepts, recent work has introduced cavity-enhanced stimulated Raman spectroscopy for sensitive H_2 detection by coupling continuous-wave pump and Stokes lasers into a high-finesse cavity. This approach combines the selectivity of stimulated Raman excitation with cavity-enhanced readout (e.g., ring-down detection), enabling ppm-level capability without spectrographs or high-power pulsed lasers [4]. The technique has been demonstrated for sensitive H_2 detection during methane plasma cracking and is readily extendable to continuous, time-resolved, in situ monitoring. Future work will focus on time-resolved, multi-species diagnostics to elucidate the formation pathways and temporal evolution of key intermediates and products during plasma cracking of hydrogen-bearing gases.

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Speaker Biography

Wei Ren is a Professor in the Department of Mechanical and Automation Engineering at The Chinese University of Hong Kong, where he also serves as Assistant Dean of the Faculty of Engineering and Director of the Energy and Environmental Engineering Programme. He received his B.S. degree in Mechanical Engineering and M.S. degree in Optical Engineering from Tsinghua University and his Ph.D. degree from Stanford University. His research focuses on optical sensing, laser spectroscopy, and combustion diagnostics, with applications in energy systems, environmental monitoring, and industrial processes. He is currently the Associate Editor of Proceedings of The Combustion Institute, Co-Editor of Applied Physics B, and Senior Editor of PhotoniX.

Non-Equilibrium Plasmas as an Enabling Technology to Improve Next-Generation Combustion Architectures

Nicholas Tsolas*

Department of Mechanical Engineering, Auburn University, Auburn AL, USA

*Contact: ntsolas@auburn.edu

Transitioning to sustainable energy fuels (i.e. oxygenated fuels, ammonia, hydrogen) is considered a critical step towards mitigating climate change, ensuring energy security and meeting energy demands. Despite their attractiveness, operability issues regarding low flames speeds leading to unstable flames, narrow flammability limits, high ignition temperatures resulting in long ignition delays, and the propensity to form NO_X emissions are potential obstacles that have hindered their widespread adoption into practical systems. Non-equilibrium plasmas (NEP) are well known to promote energy-efficient chemical reactivity via quenching and transport of electronically excited atoms and molecules, selective radical production, and fast gas heating (FGH). These effects have shown promise in improving lean flammability limits, ignition characteristics, and flame stability [1,2], making NEP a potentially viable strategy for overcoming the inherent challenges associated with sustainable fuels in air-breathing power and propulsion applications. However, closing the gap on realizing practical integration requires fundamental understanding of the plasma coupling effects on chemical reactivity of fuels in parallel with targeted technological development to optimize plasma-based technologies at practically relevant conditions. In the present work, on-going efforts are discussed that span from fundamental kinetic studies to applied demonstrations aimed at establishing NEP as an enabling technology that could potentially improve the operability of existing and next-generation combustion architectures with fuels.

From a fundamental perspective, the discussion will focus on oxygenated fuels, wherein a purpose-built plasma coupled flow reactor (PFR) experimental facility and numerical techniques are described to elucidate plasma chemical insights while developing plasma-specific kinetic mechanisms. Such mechanisms are critical to support high-fidelity predictive simulation tools needed for the design, integration, and optimization of NEP-based technologies for practical, device-scale applications. Examples will be drawn from methanol studies, with implications on overall reactivity, ignition and emission characteristics, while highlighting the remaining challenges and natural opportunities to improve the development of accurate plasma-specific kinetic mechanisms.

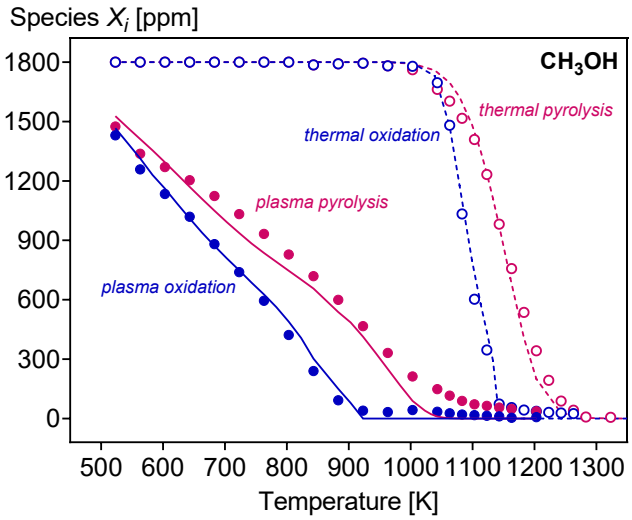

Figure 5: Comparison of methanol/air consumption with and without the effects of NEP as a function of temperature; data points - experiments; solid/dashed lines - model

Experimental results demonstrate considerable enhancement in overall fuel reactivity for both plasma-assisted pyrolysis and oxidation below 900 K compared to thermal reactions (see Fig. 1). For plasma-pyrolysis, methanol exhibits a change in decomposition rate, indicating a transition in the dominant chain-reaction sequence. At low-to-intermediate-temperatures, several intermediates are seen in the plasma-pyrolysis reaction that were not observed in the thermal reaction (not shown), including several oxygenates, and considerable HCN formation likely due to efficient N_2 dissociation and fuel radical formation. Enhanced reactivity is attributed to collisional quenching processes of methanol with electronically-excited $N_2(A^3\Sigma_u^+)$ generated by the plasma to enhance the initial formation of radical pools (i.e. fuel fragments and H-atoms) at early ~ns timescales (i.e. during applied voltage pulse). As such, the enhancement of radicals subsequently leads to driving propagating chain-reactions of the neutral-chemistry (i.e. H/OH+CH_3OH radical attack channels) to sustain reactivity at longer ~ms timescales (i.e. plasma afterglow). For plasma-assisted oxidation, plasma effects are observed to enhance methanol decomposition reactivity across all temperatures compared to both thermal oxidation and plasma pyrolysis. In parallel, enhanced plasma chemical reactivity in N_2/O_2 mixtures leads to appreciable NO_X formation, which are absent under thermal conditions below 1200 K. Similarly, enhanced reactivity is attributed to $N_2(A^3\Sigma_u^+)$ which continues to consume fuel, but its dominant role shifts towards enhancing the O-atom radical pool to

instigate direct fuel-attack. This subsequently drives the neutral chemistry to enhance propagating chain-reaction (i.e. $O+CH_3OH = CH_2OH+OH$) sequences to sustain reactivity in the afterglow. Towards discharge timescales, the neutral chemistry then controls the reactivity behavior with temperature, where hydrogen peroxide (HO_2) formation and terminating reactions play a preferential role to inhibit overall reactivity. For T < 833 K, the enhanced formation of N-atoms through direct electron-impact dissociation of N_2, leads to the immediate formation of NO (i.e. $N+O_2 = NO+O$) on the local pulse timescales. In the radical-rich environment established by the plasma, interactions of radicals and NO can promote NO_X catalytic effects [3], contributing up to 50% of the total OH-flux to overcome radial termination to sustain overall reactivity.

From a practical perspective, demonstrating plasma-assisted ignition (PAI) at elevated pressures remains challenging. At high pressures, breakdown voltage scales with pressure–distance product, requiring higher electric fields and hence higher energies [4]. These conditions can also alter the electron energy distribution, reduce excitation efficiency and shorten radical lifetimes, thereby potentially diminishing the advantages of NEP. Additionally, regime-dependent plasma behavior (e.g., glow versus spark) are expected to alter the distribution of deposited energy between plasma chemical and local thermalization pathways, thereby influencing ignition sensitivity and subsequent flame propagation [4]. Despite successful demonstrations of PAI to improve hard to ignite fuels (e.g., methane, gasoline, ammonia) a limited understanding remains of how PAI can be effectively leveraged to enhance burn rates and ignition. This knowledge gap limits the ability to optimize PAI performance for high-pressure combustion applications, but also the technological development of advanced igniters necessary for effective integration.

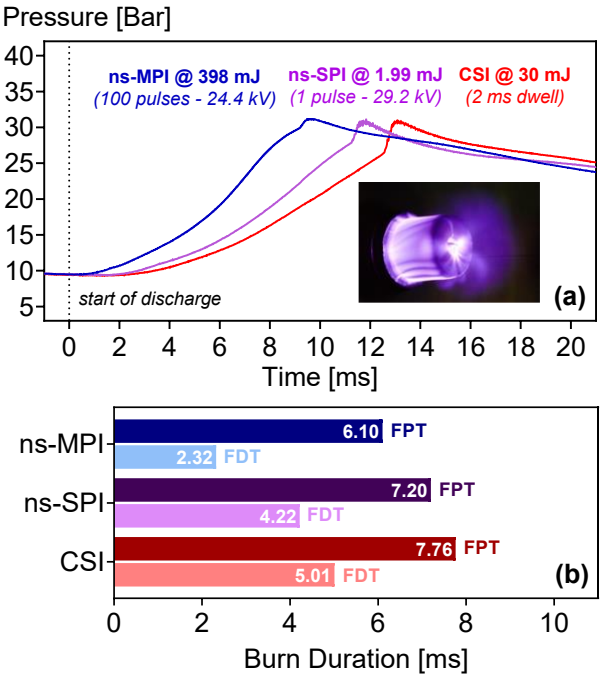

Figure 6: Comparing ns-PD to CSI at 10 bar and 664 K (a) pressure profiles and (b) measured FPT and FDT.

To demonstrate practical relevance a purpose-built plasma coupled rapid compression machine (PRCM) facility has been designed, developed and characterized to explore nanosecond-duration pulsed discharges (ns-PD) at elevated pressures. Results are directly compared with conventional inductive-coil spark ignition (CSI) systems to identify mechanisms responsible for performance enhancements, but also potential limitations that could influence practical implementation. Ignition performance was assessed through changes in flame development (FDT) and flame propagation time (FPT) for stoichiometric n-butane/air at 10 bar (see Fig. 2). For CSI, performance was shown to be primarily limited by the voltage rise rate, with ignition and kernel growth governed by breakdown. This behavior highlights the inherent inefficiency of prolonging arc-phase energy deposition, which provides no measurable improvement in burn rate. To overcome CSI performance limitations, ns-PD are utilized that exhibit both glow-like and spark-like modalities. For ns-single pulse ignition (ns-SPI), the voltage rise rate was approximately 3-orders of magnitude faster than CSI, enabling enhanced burn durations with nearly 15x lower energy expenditure. This enhancement was attributed to ns-glow discharge characteristics that promote NEP chemistry and increase radical production, thus reducing chemical induction time to facilitate kernel growth. Additional reductions in burn duration were observed with ns-multi-pulse ignition (ns-MPI), where the performance enhancement showed greater sensitivity in FPT than in FDT. As the number of pulses increases, the chemically dominated processes associated with the ns-glow phase begin to diminish, while mechanisms governed by localized heating and acoustic perturbations increasingly influence flame-kernel growth and propagation due to the growing contribution of ns-spark discharges. However, these improvements are achieved at the cost of significantly higher energy input, requiring nearly 13x more energy than CSI. Future work will focus on optimizing discharge strategies to minimize energy input while maximizing ignition performance.

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Speaker Biography

Nicholas Tsolas is an Associate Professor in the Department of Mechanical Engineering at Auburn University. He received his BASc and MASc degrees from the University of Toronto and his PhD from The Pennsylvania State University. Prior to joining Auburn, he was a postdoctoral associate at MIT. As the Principal Investigator of the Advanced Energy and Thermal Research Laboratory (AETHERLab), his research is broadly related to advancing next-generation energy conversion technologies, that span fundamental and applied initiatives in heat transfer, combustion, and low-temperature plasma phenomena. To date, he has successfully managed research collaborations with industry and government stakeholders, including L3Harris, the U.S. Department of Energy, NASA, and the U.S. National Science Foundation. In recognition of his early-career contributions, he is the recipient of the NSF CAREER Award.

Topic 4. AI-TST-ME: automation, benchmarking and knowledge transfer.

Invited contributions

Edge Migration of Aromatic Rings by Radical Reactions—Kinetics and Directionality: Can the Outcome of an Aromatic Edge Migration Be Predicted on the Fly?

Alexander M. Mebel[1,*], Michael Frenklach[2,*]

[1] *Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199, United States*
[2] *Department of Mechanical Engineering, University of California, Berkeley, California 94720-1740, United States*

*Contacts: mebela@fiu.edu, frenklach@berkeley.edu

Elucidation of chemical reactions governing the formation and growth of polycyclic aromatic hydrocarbons (PAHs) is an active area of research. Interest in this subject stems from the role of PAHs in the formation and growth of carbonaceous materials such as carbon black, combustion soot, graphene, and interstellar dust. Initial efforts in detailed kinetic modeling of PAH formation and growth relied on the postulate of chemical similarity, where the same rate constant value was assigned to all members of a homologous reaction series [1]. Subsequent theoretical studies of several such homologous PAH reaction series, such as H abstractions from aromatic molecules and C_2H_2 additions to aromatic radicals, revealed that, despite some numerical differences among the reactions, the rate constants were roughly similar in value [2,3]. One of the reaction classes identified as significantly contributing to PAH evolution at high temperatures is the migration of five-membered rings by radical reactions along PAH edges [4,5]. Initial evaluations of their rates showed that these reactions are very rapid and can be treated in kinetic modeling as partially equilibrated [6]. Based on the similarity in their reaction mechanisms, the edge migration of seven-membered rings by radical reactions was presumed to be equally rapid as that of five-membered rings [7].

Here, we examined a series of five- and seven-ring migration reactions of polyaromatic radicals theoretically. Computed reaction energetics and rate constants demonstrate the facileness of such migrations. The results show, however, that the direction of migration is not identical for homologous reactions. It is determined by strain-induced changes in molecular geometry, which is confirmed by the Harmonic Oscillator Model of Aromaticity (HOMA) [8,9] analysis. One of the notable outcomes of the present study is that fused five-membered rings can form, not split, thereby challenging the isolated pentagon rule.

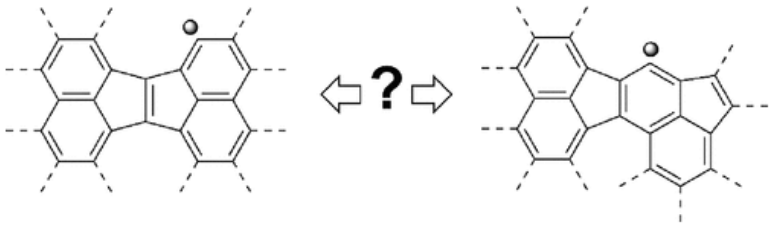

Figure 7: Is the isolated pentagon rule always valid?

Figure 2 depicts the dependence of the energy changes, ΔE, standard entropy changes at 1500 K, ΔS_{1500K}^0, and equilibrium constants at 1500 K, $K_{eq,1500K}$, on the reaction changes in HOMA. Although the displayed data exhibit a degree of scatter, they nonetheless demonstrate a clear and consistent trend. All of the puzzling features observed in the results can be attributed to strain-induced changes in molecular geometry.

Chemically, the migration processes of five- and seven-membered rings located at the edges of aromatic structures involve the transformation or isomerization of aromatic radicals that proceed rapidly at elevated temperatures—such as those found in combustion environments—and thus their outcomes are governed primarily by reaction equilibrium. Kinetic Monte Carlo (kMC) simulations showed that these migration reactions occur frequently [7,10]. In these simulations, all migrations belonging to a homologous reaction class were assumed to share the same equilibrium constant (K_{eq}). However, our analysis revealed that migration outcomes, including migration direction, vary among homologous reactions, indicating that assigning a single K_{eq} value to an entire class is not valid.

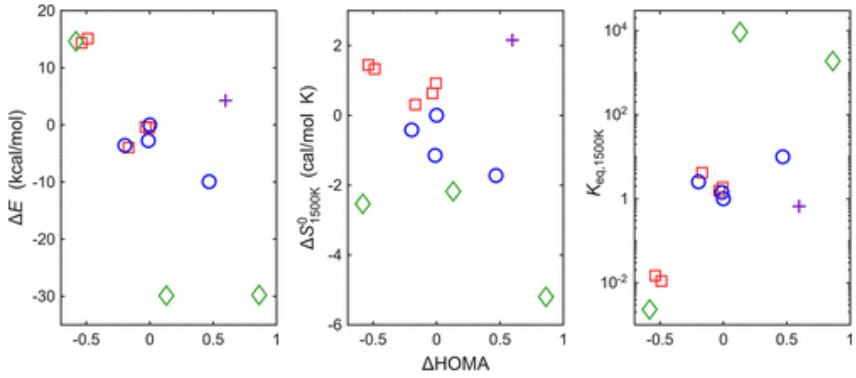

Figure 2: Reaction energy change (left panel), standard entropy change at 1500 K (central panel), and equilibrium constant at 1500 K (right panel) versus reaction change in HOMA; symbol are red squares─splitting of five-membered ring pairs; blue circles─migration of five-membered rings; purple plus─migration of seven-membered rings; green rhombi─five- and seven-membered ring migration forming two six-membered rings.

The central question of this work is whether migration reaction K_{eq} values can be predicted within the kMC simulation framework. A reliable, high-level theoretical calculation of K_{eq} is computationally too costly to incorporate directly into kMC. We observed a general trend between reaction K_{eq} and changes in HOMA. Because HOMA values are derived from molecular geometry, and because geometry can be evaluated using computationally efficient methods, a correlation between K_{eq} and HOMA could provide a practical approach for use in kMC. However, the plot of K_{eq} versus HOMA displayed a substantial amount of scatter. It is therefore our objective to determine whether this scatter is an inherent feature of the relationship or whether a higher-fidelity correlation with HOMA can be developed.

In pursuit of this objective, we investigated five-membered-ring migrations in a set of four-ring PAHs composed of two six-membered and two five-membered rings. The results showed that even for this limited set, K_{eq} does not correlate well with HOMA. However, when carbon-atom connectivity is included, a correlation of reasonable quality can be obtained. We then explored this further by extending the analysis to a larger set of migration reactions that included both five- and seven-membered rings. Based on an examination of several possible correlation models, we propose one that is suitable for use within the kMC framework.

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Speaker Biography

Alexander M. Mebel received his bachelor's degree in physical chemistry at the Moscow Institute of Steel and Alloys and his Ph.D. degree in physical chemistry at Kurnakov's Institute of General and Inorganic Chemistry of Russian Academy of Science in Moscow, Russia. After postdoctoral appointments in Germany, Japan, and USA, his first faculty position was at the Institute of Atomic and Molecular Sciences (Academia Sinica, Taiwan), and in 2003 he joined the Department of Chemistry and Biochemistry of Florida International University in Miami, Florida, USA, where he is currently Professor of Chemistry and, since 2024, Chair of the Department of Chemistry and Biochemistry. His current research interests include theoretical quantum chemical studies of mechanisms, kinetics, and dynamics of elementary chemical reactions related to combustion, atmospheric, and interstellar chemistry.

Transforming Combustion Chemistry Workflows to Handle the Big Data Deluge

William H. Green[1,*]

[1]*Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge MA, USA*

*Contact: whgreen@mit.edu

The size of combustion datasets and the complexity of combustion simulations continues to increase, making it possible to study, and guiding the design of, 'real-world-relevant' combustion systems. Our increasing ability to do accurate first-principles quantum chemistry and DNS calculations is very encouraging and often helpful. As computers, computational methods, and experimental data acquisition methods improve, combustion researchers have taken advantage of these improved capabilities to build and test higher fidelity models, and to address combustion systems with more complicated fuels and geometries.

Dealing with more complicated systems with higher fidelity has its downsides. For several decades it has been challenging for reviewers to check complicated combustion models or large datasets submitted for publication, increasing the likelihood that the archival literature contains incorrect data or flawed simulations. It can be difficult for others to use the large data sets that are published, if they are nor provided in a convenient freely-available electronic form with associated software tools. Similarly, it can be quite difficult to reproduce published simulations, or to understand why your simulations differ from those you are trying to reproduce, even if one has access to all the needed data and software.

Because of their size and complexity, it can be challenging for even the creators of the datasets or simulations to carefully check their own work, and in my experience most large datasets, whether derived from experiments or from calculations, contain some errors. If they are too big to check by hand, the authors may need to create extra software tools to help them find any errors in their data, or to help them detect any potential bugs or numerical issues affecting their complicated simulations.

Extracting valuable information from comparisons between the predictions from complex simulations and large experimental datasets is also challenging, both because of the large number of model vs. data comparisons, and because of imperfect knowledge of the uncertainties in both the simulations and the experimental data. What level of agreement is "satisfactory"?

It is also important to keep in mind Fermi's maxim: 'With four parameters I can fit an elephant, and with five I can make him wiggle his trunk'. Usually, the datasets available, even if quite enormous, do not have enough information content to determine all the uncertain parameters in the simulations. Even in the rare case that the data does has enough information content, it can be difficult to extract it: because of the poor scaling of existing global optimization methods, it is often impossible to guarantee one has found the best-fit parameters, even for rather simple systems.

The Data Science community has been dealing with similar issues, and has found useful ways to handle some of them. I argue we should move faster to learn from that community, both about what they are doing that works well, and also to avoid some pitfalls they have run into. While combustion increasingly resembles data science, it is of course distinct, both because

In this talk I will give show several illustrative examples of what can be done using today's computational capabilities, focusing on our ability to fairly accurately predict the properties of molecules and reactions, and to rapidly develop accurate combustion chemistry simulations. I will also discuss some of the challenges my group has encountered as we attempt to predict combustion kinetics with high fidelity [2,3,4], and to provide useful software [5,6,7] and clean datasets [8,9] to the community.

I will close by presenting a vision for how the combustion community can work together to modernize an improve our workflow, to make it easier for us to collaborate to do good research, and to make our community quicker at solving societal challenges.

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Speaker Biography

Bill Green received his Ph.D. in Physical Chemistry from U.C. Berkeley mentored by Brad Moore. After postdoctoral work with Nicholas Handy and Marsha Lester, he worked in industry for six years before joining the Chemical Engineering faculty at MIT in 1997. From 2008-2013 he was the Editor of the *International Journal of Chemical Kinetics*. Since 2024 he has led MIT's Energy Initiative. Most of his research focuses on developing automated methods to construct and solve chemical kinetic simulations, or to predict molecular properties. His group developed the popular open-source Reaction Mechanism Generator (RMG) and Chemprop software packages. He co-founded Thiozen (to commercialize H_2 production from H_2S) and also LNK Energies (to provide an affordable way to power vehicles with hydrogen, conveniently carried on a liquid organic hydrogen carrier (LOHC)). He leads the CLEAR project to improve cost and life-cycle greenhouse gas emission estimates for energy innovations.

Automated Kinetic Data Generation for Combustion Models: the Tabulated Model of Transition States (TMTS) Method

Baptiste Sirjean[1,*], Fabiola Citrangolo Destro[1], Pierre-Alexandre Glaude[1], René Fournet[1]

[1]*Université de Lorraine, CNRS, LRGP, F-54000 Nancy, France*

*Contact: baptiste.sirjean@univ-lorraine.fr

Context

The predictive capability of kinetic combustion models depends on the completeness of the reactions included in the reaction mechanism and the accuracy of the associated kinetic and thermochemical data. For hydrocarbons and major families of oxygenated compounds, such as alcohols, ethers, and esters, the knowledge of reaction mechanisms is generally no longer a significant source of error in model predictions. Thus, the accuracy of combustion property predictions for these systems relies primarily on the precision of thermo-kinetic data. Generating kinetic models is a long-standing challenge that has engaged numerous research groups over the past decades [1]. Pioneering work in automation was conducted there, advancing chemo-informatics and high-throughput generation of thermochemical and kinetic data. These efforts have aligned with the intended applications of combustion models, as the typical size of fuel molecules directly determines the size of the mechanism. The first generated models were closely tied to applications in spark-ignition and Diesel engines, with fuel sizes of ~C_8 and ~C_{16}, respectively, and kinetic model construction quickly emerged as a prime candidate for computer-assisted generation. Several methods have been proposed for generating high-throughput kinetic data, but their accuracy may be limited compared to that achievable with ab initio kinetics [2]. For energy production in gas turbines, gas combustion can be modeled with mechanisms containing 1 to 4 carbon atoms. For systems of this size, automated ab initio theoretical calculations using transition state theory or master equation methods (with partition function corrections and tunneling effects, i.e., Ab Initio-TST-ME) to generate kinetic data on-the-fly is a promising approach to increase the accuracy of the model prediction [3]. However, precise on-the-fly calculations for larger fuels (jet, diesel and gasoline) is currently not feasible. Progress in this area will require advancements in numerical methods and theories for ab initio calculations and, potentially, the use of AI to construct accurate potential energy surfaces and partition function corrections.

Our work explores an alternative to on-the-fly calculations, aiming to propagate the precision of Ab Initio-TST for reactions of small systems to those of heavier fuels, while enabling high-throughput kinetic data generation.

TMTS method

The method we developed is the Tabulated Model of Transition States (TMTS) [4]. For a given reaction type, this approach involves: 1) Geometry optimization of minimal-size reactants, transition states (TS), and products; 2) Identification of a minimal representative substituent group for larger substituents; 3) Calculation of rate coefficients for all possible combinations of representative groups on the minimal reactants, TS, and products; 4) Transferring this information into comprehensive tables, where rate coefficients are read based on the substituents along the carbon chain.

Implementing the TMTS method for alkyl radical isomerizations demonstrated the need to account for "spectator" alkyl groups to compute precise kinetic data, as the level of branching in the TS can induce variations of several orders of magnitude in the rate coefficients [4]. This work also highlighted the importance of considering diastereoisomers for accurate kinetic calculations. The combinatorial nature of the substitution along the chain and the existence of multiple configurations result in an extremely large number of calculations, making manual construction of TMTS table nearly impossible. To address this, we developed AutoTMTS, a code capable of automatically generating TMTS tables [4]. The AutoTMTS workflow creates all possible substituent combinations on the minimal structures, generates Gaussian input files for geometry optimization, frequency calculations, and relaxed scans around single bonds, and analyzes the electronic structure calculation results. Once the electronic structure calculations are performed, AutoTMTS identifies symmetries and optical isomers in the optimized structure, treats internal rotors as hindered or free rotors, links optimized TSs to their corresponding reactants and products, and extracts data from output files for canonical Ab Initio-TST rate coefficient calculations using the ThermRot code. Finally, it writes the calculated kinetic data into tables for each model TS. Figure 1 illustrates the workflow implemented in AutoTMTS, from the input to the TMTS table.

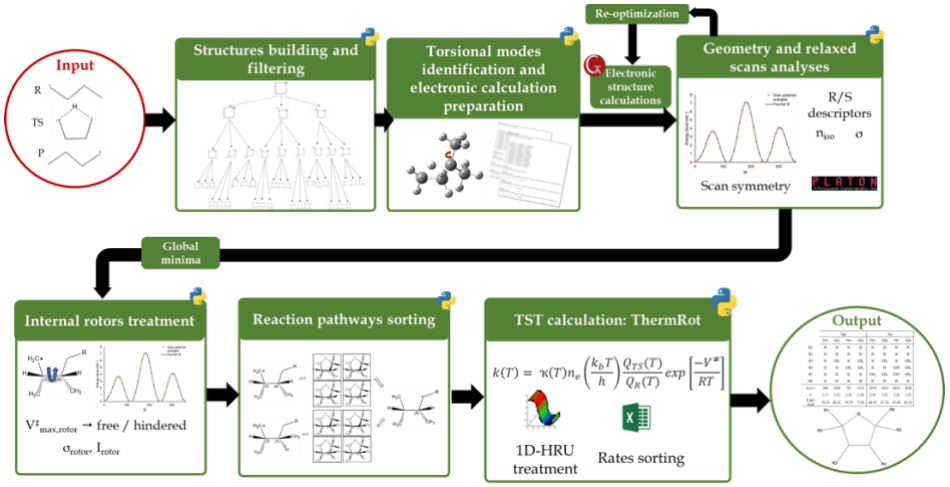

Figure 8: Automated workflow for the Tabulated Model of Transition State construction with AutoTMTS.

This automated workflow was applied to 3- to 6-center isomerizations of alkyl radicals. In the latter case, 72 rate constants were calculated, requiring the computation of 405 transition states due to the multiple configurations in the TS rings [6]. The TMTS data underscored the necessity of accounting for multiple TS configurations to precisely calculate a single reaction rate coefficient. The TMTS approach has been demonstrated as applicable to other reaction types, such as C-C and C-H β-scissions in alkyl radicals, as well as H-abstraction by H, OH, HO_2, RO, and ROO radicals from linear and branched alkanes [7].

This approach enables high-throughput estimation of canonical kinetic data for real-world fuels (up to ~C_{20}), with accuracy likely approaching that of on-the-fly calculations. The TMTS method proved effective for these reactions by leveraging error cancellations and balances between entropy and activation energy variations.
The TMTS kinetic data for H-abstractions, β-scissions, and isomerizations of alkyl radicals were implemented in EXGAS, our software tool for the generation of combustion kinetic models. A pyrolysis model for a highly branched alkane, iso-dodecane, was generated and used to simulate recent speciation data obtained in a plug-flow reactor. The simulation results showed significant improvements in predicting the selectivity of primary products compared to the model generated using the legacy reaction rate rules based on semi-empirical correlations. The simulation results also emphasized the importance of incorporating precise sub-mechanisms for the decomposition of major primary products, here, branched alkenes, to improve the accuracy of the predicted small pyrolysis products. The challenge of improving the predictive capabilities of kinetic models is closely linked to the well-identified issue of target data used to constrain the models, and thus to the broader quantification and minimization of uncertainties in combustion models, as well as the accuracy required on the local or global combustion characteristics that depends on the target combustion system to be simulated.

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Speaker Biography

Baptiste Sirjean obtained his PhD in 2007 from the National Polytechnic Institute of Lorraine, focusing on the development of theoretical chemistry methods for modeling combustion processes. After his PhD, he worked as a postdoctoral researcher for two years in Professor Hai Wang's group at the University of Southern California in Los Angeles. In 2009, he joined the Reaction and Process Engineering Laboratory as a CNRS Research Associate. Now a CNRS Research Director, his primary research focuses on the kinetics of combustion and liquid-phase oxidation of organic compounds, using experiments and modeling based on theoretical chemistry. His research focuses on improving the efficiency and environmental impact of combustion, liquid-phase oxidation, and toxic destruction processes.

Topic 5. Chemical Kinetics Mechanisms: Progress in accuracy and details.

Invited contributions

Details in Elementary Kinetics: Setting the Foundations for Combustion Kinetics Modeling

Raghu Sivaramakrishnan[1,*]

[1]*Chemical Sciences & Engineering Division, Argonne National Laboratory, Lemont, IL-60439, USA.*

*Contact: raghu@anl.gov

Modern combustion modeling relies on a highly quantitative description of the underlying elementary chemical processes. This places an increased emphasis on not just understanding the mechanisms of elementary reactions but also obtaining and representing their rate coefficients accurately over a wide range of conditions relevant in practical combustion applications. The flame chemistry perspectives article [1] highlights frontier research areas and challenges in mechanism development and here I would like to talk about two related and interwoven areas of relevance. The first topic involves the development of a theory-based kinetics mechanism [2] for core species (H_2-C_3) in combustion and the second topic (as a direct offshoot of the first) involves the identification and implementation of non-thermal phenomena [3] within this model. Over the course of several years now we have been actively involved in the development of a theory informed kinetics model that includes *a priori* high-level theoretical predictions for the elementary reactions as well as thermochemistry and transport parameters for species involved in small molecule combustion chemistry (H_2 and C_0 – C_3 species). A particular aspect to highlight is the analysis of pressure dependence with theory-based representations of pressure fall-off that are in agreement with direct kinetics experiments (where available) for key recombination and dissociation reactions within this model [2]. Inadequate treatment of fall-off can lead to mis-interpretation of simulation results as highlighted in recent studies [4,5]. Pressure fall-off has always been a topic of relevance in combustion kinetics [6] and a proper treatment of fall-off in radical dissociations within our ThInK model [2] provided the foundations for elucidating the role of non-thermal phenomena such as radical prompt dissociations in combustion [3,7,8]. Prompt dissociation phenomena are an inherent feature of pressure fall-off and neglect of either phenomena can lead to noticeable effects in flame modeling. Fig. 1 depicts simulated laminar flame speeds for CH_2O-air flames at standard conditions (1 atm, T_u = 300 K) using our ThInK model that includes a fall-off analysis for the thermal dissociation of HCO as well as the consideration of its prompt disociation due to rovibrational excitation from CH_2O+H/OH abstractions. Neglect of either effect, pressure fall-off or prompt dissociation in HCO, can have noticeable consequences in the flame simulations as depicted below. The present work will discuss the theory-based core model [2] as well as non-thermal phenomena such as prompt dissociations [3] and chemically termolecular reactions [3,9,10] represented here.

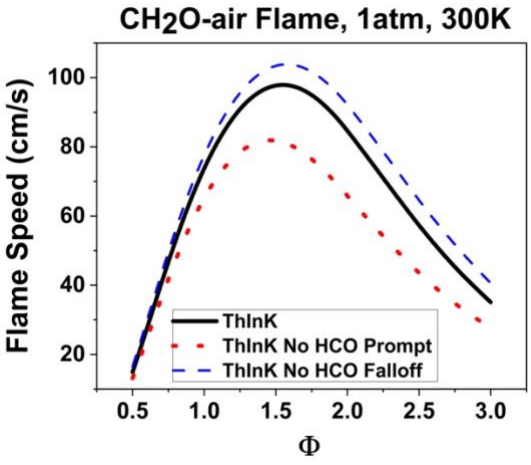

Figure 9: Laminar flame speed simulations using ThInK [2] for CH_2O in air at P = 1 atm and T_u = 300 K.

Acknowledgments
RS acknowledges the contributions of all the collaborators involved in the development of the ThInK model. This work was supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences (BES), Division of Chemical Sci- ences, Geosciences, and Biosciences (CSGB) under contract No DEAC02- 06CH11357 as part the Argonne-Sandia Consortium on PressureDependent Chemistry under ANL FWP 59044.

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Speaker Biography
Raghu Sivaramakrishnan is a Scientist in the Chemical Dynamics group at Argonne National Laboratory. He received a B. Tech. in Chemical Engineering from the University of Madras, and an MS and PhD in Chemical Engineering from the University of Illinois at Chicago (Advisor - Kenneth Brezinsky). He continued as a post-doc and research staff member in Ken Brezinsky's group before moving to Argonne as a post-doc to work with Joe V. Michael to characterize the kinetics of elementary reactions. In 2010, he was hired as a research staff at Argonne where his research interests involve applications of theoretical and experimental chemical kinetics to model reactions of gas-phase molecules relevant in complex reacting systems such as in combustion and propulsion, atmospheric chemistry, and practical chemical conversions.

Speciation experiments in kinetics: what do we learn from modeling?

Guillaume Dayma*

Université d'Orléans, ICARE-CNRS, Orléans, FRANCE

*Contact: guillaume.dayma@univ-orleans.fr

Experimental data are essential benchmarks for assessing the validity of the thousands of reactions and associated rate constants that make up a detailed kinetic mechanism. These data may consist of global quantities, such as ignition delay times or flame speeds, which reflect the combined effect of a large network of reactions, or more targeted observables, such as species mole fraction profiles, which result from a more limited sequence of reaction pathways. Comparing experimental results obtained under a wide range of thermodynamic conditions with numerical simulations is a key step in demonstrating the robustness of a kinetic mechanism. Once validated, the mechanism can be used not only to reproduce experimental observations, but also to predict quantities that are difficult to measure experimentally. It can also be incorporated into computational fluid dynamics solver to model complex systems. After demonstrating its ability to reproduce experimental data, a detailed kinetic mechanism can also be used to interpret and better understand experimental observations. In this context, rate-of-production and sensitivity analyses are no longer primarily aimed at identifying the optimal thermokinetic parameters for fitting experiments, but rather at elucidating the reaction pathways responsible for the observed phenomena. A detailed kinetic mechanism therefore makes it possible to track the sequence of reactions leading, for example, to heat release or to the formation of a specific chemical species.

Two examples have been selected to illustrate the value of reaction mechanisms for interpreting species profiles. The reactivity of five-carbon esters studied in a jet-stirred reactor (JSR) will first be analyzed at the light of a mechanism published by Dayma et al. [1], while the time-resolved history of CO measured in a shock tube will be interpreted using the mechanism reported by Grégoire et al. [2].

In the first example, the oxidation of butyl formate (BF), propyl acetate (PA), ethyl propanoate (EP), and methyl butanoate (MB) was investigated in a JSR under conditions of $\varphi = 1$, $p = 10$ atm, and a residence time of 0.7 s. Figure 1 presents the evolution of the mole fractions of the four fuels as a function of the temperature of the reactor. Under these conditions, it can easily be observed that methyl butanoate (MB) is less reactive than the other three. This difference in reactivity between these four isomers can be explained by the kinetic mechanism developed in this study, but a deeper analysis using this mechanism reveals other surprises.

In the second example, the pyrolysis and oxidation of propan-1-ol was studied near atmospheric pressure, measuring CO time-history profiles behind reflected shock waves using laser absorption diagnostics. Figure 2 shows the time evolution of the mole fraction of CO measured experimentally and compared with the mechanism prediction. Thanks to the mechanism developed in this work, the increase in CO mole fraction observed within the first 2 ms can be correlated to the consumption of propan-1-ol, but the mechanism can also be used to understand the second rise in CO mole fraction as it will be shown in the presentation.

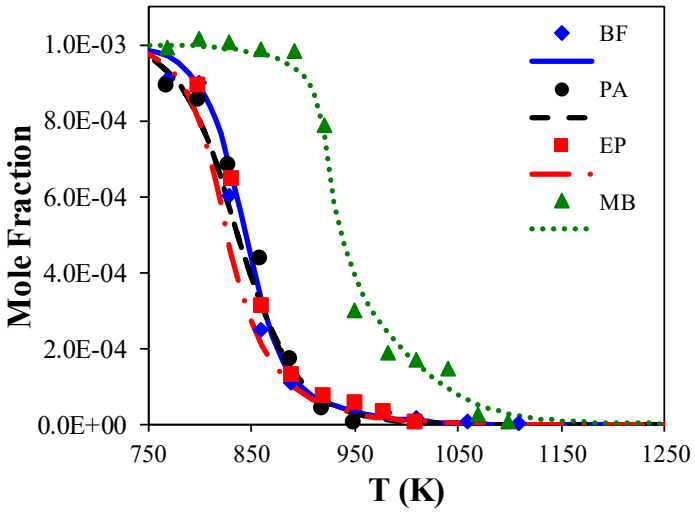

Figure 1: Experimental (symbols) and computed (lines) mole fraction profiles obtained from the oxidation of methyl butanoate (green), ethyl propanoate (red), propyl acetate (black), and butyl formate (blue) in a JSR at φ = 1, p = 10 atm, τ = 0.7s.

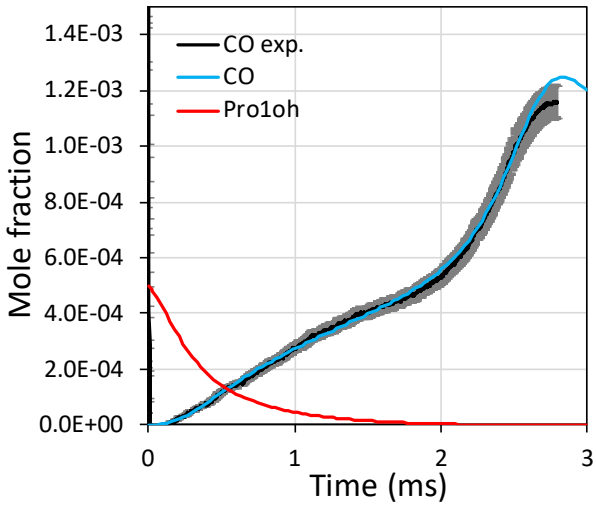

Figure 2: Evolution of the experimental mole fraction of CO (black) and the calculated mole fractions of propan-1-ol (red), and CO (blue) vs. time with X_{fuel} = 0.05%, φ = 0.5, T_5 = 1302 K and p_5 = 1.35 atm.

Acknowledgements

Claire M. Grégoire, Océane Clément, Olivier Mathieu, and Eric L. Petersen from Texas A&M University, Maristella Di Teodoro, Sarah N. Elliott, and Carlo Cavallotti from Politecnico di Milano, Zeynep Serinyel, Sébastien Thion, Maxence Lailliau, and Philippe Dagaut from Univresity of Orléans and CNRS are warmly acknowledged for their participation in this work.

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[1] Dayma G., Thion S., Lailliau M., Serinyel Z., Dagaut P., Oxidation of C5 esters: influence of the position of the ester function, Int. J. Chem. Kinet. 53 (2021) 1124–1132.
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Speaker Biography

Guillaume Dayma has been professor at the University of Orléans since 2012. He obtained his PhD from the Institut National Polytechnique de Lorraine (Nancy, France) in 2003. He was a post-doc fellow at the Institute for Aerospace Studies (University of Toronto, Canada) in 2005. He started as assistant professor at Pierre and Marie Curie University (now Sorbonne University, Paris, France) from 2006 to 2009 before moving to Orléans. His research activities aim at understanding the chemical phenomena during combustion. He develops detailed chemical kinetic mechanisms for a variety of fuels. He is also teaching physical chemistry, thermochemistry and kinetic mechanism development at the University of Orléans. He is the author of more than 120 publications in peer-reviewed scientific journals.
He obtained the Research Excellence Award for high-impact scientific contributions in 2020 and was elected Fellow of the Combustion Institute for significant contribution to the experimental and modeling study of the combustion chemistry of oxygenated fuels in 2023.

Developing Detailed Chemical Kinetic Mechanisms for Fuel Combustion

Henry Curran

Combustion Chemistry Centre, University of Galway, Galway, Ireland

*Contact: henry.curran@universityofgalway.ie

Developing detailed chemical kinetic mechanisms, including their low-temperature chemistry is very complex requiring hundreds of species and thousands of reactions. In addition, the chemistries of alkanes, alkenes, alcohols and aldehydes show interdependent relationships, Fig. 1, and it is not usual for one chemical kinetic mechanism to be used to simulate all four types of fuels simultaneously. In order for a model to be proven reliable and chemically accurate it must be proven to be valid for all fuels by being able to simulate a wide range of experimental targets simultaneously.

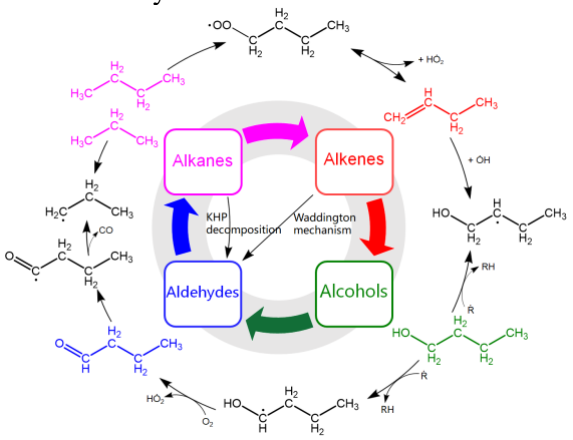

Figure 1: The inter-dependent relationship between the low-temperature chemistry of alkanes, alkenes, alcohols and aldehydes.

Moreover, the combustion community has been/is studying alternative fuels, including ammonia and this requires the development of an accurate chemical kinetic model describing its chemistry. The chemistry of ammonia (or any fuel) can be developed in a similar way to that of a hydrocarbon, Fig. 2, and their interaction chemistry can also be described. This presentation will open the discussion on the development of detailed chemical kinetic mechanisms, what we have learned, and what we can do to improve the mechanisms that we have.

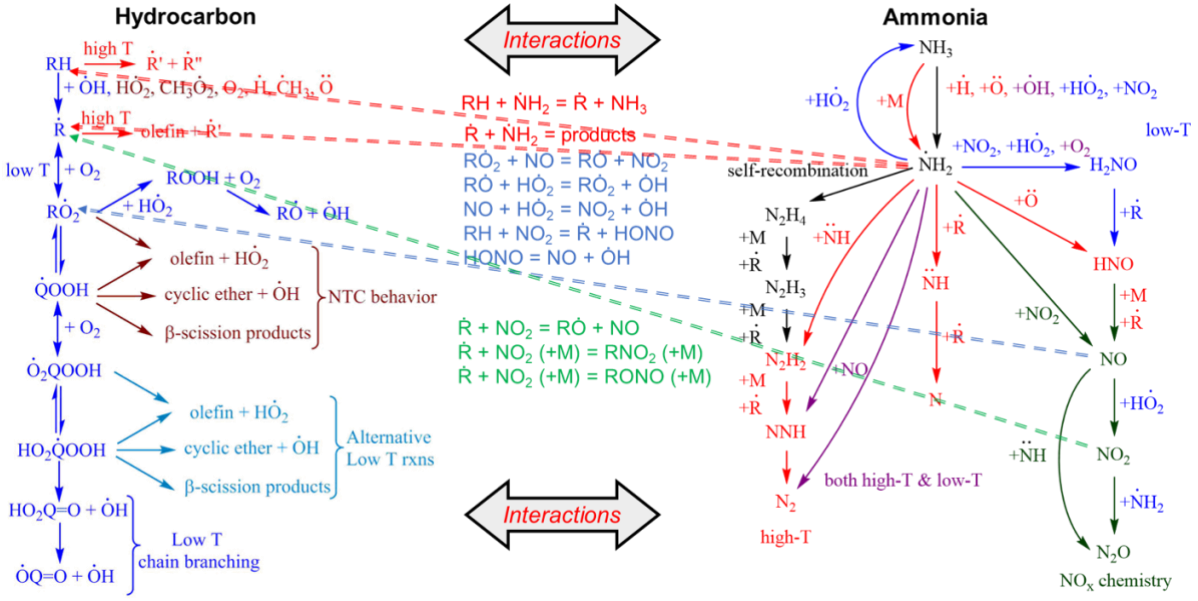

Figure. 2: The chemistry of ammonia is developed in a similar way to that of a hydrocarbon. Moreover, their interaction chemistry can be described in a general way.

Speaker Biography

Prof. Curran received his PhD degree in experimental and numerical studies of combustion kinetics from the University of Galway, Ireland in 1994 and a DSc degree by research from the National University of Ireland in October 2011. He is director of the Combustion Chemistry Centre and a member of the Board of Directors of the Combustion Institute. He is a member of the editorial board of Progress in Energy and Combustion Science and has served on the editorial boards of Combustion and Flame, the Proceedings of the Combustion Institute and Combustion Theory and Modeling. He is a founder member of the Irish Section of the Combustion Institute, a fellow of the Combustion Institute, the Institute of Chemistry of Ireland and the Royal Society of Chemistry. He was elected a member of the Royal Irish Academy in March 2015. He was awarded the Boyle-Higgins Gold Medal in Chemistry by the Institute of Chemistry of Ireland in April 2017 and the Yakov B. Zeldovich Gold Medal by the Combustion Institute in July 2022. He was given the Friendship Award of China in September 2025. He has been named by Clarivate Analytics as being among the top 1% of researchers cited in his field every year from 2014–2022, 2024 and 2025. He was appointed Chief Technical Advisor for Chemical Kinetic Modelling by Convergent Science in 2017. He has more than 35 years' experience in developing detailed chemical kinetic models to describe the combustion of hydrogen, syngas, hydrocarbon, ammonia and oxygenated hydrocarbon fuels.

Poster presentations

- Joint poster session and reception of the Pre-ISOC workshops - Saturday 25th July, 17.30-19.30
- Continue the discussion on Slack!

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FC3 | *Plasma-driven NH3 Reforming: Numerical and Experimental Analysis with Integrated CRDS* | Max Bernard, Brian C. Harrod, Galia Faingold, Si Shen, Victorien Blanchard, Nir Druker, Bret C. Windom, Azer P. Yalin, Joseph K. Lefkowitz

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FC6 | *An Exploration of Ignition Limits for High-speed Flight Applications* | Weronika Senior-Tybora, Si Shen, Joseph K. Lefkowitz

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FC8 | *The RMMD Schema for Improving the Findability, Accessibility, Interoperability and Reusability of Reaction Models* | Florian Solbach, Andreas V. Copan, Raymond Langer, Sanket Girhe, Heinz Pitsch, Luna Pratali Maffei, Sarah N. Elliot, Kai Leonhard

FC9 | *A Combined Ab Initio and Experimental Investigation of the Combustion Mechanism of Trimethyl Phosphite* | Timothée Fages, Axelle Le Cadre, René Fournet, Baptiste Sirjean, Olivia Venot, Pierre-Alexandre Glaude

FC10 | *Flame synthesis of iron-silica nanoparticles* | Munko Gonchikzhapov, Tina Kasper

FC11 | *Direct uncertainty quantification of high-dimensional combustion kinetic models through deep reinforcement learning* | Hao Hu, Peng Ma, Shumeng Xie, Mengjie Li, Christine Mounaïm-Rousselle, Huangwei Zhang

FC12 | *A review of the current PH3 decomposition mechanism* | Mats-Ole Dewerth, Munko Gonchikzhapov, Tina Kasper

FC13 | *Flame Temperature Measurement via Transient Thermocouple Junction Heating Analysis* | A. Wortmeier, M. Gonchikzhapov, T. Kasper

FC14 | *Development of a kinetic mechanism for trimethylphosphine: Ab initio calculations and experiment* | A. Le Cadre, O. Venot, B. Sirjean, R. Fournet, P.-A. Glaude

FC15 | *Potassium Radiative Emissions for Wildfire Detection: Developing a Path Toward Laser Heterodyne Radiometry* | Erin E McCaughey, Phillip R. Westmoreland, J. Houston Miller

FC16 | *Impact of chemical mechanisms on NH3/diesel dual-fuel combustion via two-zone model* | Salih Baykal, Sascha Jacobs, Torsten Methling, Andreas Huber, Markus Köhler

FC17 | *Kinetic Parameter Optimization of a Detailed NH3/H2 Combustion Mechanism Using Extensive Direct and Indirect Combustion Data* | A. G. Szanthoffer, M. Papp, T. Nagy, T. Turányi

FC18 | *A novel data consistency analysis for experimental laminar burning velocities of NH3-H2 mixtures for kinetic model validations* | Xinlu Han, Kaidi Wan, Tibor Nagy

FC19 | *From Fuel/O2 Oxidation to Fuel/CO2 Reforming: Plasma-Enabled Oxygen Transfer and Oxygenate Formation* | Haodong Chen, Zhaoying Li, Bin Yang

FC20 | *Combustion experimental data, reaction mechanisms, and computer codes for model analysis and development in the ReSpecTh Information System* | Tamás Turányi, István Gy. Zsély, Máté Papp, Tibor Nagy

FC1

Influence of CO_2 on Energy Deposition in Nanosecond Pulsed Discharges

Nicholas S. Dewey[1,*], Tanvir I. Farouk[1,2], Christopher B. Reuter[1]

[1]*Chemistry Division, U.S. Naval Research Laboratory, Washington, DC 20375, USA*

[2]*Department of Mechanical Engineering, University of South Carolina, Columbia, SC 29208, USA*

*Contact: nicholas.s.dewey.ctr@us.navy.mil

Keywords: Nanosecond discharge; plasma kinetics; non-equilibrium plasma; optical emission spectroscopy; plasma-assisted flow tube

Nanosecond repetitively pulsed discharges generate radicals and excited state species that accelerate gas-phase combustion kinetics and stabilize flames, which is important for mitigating some of the safety and operability issues faced by modern propulsion systems. For applications of these plasmas in engines, the electrodes are typically placed in the gas recirculation zone, where combustion products form due to efficient mixing of the fuel and oxidizer. Therefore, it is important to understand the impact of product formation on the discharge. The present work utilizes a plasma-assisted flow tube at atmospheric pressure to investigate the effect of CO_2 on nanosecond-pulsed discharges over a range of pulse repetition frequencies and electrode gap distances. Varying fractions of CO_2, from 0–50% in gas mixtures with N_2, are used to study the impact on energy per pulse and breakdown time of the plasma via measurements of voltage and current waveforms. Optical emission spectroscopy is also used to obtain temporally resolved temperatures of N_2. In addition, a trace amount (1%) of H_2 is added to the flow to obtain electron number densities via measurements of the H_α Balmer line. Negligible effects of CO_2 on energy per pulse and breakdown time are observed, and electron densities are typically within the uncertainty of the measurements. However, the presence of CO_2 in the mixture increases rotational and vibrational temperatures by up to ~50% at the time of breakdown. This result is supported by kinetic simulations showing that electronic excitation into the v = 0.083 eV vibrational state of CO_2 and the v = 0.29 eV states of CO_2 and N_2 occur on similar timescales at the E/N at breakdown, which enables rapid energy transfer between near-resonant vibrational modes. The results herein may be used to improve computational models of plasma-assisted combustion in practical reacting flows.

FC2

Characterizing Sustainable Aviation Fuels (SAFs) Using AI-Physics Hybrid Models

Qiren Zhu[1], Sirio Brunialti[2], Chuangchuang Cao[1], Qi Wang[1,*], S. Mani Sarathy[1,2]

[1]*Clean Energy Research Platform (CERP), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia*

[2]*Institute of Fluid Science, Tohoku University, 2-1-1 Katahira, Aoba, Sendai, Miyagi 980-8577, Japan*

*Contact email address: qi.wang@kaust.edu.sa

Keywords: FGMech; Lumped modeling; Real fuel combustion; Sustainable aviation fuels

Sustainable Aviation Fuels (SAFs) have emerged as promising for reducing greenhouse gas emissions from the aviation sector while maintaining compatibility with existing aircraft engines and fuel infrastructure. This study presents an AI-physics hybrid framework for characterizing SAF combustion using a functional-group-based approach for mechanism development (*i.e.*, FGMech). This approach combines physics-based combustion modeling with data-driven techniques to improve both predictive accuracy and computational efficiency. A key advancement of the present work is the enhancement of the underlying chemical kinetic mechanism through the incorporation of updated high-temperature reaction pathways and the addition of comprehensive low-temperature chemistry. The improved high-temperature chemistry enables more accurate prediction of ignition delay times, premixed flame propagation, and species evolution under elevated-temperature, non-diluted conditions relevant to gas turbine operation. Meanwhile, the newly integrated low-temperature chemistry captures fuel oxidation pathways that govern ignition characteristics in intermediate and low-temperature regimes, extending the applicability of the model to a wider range of combustion environments. The AI component is trained on datasets generated from the enhanced FGMech framework, allowing rapid prediction of real fuels using their functional group distributions without the need for surrogate model development. Model validation against available experimental measurements demonstrates improved agreement across multiple operating conditions, including ignition delay, flame propagation, and major species concentrations. Overall, the proposed AI-physics hybrid FGMech framework provides a robust and computationally efficient tool for evaluating the combustion performance of emerging SAF formulations. The methodology supports accelerated fuel screening, mechanism development, and the design of next-generation low-emission aviation propulsion systems, contributing to the broader transition toward sustainable aviation.

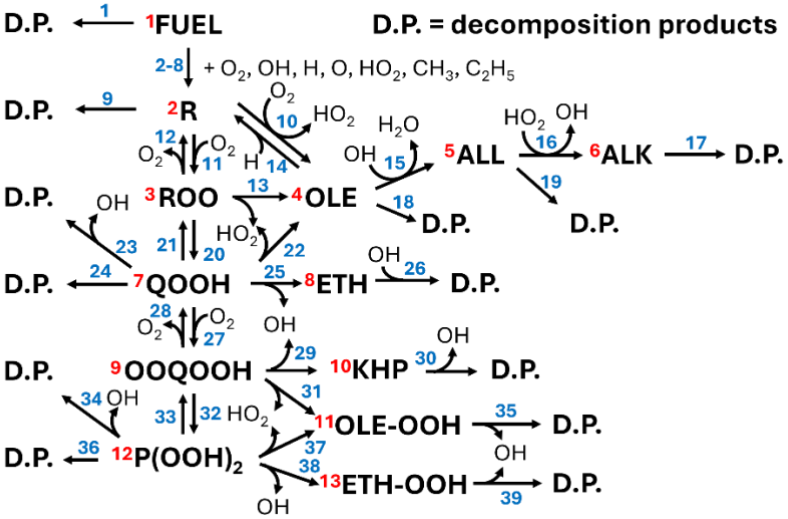

Figure 1: Structure of the low-temperature FGMech sub-mechanisms. Species numbered in red; reactions numbered in blue. Decomposition products are exclusively species from the base mechanism.

FC3

Plasma-driven NH_3 Reforming: Numerical and Experimental Analysis with Integrated CRDS

Max Bernard[1*], Brian C. Harrod[2], Galia Faingold[3], Si Shen[1], Victorien Blanchard[2], Nir Druker[1], Bret C. Windom[2], Azer P. Yalin[2], Joseph K. Lefkowitz[1]

[1]*The Stephen B. Klein Faculty of Aerospace Engineering, Technion – Israel Institute of Technology*

[2]*Department of Mechanical Engineering, Colorado State University*

[3]*CAPS Laboratory. Department of Mechanical and Process Engineering, ETH Zurich*

*Contact: max.bernard@campus.technion.ac.il

Keywords: Plasma-assisted combustion; Plasma reforming; NH_3 oxidation, Cavity ring-down spectroscopy, NH_2 radical

In this work, two stirred plasma reactors are utilized to provide a characterization of NH_3 plasma-reforming and oxidation in terms of gas temperature (T_{gas}) and species distribution measurements. One reactor was designed with optical access for optical emission spectroscopy (OES) to quantify the rotational temperature of the N_2 second positive system and another in-situ detection of radical species (NH_2) via cavity ring-down spectroscopy (CRDS). The exhaust species distribution was characterized in terms of the NH_3 conversion and the H_2 yield by Fourier transform infrared (FTIR) spectroscopy and gas chromatography with a thermal conductivity detector (GC-TCD), respectively. By combining these techniques with simulated results from plasma-gas kinetic modeling, valuable insight of the chemical mechanism driving plasma-assisted NH_3 cracking and oxidation was gained. Transient NH_2 measurements and model comparison demonstrate accurate prediction of formation and consumption timescales in a pure NH_3 plasma. Ex-situ speciation of a range of gas mixtures, including pure NH_3, N_2-diluted, and air-diluted formulations, revealed unique reaction pathways. For air-diluted mixtures, oxidation reactions are shown to significantly dominate NH_3 consumption pathways, particularly in lean warm-temperature plasmas, whereas in N_2-diluted mixtures H_2 yields are optimized, particularly in highly diluted cases or with maximized specific energy input.

FC4

Seeing the Unseen: Isomer-Resolved Intermediates in C_8 *Iso*-Alkane Oxidation observed by FTIR-MBMS

M. Groß[1*], T. Bierkandt[1], S. Schmitt[1], N. Gaiser[1], A. Huber[1], M. Köhler[1]

[1]*Institute of Combustion Technology, German Aerospace Center (DLR), Pfaffenwaldring 38-40, 70569 Stuttgart, Germany*

*Contact: melena.gross@dlr.de

Keywords: FTIR spectroscopy, laminar flow reactor, iso-alkanes, molecular-beam mass spectrometry, isomer separation

Understanding the reaction pathways of renewable synthetic fuels is essential for optimizing combustion processes, predicting emissions and assessing their environmental impact. *Iso*-alkanes form key hydrocarbon intermediates that often occur as structural isomers that cannot be distinguished by conventional mass-based diagnostics. To address this challenge, an electron-ionization molecular-beam mass spectrometry (EI-MBMS) system was combined with FTIR spectroscopy to enable isomer-resolved measurements.

A systematic investigation of five C_8 *iso*-alkanes (2-methylheptane, 3-methylheptane, 2,4-dimethylhexane, 2,5-dimethylhexane, and 2,3,4-trimethylpentane) was performed in a laminar tubular quartz flow reactor with a linear temperature ramp from 1223 to 773 K, corresponding to residence time of 1.7 s - 2.7 s. Fuel-oxidizer mixtures diluted with 99% argon were analyzed using EI-MBMS (nominal ionization energy of 13.5 eV). Reaction products and intermediates were sampled at the reactor outlet, rapidly quenched, and detected by reflectron TOF-MS. In parallel, FTIR spectra were recorded between 800 and 4000 cm^{-1} with 0.5 cm^{-1} resolution and quantified using a commercial reference spectra database (Bruker). Measurement uncertainties of species mole fractions were estimated at 20-30% for both techniques.

FTIR spectroscopy enabled the identification and quantification of individual C_4H_8 isomers during the oxidation of the investigated fuels, even near detection limits. The summed mole fractions of the C_4H_8 isomers obtained from FTIR showed excellent agreement with the total C_4H_8 mole fraction measured by EI-MBMS, demonstrating the consistency of the combined approaches using the two complementary techniques (see Fig. 1).

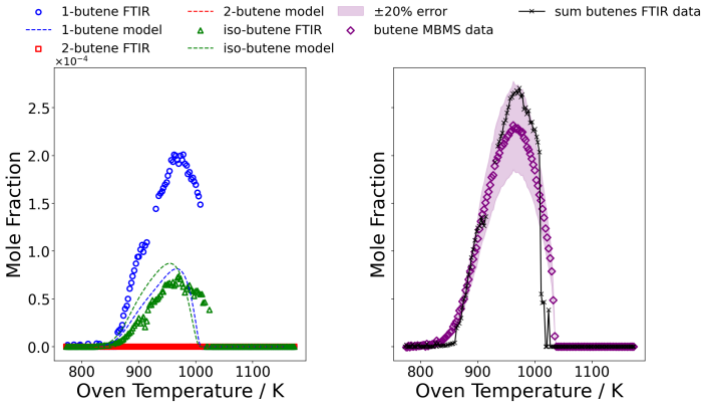

Fig 1. FTIR data showing the resolved C_4H_8 isomers from the rich oxidation (Φ = 1.5) of 2-methylheptane in comparison with the kinetic model from Sarathy et al.[1] (left) and the summed up resolved isomers in comparison to MBMS data (right).

Current work extends this methodology to C_3H_4 isomers and other smaller reaction intermediates to investigate the formation of small intermediates. Their conversion through propargyl recombination to benzene is examined to establish links between fuel structure, aromatic formation, and soot propensity.

The combined FTIR-MBMS methodology provides complementary, isomer-resolved information on combustion chemistry and generates high-quality data for validating and improving predictive combustion models.

FC5

Hypergolic ignition of sodium borohydride-polyethylene fuel under hydrogen peroxide sprays

Saar Levi[1], David Peles[1], Keren Mizrahi[1], Syamantak Nath[2], Joseph K. Lefkowitz[1*]

[1]*Stephen B. Klein Faculty of Aerospace Engineering, Technion - Israel Institute of Technology, Haifa, Israel*
[2]*Letara Ltd., Sapporo, Hokkaido, Japan*

*Contact: saar.levi@campus.technion.ac.il

Keywords: Hypergolic; hydrogen peroxide; hybrid rocket; high-density polyethylene

Hypergolic propellants are defined by their ability to ignite immediately upon contact, resulting in rapid exothermic reactions occurring without the need for an external ignition source. In hybrid rocket engines, this spontaneous reaction simplifies thruster management, reduces system mass, and enables engine re-ignition. The present research investigates hypergolic ignition using a propellant combination of high-density polyethylene (HDPE) fuel embedded with sodium borohydride (SBH) additive, with rocket-grade hydrogen peroxide (RGHP) as the oxidizer. This HDPE-SBH-RGHP system offers a "green" propellant option, which is a less toxic alternative to traditional, highly hazardous hypergolic propellants, enhancing operational safety and reducing production costs. Our experimental framework utilizes spray ignition tests designed to emulate the operational environment of a hybrid rocket motor. This approach provides foundational data on the interaction between multiple ignition points, the dynamics of flame propagation, and the fuel's response to a continuous oxidizer supply. The primary focus is on the critical influence of pressure as a key condition governing the initiation and sustainment of hypergolic reactions. The investigation confirms that the initial pressure and the O_2/N_2 ratio are the primary factors determining the ignition threshold. While success is consistent above 5 bar (with 2 bar marking a critical 50% probability), ignition at atmospheric pressure was only achieved by increasing the O_2 concentration to 35%. Furthermore, this high initial pressure not only enables ignition but also promotes superior flame stability, resulting in more robust heat release compared to lower-pressure cases. Other operational configurations were also explored, including sample exposure to humidity, sample orientation with respect to oxidizer flow direction, liquid accumulation on the fuel surface, and potential for re-ignition. It is concluded that the reliability of ignition in hypergolic solid fuels is a strong function of the initial conditions in the reactor, even for highly reactive propellant combinations.

FC6

An Exploration of Ignition Limits for High-speed Flight Applications

Weronika Senior-Tybora[1*], Si Shen[1], Joseph K. Lefkowitz[1]

[1]*The Stephen B. Klein Faculty of Aerospace Engineering*
Technion – Israel Institute of Technology, 32000 Haifa, Israel

*Contact: weronikatybora@campus.technion.ac.il

Keywords: Plasma-assisted combustion; Ignition; High-speed propulsion; Minimum Ignition Energy

Ignition in high-speed systems faces significant challenges due to the brief gas residence time within the combustion chamber, where high velocity and turbulence can easily extinguish the ignition kernel. This is particularly problematic for ramjet or scramjet engines during cold-starts and for turbofan engines at high altitudes. The nanosecond-pulsed high-frequency discharge (NPHFD) ignition technique addresses these issues by enabling precise control over pulse repetition frequency, pulse number, and energy per pulse, thereby influencing total discharge energy and duration. This study explores the effects of NPHFD on ignition in flowing ethylene–air mixtures under simulated aerospace conditions, with a focus on scramjet cavity cold-starts. We assessed ignition probability across various initial temperatures (20 - 300°C), velocities (10 - 140 m/s), equivalence ratios (0.2 - 0.6), pulse repetition frequencies (1 - 200 kHz), and pulse numbers (2 - 100). High-speed infrared and Schlieren imaging systems captured kernel development. Results indicated that higher temperatures and pulse repetition frequencies significantly enhance ignition probability. Conversely, increased velocity suppresses ignition, resulting in narrower ignition limits than in quiescent or low-speed flows. Interestingly, larger kernels formed with higher velocities, suggesting a trade-off between ignition probability and kernel growth. Analysis of pulse coupling showed that the total deposited energy has a secondary effect on ignition. In contrast, the primary parameter influencing its success is energy efficiency for ignition, which defines the number of pulses coupled into a single kernel. Energy efficiency for ignition increased with higher pulse repetition frequency and showed a minor effect on the equivalence ratio. Comparisons to recent ignition studies in scramjet cavity flame-holders showed that our tunnel conditions offered higher ignition probabilities, likely due to reduced local turbulence near the igniter, which aids kernel stabilization.

FC7

Experimental and Numerical Study of Rich–quench–lean Combustion of Methane–hydrogen Blends in a Micro-Turbine Combustor

Guguloth Mahesh Nayak[1], Silky Elanjickal[1], Lev Filimonov[1], Salmon Nabwani[1], Beni Cukurel[1], and Joseph K. Lefkowitz[1]

[1]*Stephen B Klein Faculty of Aerospace Engineering, Technion, Haifa, Israel, 3200003*

*Contact: gmaheshnayak@campus.technion.ac.il

Keywords: Hydrogen combustion, Rich-quench-lean combustion, Micro gas turbine, chemical reactor network, Methane-hydrogen blends

This study presents an experimental and computational investigation of a Rich-Quench-Lean (RQL) combustor operating on methane-hydrogen (CH_4/H_2) fuel blends across hydrogen volumetric fractions of 0–100%. The work addresses the need for fuel-flexible combustion systems compatible with low-carbon energy transition, with particular focus on the development and validation of a chemical reactor network (CRN) as a cost-effective predictive tool, complemented by 3D LES-CFD for high-fidelity flow field characterization.

Experiments were conducted at atmospheric pressure with elevated inlet air temperatures (473, 573, and 673 K), varying hydrogen content and global air-fuel equivalence ratio. NO_x emissions remained below 15 ppm across the operational envelope, attributed to effective quench-zone air mixing suppressing stoichiometric pocket formation under varied preheated air, hydrogen fraction, and part-load modulation. CO showed stronger sensitivity to operating point, reflecting competing effects of residence time and reaction temperature on carbon burnout. These measurements provided the validation dataset for both computational approaches.

The CRN was constructed to represent the RQL zone architecture using Perfectly Stirred Reactors (PSRs) and Plug Flow Reactors (PFRs) (Fig.1). Fuel-air mixing non-uniformity in the rich primary zone was captured through a Gaussian distribution of five parallel PSRs, each operating at a distinct local equivalence ratio, replicating spatial inhomogeneity without the computational cost of full CFD. CRN predictions demonstrated close agreement with experimental NO_x and CO measurements across all CH_4/H_2 blends. Complementarily, CRN predicted pollutant emission corroborates with CFD, carried out at full-scale operating conditions of 965 K and 3.15 bar

Kinetic mechanism evaluation revealed that GRI 3.0 systematically overpredicts NO_x relative to dedicated nitrogen combustion chemistry, highlighting the importance of mechanism selection for hydrogen-enriched flames. Together, the validated CRN and LES-CFD form a complementary multi-fidelity framework for the design of low-NO_x RQL combustors in hydrogen-blended gas turbine applications

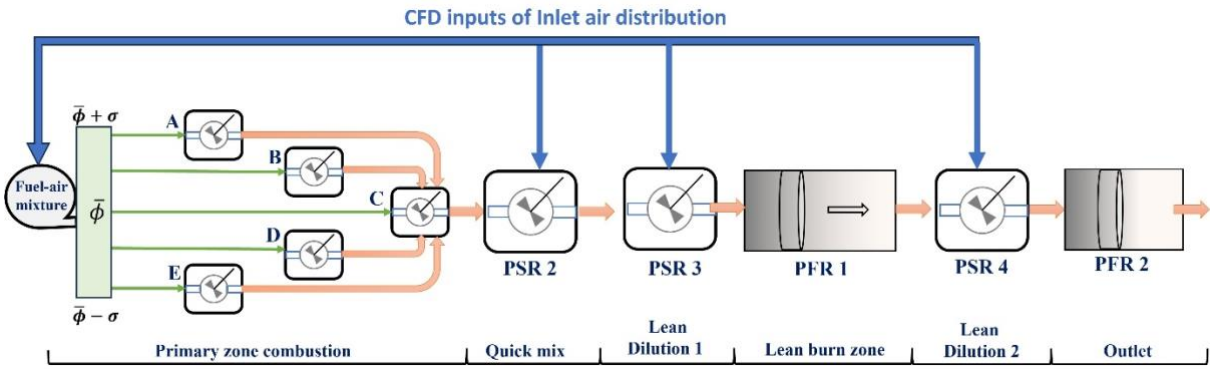

Fig.1 Schematic of chemical reactor network representing RQL architecture.

FC8

The RMMD Schema for Improving the Findability, Accessibility, Interoperability and Reusability of Reaction Models

Florian Solbach[1], Andreas V. Copan[2,3], Raymond Langer[4], Sanket Girhe[4], Heinz Pitsch[4], Luna Pratali Maffei[5], Sarah N. Elliot[6], Kai Leonhard[1]

[1]*Institute for Technical Thermodynamics, RWTH Aachen University*

[2]*College of Engineering, University of Georgia*

[3]*Department of Chemistry, University of Georgia*

[4]*Institute for Combustion Technology, RWTH Aachen University*

[5]*Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta", Politecnico di Milano*

[6]*Argonne National Lab*

*Contact: Kai.Leonhard@LTT.RWTH-Aachen.de

Keywords: FAIR, reaction model, meta data, database, potential energy surface

As discussed during the last Flame Chemistry Workshop in Milano, the FAIR (Findable, Accessible, Interoperable, and Reusable) publication of reaction mechanisms is challenging because of diverse requirements from theoreticians, experimentalists, and modelers. Based on this initial discussion, we held several meetings with interested researchers and identified main objectives, and have started their implementation in the "Reaction Model MetaData format", RMMD (https://git-ce.rwth-aachen.de/ltt/reaction-model-metadata/). RMMD is a YAML-based file format designed to help researchers add meaningful and detailed metadata to their reaction models, quantum chemistry data, rate constant parameters, etc., to facilitate reuse and improve machine-readability, e.g., for machine-learning applications.

Main objectives of RMMD are:

- Species identification and their relation to the potential energy surface: Species and reactions in chemical kinetics models are usually identified by names such as "CHFCHCF3", which are not always sufficient to identify the intended chemical species. RMMD associates the species name with canonical and machine-readable identifiers, making it easy to find appropriate parameters in a model for humans and for databases that pull data from publications, such as the NIST Chemical Kinetics Database (https://kinetics.nist.gov/kinetics/), for combustion and beyond.
- Support diverse data: RMMD supports empirical parameters as well as quantum-chemistry data, the latter of which is often used to obtain the former.
- Provenance: Every parameter should remain traceable to its primary source, including the original method and any subsequent modifications, or, where this is not possible, the reasoning behind the chosen parametrization must be documented. RMMD allows for providing detailed provenance through literature references and by linking empirical parameterizations to quantum chemistry calculations.
- Many more: declaring a data usage license, specifying thermodynamic reference states, ...

With this poster, we present more details on the concept and the current implementation status of RMMD.

FC9

A Combined Ab Initio and Experimental Investigation of the Combustion Mechanism of Trimethyl Phosphite

Timothée Fages[1*], Axelle Le Cadre[2], René Fournet[1], Baptiste Sirjean[1], Olivia Venot[2], Pierre-Alexandre Glaude[1]

[1] Université de Lorraine, CNRS, LRGP, 54000 Nancy, France
[2] Université Paris Cité and Univ Paris Est Creteil, CNRS, LISA, F-75013 Paris, France
timothee.fages@univ-lorraine.fr

The combustion of organophosphorus compounds is crucial for understanding their role as flame retardants, as well as their behavior in battery fire, or during the destruction of pesticides and chemical agents. While pentavalent organophosphorus compounds have been extensively studied, trivalent species remain under-investigated due to their lower stability.

In most mechanisms involving pentavalent organophosphorus compounds, trivalent species larger than CH_3OPO are rarely considered (e.g., Jayaweera et al. [1]). However, Kanayama et al.'s study [2] on trimethyl phosphate (TMP) revealed that, at low temperatures, the primary unimolecular decomposition of TMP produces a trivalent species, $P(OH)(OCH_3)_2$, one that is typically not included in reaction mechanisms. The lack of research on trivalent systems means that such reactions are often overlooked. Incorporating these species would require not only adding the species to the mechanism but also detailing all related decomposition reactions, even in the absence of literature. Additionally, the reactivity of trivalent organophosphorus compounds differs so significantly from pentavalent ones that direct analogies cannot be drawn between their mechanisms.

To address this gap, our study focuses on the decomposition of trimethyl phosphite (TMPI), as a model molecule of trivalent species, for which no kinetic mechanism has yet been reported. The species and reaction pathways identified in its mechanism may provide insights that help connect trivalent and pentavalent organophosphorus chemistry.

A kinetic mechanism was constructed based on ab initio calculations made at the QCISD(T)/cc-pv∞z//B2PLYPD3/6-311+g(2d,d,p). Rate constants were derived from transition state theory, and master equation simulations with the Master Equation System Solver (MESS) when pre-reaction complexes were observed. Variational Reaction Coordinates Transition State Theory was also used to evaluate the rate constant of some combination reactions. Ignition delay times of $TMPI/O_2/Ar$ and $CH_4/TMPI/O_2/Ar$ mixtures were measured in a shock tube under 7 and 9 bars between 1400 and 1800 K in stoichiometric conditions in order to validate the new mechanism.

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FC10

Flame synthesis of iron-silica nanoparticles

Munko Gonchikzhapov[1], Tina Kasper[1]

[1]*Technical Thermodynamics, Paderborn University, Paderborn 33098, Germany*

*Contact: munko@mail.uni-paderborn.de

Keywords: flame synthesis, multiple complex nanoparticles, flame structure

Multicomponent nanoparticles form new unique structures with synergistic functionality, which allow them to perform multiple tasks simultaneously. Flame synthesis is one of the most effective methods for producing nanoparticles. The synthesis of iron and silicon nanoparticles is well studied individually. However, fundamental knowledge of iron-silica nanoparticles synthesis is still not sufficiently represented in literature. In this study, the chemical and thermal structure of a hydrogen flame doped with iron pentacarbonyl (IPC) and tetramethyl silane (TMS) was investigated.

The premixed laminar hydrogen flame (φ=0.6) is stabilized on a sintered bronze matrix. For the flame dopped with one additive, the additive mole fraction is 600 ppm, for the mixture doping is IPC – 600 ppm, TMS – 300 ppm. Distribution of species in the flames was measured using mass-spectrometry. Temperature distribution was measured with a type R thermocouple, coated with SiO_2. A quartz crystal micro balance (QCM) setup was used to investigate particle formation in the gas phase. The morphology of the nanoparticles was determined using transmission electron microscopy (TEM).

QCM measurements show fundamentally different behaviors of solid phase formation in individual flames of the precursors and in the flame of the mixture. In a single-precursor flame, two solid-phase formation zones are observed: the near zone and the far zone. In a mixture flame, there is only one large, broad zone. Mass spectrometric measurements showed that in the mixed flame, the reaction zone for IPC and TMS is significantly wider than in the individual flames. At the same time, significant hydrogen unburned amount is observed despite the sufficient presence of oxygen. TEM analysis of the nanoparticles indicates that the smallest particles are found in IPC doped flame. The average particle size was 2–4 nm. When TMS is added to the IPC, the particles grow to a size of 10–20 nm.

FC11

Direct uncertainty quantification of high-dimensional combustion kinetic models through deep reinforcement learning

Hao Hu[1,2], Peng Ma[2], Shumeng Xie[1], Mengjie Li[1], Christine Mounaïm-Rousselle[3], Huangwei Zhang[1,2,*]

[1]*Department of Mechanical Engineering, National University of Singapore, 9 Engineering Drive 1, Singapore 117575, Republic of Singapore*

[2]*Centre for Hydrogen Innovations (CHI), National University of Singapore, 1 Engineering Drive 3, Singapore 117580, Republic of Singapore*

[3]*Université Orléans, INSA CVL, PRISME, UR4229, Orléans, France*

*Contact: mpezhu@nus.edu.sg

Keywords: Combustion kinetics; Ammonia combustion; Uncertainty quantification; Deep reinforcement learning; Transfer learning

Accurate uncertainty quantification (UQ) of combustion kinetic models is challenging due to the nonlinear, high-dimensional nature of reaction mechanisms and the presence of uncertainty in experimental measurements. Conventional UQ approaches often rely on pre-trained surrogate models and sampling-based inference that introduce additional approximation errors and computational costs. To address these limitations, a deep reinforcement learning (DRL)-based UQ framework is proposed, which learns a direct mapping from uncertain experimental targets to optimal reaction rate parameters that minimize the model error with respect to the targets. The framework employs a neural network trained to minimize a group-based error metric between kinetic model predictions and experimental targets while respecting prescribed experimental uncertainty bounds, thereby avoiding reliance on pre-trained surrogate construction and extensive Monte Carlo sampling. The method is applied to an ammonia combustion mechanism and benchmarked against a surrogate-assisted genetic algorithm and a Bayesian UQ approach. Results show that the DRL-based framework achieves faster convergence, lower nominal model error, and reduced variability across independent runs under a fixed kinetic simulation budget, while producing posterior ensembles that remain largely confined within experimental uncertainty ranges and exhibit scalable behavior under tightened confidence levels. Furthermore, by leveraging transfer learning, the trained DRL policy can be efficiently adapted to new experimental datasets at different operating conditions, with significantly accelerated retraining efficiency and improved accuracy compared to training from scratch. These findings demonstrate that DRL-based UQ provides an accurate, sample-efficient, and adaptable alternative for complex combustion kinetic systems.

FC12

A review of the current PH_3 decomposition mechanism

Mats-Ole Dewerth[1], Munko Gonchikzhapov[1], Tina Kasper[1]

[1]*Technical Thermodynamics, Paderborn University, 33098 Paderborn, Germany*

*Contact: mats.ole.dewerth@mail.uni-paderborn.de

Keywords: phosphine, kinetics, chemiluminescence, phosphorus oxides

Phosphorus is an essential building block of life, and phosphorus recovery from waste streams such as sewage sludge is gaining importance. Since sewage sludge is often utilized thermally and thermal recovery processes are still being developed, a closer look at the kinetics of phosphorus species in the gas phase is warranted.
Phosphine, or PH_3, is the simplest gaseous phosphorus species and can serve as a stand-in for more complex species in experiments. Its decomposition mechanism has not been examined closely and the current mechanism is mostly based on the research of Norrish, Hamilton and Murrells, suggesting reactions analogous to NH_3.
Initial experiments using a plug flow reactor (PFR) show that PH_3 reacts at far lower temperatures than expected. CHEMKIN simulations fail to simulate reactions below 700°C. Mass spectrometric measurements of a reactive flow consisting of PH_3, NH_3, O_2 and H_2, highly diluted by Ar show that PH_3 rapidly decomposes between roughly 200°C and 300°C. Main reaction pathways of PH_3 decomposition suggest O, OH and H as reaction partners. The low temperatures at which PH_3 reacts and where we do not expect strong radical formation indicate either missing reaction pathways with elemental H_2 and O_2, or catalytic effects taking place. Further PFR experiments with an optical spectrometer using only PH_3, H_2 and O_2 show the characteristic signal of phosphorus chemiluminescence at temperatures around 400°C (see Fig. 1). The reaction pathways in the current mechanism fail to account for the proposed chemiluminescence pathways of phosphorus species: PO + O → PO_2 and HPO + O → HOPO.

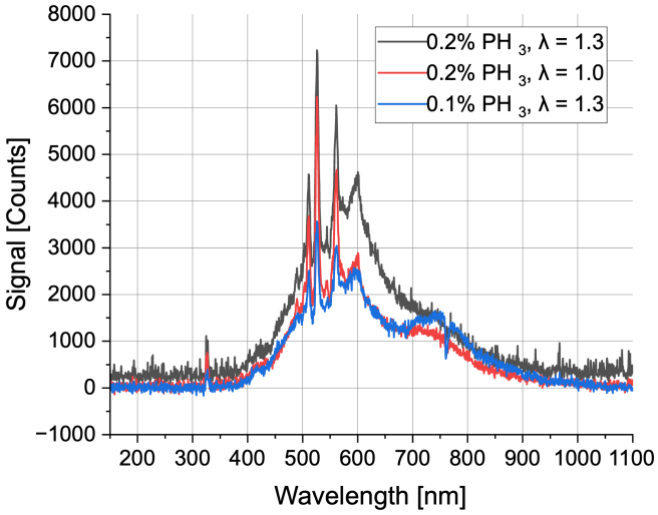

Fig. 1: Chemiluminescence signal of phosphorus species

FC13

Flame Temperature Measurement via Transient Thermocouple Junction Heating Analysis

A. Wortmeier*, M. Gonchikzhapov, T. Kasper

Technical Thermodynamics, Paderborn University, Paderborn, Germany

*Contact: andreas.wortmeier@uni-paderborn.de

Keywords: combustion; temperature; measurement; thermocouples; flame

Flame temperature is one of the most important quantities for kinetic simulations of flames and must be measured with high accuracy even in challenging flame conditions.

Thermocouples provide a simple and robust means of measuring flame temperatures and are often preferred over optical diagnostics in challenging combustion environments, particularly when particle formation occurs. However, at the high temperatures encountered in combustion processes, thermocouples lose a significant fraction of the absorbed heat through thermal radiation, causing the measured temperature to underestimate the actual gas temperature. Accurate radiation correction therefore requires knowledge of both the flow conditions surrounding the thermocouple and its emissivity.

Protective coatings are commonly applied to suppress catalytic surface reactions that may distort temperature measurements. In addition, such coatings modify the emissivity of the thermocouple and can extend its operating range to gas temperatures exceeding the melting point of the thermocouple material. An alternative approach for measurements under these extreme conditions is to expose the thermocouple to the flame onlybriefly, preventing it from reaching thermal equilibrium with the hot gases. In this case, the challenge lies in determining the flame temperature from the transient heating response of the thermocouple junction.

This study compares these different approaches for gas temperature determination in a model flame and discusses methods for evaluating transient thermocouple measurements. The setup is shown below in figure 1.

Figure 1: Burner with glowing thermocouple.

FC14

Development of a kinetic mechanism for trimethylphosphine: *Ab initio* calculations and experiment

A. Le Cadre[1], O. Venot[1], B. Sirjean[2], R. Fournet[2], P.-A. Glaude[2]

[1] *Université Paris Cité and Univ Paris Est Creteil, CNRS, LISA, F-75013 Paris, France*
[2] *Université de Lorraine, CNRS, LRGP, F-54000 Nancy, France*

The combustion of organophosphorus compounds is of particular interest due to their wide range of applications, such as in pesticides, batteries, flame retardants and the destruction of chemical weapons [1, 2]. Compared to the mechanisms governing hydrocarbons, there is far less research on the mechanisms of organophosphorus compounds. In fact, the current mechanisms reported in the literature stem mainly from the work of Jayaweera et al. [3] dating from 2005 and building on earlier work by Twarowski [4], Glaude [5] and Korobeinichev [6]. In recent years, numerous studies have been conducted on various pentavalent organophosphorus compounds such as dimethyl methylphosphonate (DMMP) [7,8], trimethylphosphonate (TMP) [9], diisopropyl Methylphosphonate (DIMP) [10,11], diethyl methylphosphonate (DEMP) [11] and triethyl phosphate (TEP) [11,12] . However, trivalent organophosphorus compounds such as trimethylphosphine and trimethyl phosphite (TMPi) have been overlooked despite their promising properties as additives in batteries or flame retardants.

In this work, we therefore aim to develop a first kinetic mechanism for trimethylphosphine based on quantum chemistry methods. The thermodynamic properties are calculated at the QCISD(T)/∞Q(Z)//B2PLYPD3/6–311+G(2d,d,p) level. The contribution of hindered rotors was included with the 1D-HR-U approach. The rate constants were determined at the QCISD(T)/∞Q(Z)//B2PLYPD3/6–311+G(2d,d,p) level and we solved the master equation using the MESS [13] code. The mechanism has been validated using experimental data obtained from shock tube measurements. The experiments were conducted in a mixture of 3.65% CH_4, 7.3% O_2, 0.375% trimethylphosphine and 88.675% argon at pressures between 6.5 and 8.5 bar.

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FC15

Potassium Radiative Emissions for Wildfire Detection: Developing a Path Toward Laser Heterodyne Radiometry

Erin E McCaughey[1], Phillip R. Westmoreland[2], J. Houston Miller[1]

[1] George Washington University, [2] North Carolina State University

*Contact: houston@gwu.edu

Keywords: wildfire, heterodyne, potassium

Optical techniques for fire detection have evolved from simple visual observation to more advanced hyperspectral imaging systems, yet there remains a need for compact, selective and field-deployable tools capable of quantifying and characterizing both intensity and spectral signatures of flames. George Washington University is developing a novel approach to characterizing wildfires that leverages spectral emissions from potassium, a key tracer of flaming biomass combustion, based on laser heterodyne radiometry. This contribution focuses on the development and testing of this technique in a model, laboratory system using both absorption spectroscopy to profile $^2S_{1/2}$ ground state potassium and emission spectroscopy for the $^2P1/2$ excited state, both monitored at 769.9 nm. To interpret the signals, we are also modeling potassium chemistry by following reaction paths along diffusive trajectories in the flame.

Preliminary profiles for potassium ground state concentrations show that atomic potassium occurs where the diffusive trajectories approach the high-temperature reaction zone rich in H-atom, O-atom, and hydroxyl radical, are known to be present in super-equilibrium concentrations (Smyth et al., 1990). QC results suggest that exothermic reactions involving intermediate potassium species (notably KO·.) may directly form potassium atoms in the excited $^2P_{1/2}$ state.

FC16

Impact of chemical mechanisms on NH3/diesel dual-fuel combustion via two-zone model

Salih Baykal*, Sascha Jacobs, Torsten Methling, Andreas Huber, Markus Köhler

German Aerospace Center (DLR), Institute of Combustion Technology, Stuttgart

*Contact: salih.baykal@dlr.de

Keywords: Ammonia, Diesel, Internal combustion engine, Applied simulation, Modeling

The reduction of greenhouse gas emissions in the transport sector demands climate neutral solutions e.g. by the use of sustainable fuels. Promising alternative candidates to replace fossil diesel (B0) are ammonia (NH_3) and biodiesel (B100). Their implementation in transport applications requires an accurate understanding of their implications on combustion and emission characteristics in engines. In this study, the impact of chemical kinetic mechanisms on the combustion and emission behavior of NH_3/B0 and NH_3/B100 dual-fuel operation is investigated using a newly developed quasi-dimensional two-zone model.

This study investigates four distinct use cases across two engine configurations [1, 2] (large and small diesel engine): pure B0, pure B100, and their respective dual-fuel combinations with NH_3. Numerical results of different NH_3/NO_x sub-mechanisms [3-5] from the literature are compared in terms of in-cylinder pressure histories and NO_x emissions. The results reveal that for the pure B0 baseline the choice of chemical kinetic mechanism yields no notable differences in emission predictions exclusively. In contrast, significant discrepancies in emission modeling emerge in all other cases. For the pure B100 baseline, variations exist among the mechanisms due to the fuel chemistry, while the introduction of ammonia in both dual-fuel configurations leads to highly divergent NO_x emission pathways. To identify the underlying chemistry, sensitive reaction pathways responsible for NO_x formation and consumption are thoroughly investigated by means of a rate of progress (ROP) analysis to isolate the specific elementary steps driving the observed kinetic discrepancies.

Demonstrating its capability to reliably represent engine-relevant boundary conditions, the deployed two-zone model serves as an efficient tool for mechanism testing and comparison. The analysis underscores how heavily emission modeling in applied combustion systems depends on the selection and formulation of specific chemical kinetic (sub-)mechanisms. These findings highlight the necessity of validating chemical mechanisms within applied simulations to ensure accurate emission predictions for future low-carbon powertrains.

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FC17

Kinetic Parameter Optimization of a Detailed NH_3/H_2 Combustion Mechanism Using Extensive Direct and Indirect Combustion Data

A. G. Szanthoffer[1,2,*], M. Papp[1], T. Nagy[3], T. Turányi[1]

[1] *Institute of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary*
[2] *Hevesy György PhD School of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary*
[3] *Institute of Materials and Environmental Chemistry, HUN-REN Research Centre for Natural Sciences, Budapest, Hungary*

*Contact: andras.gyorgy.szanthoffer@ttk.elte.hu

Keywords: ammonia combustion, carbon-free fuel, renewable energy, detailed kinetic mechanism, parameter optimization

Ammonia (NH_3) is a promising carbon-free fuel that has attracted growing interest as a sustainable energy carrier. However, its combustion characteristics are less favorable than those of hydrocarbons. NH_3 is therefore often blended with hydrogen (H_2) or partially cracked to generate H_2 in situ, improving fuel reactivity. The development of ammonia-fueled combustion devices requires accurate chemical kinetic models reliably predicting the combustion behavior of NH_3/H_2 mixtures. This work presents an optimized NH_3/H_2 combustion mechanism designed to reproduce experimental data more accurately than previously published models.

The starting mechanism was derived from the NUIG-2024 mechanism [1] by modifying selected rate parameters and introducing realistic NH_3 third-body efficiencies (TBEs). Optimization was performed by minimizing a mean-squared objective function using both direct rate coefficient measurements and indirect combustion data. The indirect data include ignition delay times, laminar burning velocities, and species concentration measurements from homogeneous reactors. Comprising 7,259 data points from 578 data series, this is, to our knowledge, the largest indirect NH_3/H_2 combustion data collection used for mechanism development. The optimized parameters included the Arrhenius (A, n, E) parameters of 25 reaction rate coefficients and the NH_3 TBE for the H + O_2 (+M) = HO_2 (+M) reaction. All parameters were constrained within prior uncertainty bounds derived from direct measurements and previous optimization studies.

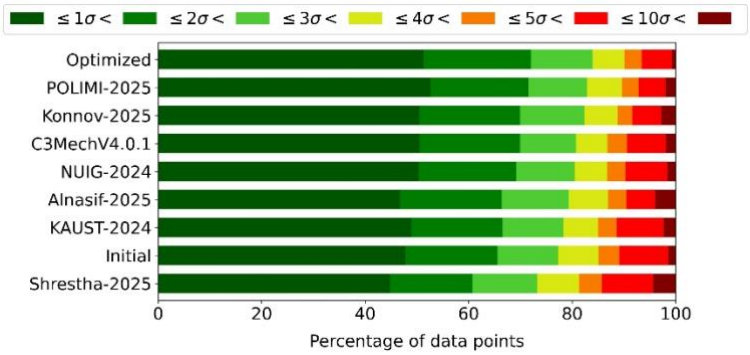

Figure 1: Percentages of the NH_3/H_2 indirect experimental data points that the investigated mechanisms could reproduce within given thresholds of the standard deviations (σ) of the experimental results.

The optimized mechanism substantially outperforms both NUIG-2024 and the initial mechanism. It reproduces all types of indirect experimental data within or close to their 3σ uncertainty limits on average. Overall, it reproduces the most experimental data within their 3σ uncertainty limits (84%) and the fewest beyond the 10σ limits (<0.8%) (Figure 1).

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FC18

A novel data consistency analysis for experimental laminar burning velocities of NH_3-H_2 mixtures for kinetic model validations

Xinlu Han[1]*, Kaidi Wan[2,3], Tibor Nagy[4]*

[1] *College of New Energy, China University of Petroleum (East China), Qingdao 266580, PR China*
[2] *Aircraft and Propulsion Laboratory, Ningbo Institute of Technology, Beihang University, Ningbo 315800, PR China*
[3] *National Laboratory for Computational Fluid Dynamics, School of Aeronautic Science and Engineering, Beihang University, Beijing 100191, PR China*
[4] *Institute of Materials and Environmental Chemistry, HUN-REN Research Centre for Natural Sciences, Budapest, 1117, Hungary*

*Contact: hanxinlu@upc.edu.cn, nagy.tibor@ttk.hu

Keywords: Laminar burning velocity, Ammonia-hydrogen mixtures, Data consistency analysis

Ammonia (NH_3) is a promising carbon-free fuel, where the H_2 enrichment strategy often adopted to enhance the combustion. One of the fundamental combustion properties, the laminar burning velocity (S_L), has been extensively investigated in the literature. Many measurements providing laminar burning velocity data are available, but exhibited significant data scatter, i.e., inconsistency much beyond the reported uncertainties among different experimental results under the same conditions. The present study focuses on the data consistency of NH_3+H_2 laminar burning velocities. To complement the existing literature datasets for consistency analysis, experiments were performed using the heat flux method at 298 K and 1 atm, and at various equivalence ratios, oxygen ratios, and H_2 blending ratios (x_{H2}). Based on simulations of five widely-used kinetic models from Han, Stagni, Konnov, Shrestha, and KAUST, linear relationship was found between $\ln S_L$ and x_{H2} across a broad range of conditions, with sensitivity analysis highlighting the underlying physio-chemical reason. Based on this linear relationship, a new data consistency criterion was proposed. Through the new and the previously existing criteria, 12 consistent experimental datasets were identified from the 20 available datasets of NH_3+H_2+N_2+O_2 laminar burning velocities (already excluding those without stretch or heat loss corrections). The present consistency analysis noticeably reduced the data scatter ranges, e.g., for 60%NH_3+40%H_2+air laminar burning velocities at 298 K and 1 atm, it was reduced from 9 cm/s to 3 cm/s, the latter being comparable to the reported experimental uncertainties. In addition to the found consistent data sets, which were suggested for future model validation and optimization studies, the present methodology using all available data consistency criteria has potential to help other fuel systems to filter out less reliable data sets, effectively overcoming the data scatter from different measurements.

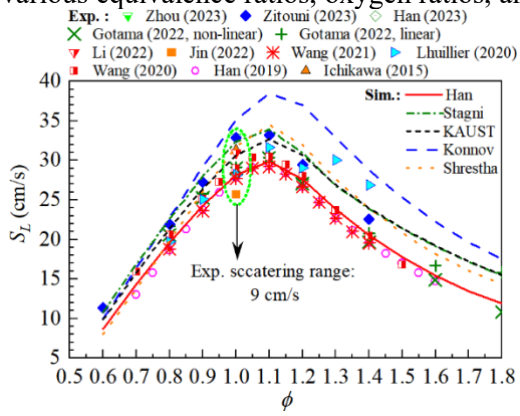

Fig.2. Laminar burning velocities of 60% NH_3 + 40% H_2 + air flames at 298 K and 1 atm

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FC19

From Fuel/O_2 Oxidation to Fuel/CO_2 Reforming: Plasma-Enabled Oxygen Transfer and Oxygenate Formation

Haodong Chen*, Zhaoying Li, Bin Yang*

[1] *Center for Combustion Energy and Department of Energy and Power Engineering, Tsinghua University, Beijing 100084, PR China*

*Contact: chd20@tsinghua.org.cn; byang@tsinghua.edu.cn

Non-equilibrium plasma activates CO_2 at low temperatures, opening fuel/CO_2 reforming chemistry. We compare CH_4/CO_2 and DME/CO_2 nanosecond discharges with fuel/O_2 plasma-assisted oxidation to show how CO_2 serves as an oxidant in plasma and becomes coupled to fuel conversion and oxygenate formation.
In fuel/O_2 plasmas, O_2 drives low-temperature oxidation through fuel + O/O(^{1}D), H-abstraction, O_2 addition, and RO_2 chemistry. Plasma-activated CO_2 opens analogous but less direct oxygen-transfer routes. In CH_4/CO_2/Ar, added CO_2 suppresses C_2H_2 and C_2H_4 formation but promotes CO, H_2O, CH_2O, and CH_3OH formation [1]. Electron- and Ar*-induced CO_2 dissociation generates CO and O atoms; together with ionic, electron-impact, and excited-species induced CH_4 consumption, the resulting O/H/OH pool shifts methane chemistry from hydrocarbon growth toward oxygenates formation.
$CH_4/^{13}CO_2$ experiments further show that CO_2 is not only an O radical source in methane conversion: carbon atoms from CO_2 are incorporated into double-oxygenated products in CH_4/CO_2 conversion, forming acids and esters through COOH/HOCO-related chemistry. In DME/CO_2, CO_2 likewise enhances H-atom abstraction of fuel by O/H/OH while suppressing direct electron- and Ar*-driven fragmentation [2]. The model identifies oxygenates formation via coupled plasma and low-temperature oxidation chemistry: ethyl methyl ether and dimethoxymethane arise from fuel decomposition and radical recombination, whereas methyl formate is promoted through RO_2-related pathways.
Therefore, the role of CO_2 is not only an O radical source: it also provides C atoms in oxygenate formation and enables low-temperature oxidation pathways like RO_2 chemistry in fuel/CO_2 conversion activated by plasma. This expands dry reforming from syngas production toward direct, one-step formation of value-added oxygenates and provides a kinetic basis for selectivity control.

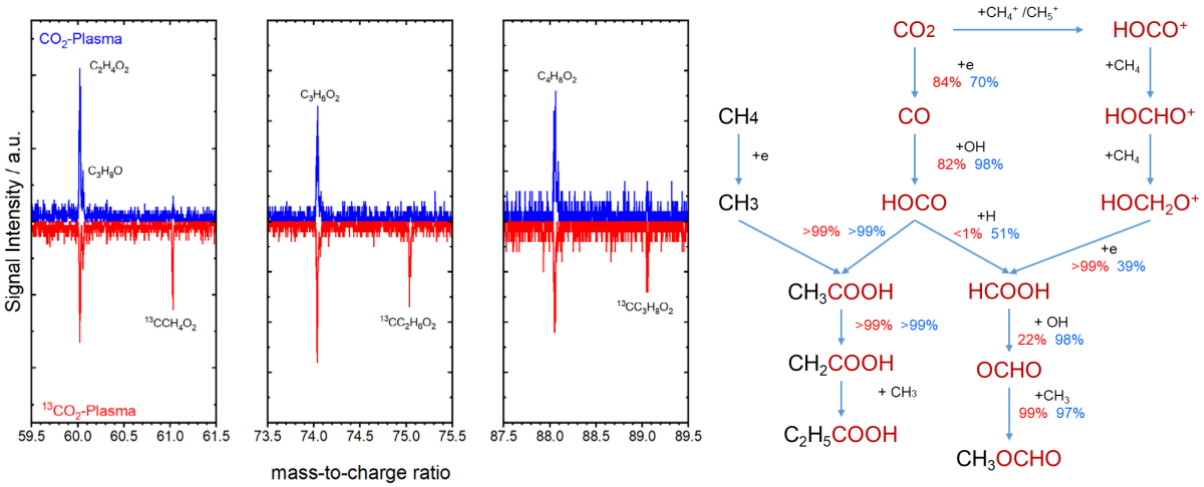

Fig. 1. Left: CH_4/CO_2 (upper) and $CH_4/^{13}CO_2$ (lower) mass spectra near $C_2H_4O_2$, $C_3H_6O_2$, and $C_4H_8O_2$. Right: pathway analysis at 340 K and 760 Torr for HCOOH and CH_3COOH.

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Combustion experimental data, reaction mechanisms, and computer codes for model analysis and development in the ReSpecTh Information System

Tamás Turányi[1,*], István Gy. Zsély[1], Máté Papp[1], Tibor Nagy[2]
[1]*Institute of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary*
[2]*HUN-REN Research Centre for Natural Sciences, Budapest, Hungary*

*Contact: turanyi@chem.elte.hu

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The ReSpecTh Information System [1] was created in 2014 as a joint website [2] for publishing datasets, models, and utility codes in the fields of gas-phase reaction kinetics (Re), high-resolution molecular spectroscopy (Spec), and thermochemistry (Th). The datasets contain validated experimental, empirical, and computed, machine-searchable data, and the corresponding metadata. The reaction kinetics (Re) branch contains directly measured and theoretically calculated rate coefficients, as well as indirect experimental data (ignition delay times, laminar burning velocities, and concentrations measured in flow reactors, jet-stirred reactors, micro-reactors, and flames). These data are stored in ReSpecTh Kinetics Data (RKD) format files [3]. The amount of published data continuously increases and now includes a large number of indirect (237,326 datapoints in 4,626 RKD data files) and direct (9,092 datapoints in 470 RKD data files) values. These data are related to the combustion of hydrogen, syngas, methanol, ethanol, methane, ethylene, H_2/O_2/NOx, syngas/NOx, methanol/NOx, ammonia, butanol, pentane and dimethyl carbonate. Several hundred published detailed reaction mechanisms in CHEMKIN format are provided for these combustion processes. The published utility codes include Optima++ [4] (creation and utilization of RKD format files; framework code for simulations using simulation codes Cantera, OpenSMOKE++, FlameMaster and Zero-RK; automatic testing and comparison of combustion mechanisms, sensitivity analysis; mechanism optimization). Additional codes are available for assessing the uncertainty of experimental data, mechanism reduction, and global uncertainty analysis.

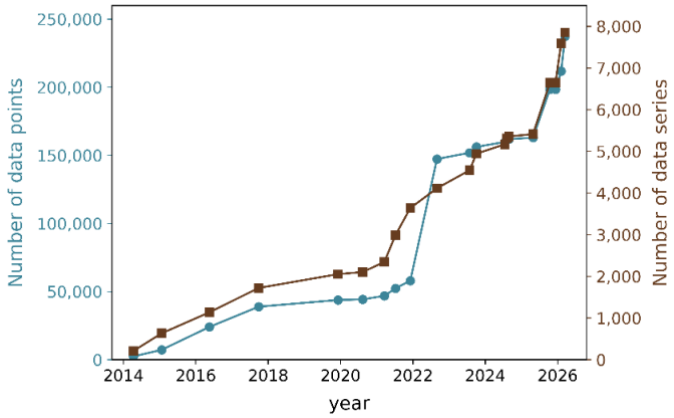

Figure 1. Increase in the number of indirect datapoints and data series in the ReSpecTh database.

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