



Flame Chemistry Workshop: a perspective on challenges and strategic actions in combustion experiments and chemical kinetics modeling[☆]

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ABSTRACT

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 present article concisely describes 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.

1. Introduction

The accurate prediction of combustion behaviors depends critically on the fidelity of chemical kinetics models that describe ignition, flame propagation, and pollutant formation. While substantial progress has been made over the past decades, new challenges are emerging as combustion research expands into sustainable aviation fuels, ammonia,

hydrogen, and plasma-assisted processes. In parallel, rapid advances in diagnostics, automation, and theoretical chemistry provide unprecedented opportunities to probe and model reacting systems. Yet the pace of these developments has revealed persistent gaps in data quality, model validation, and knowledge transfer, underscoring the need for a coordinated community effort that bridges experiments, theory, and modeling.

[☆] Supplemental Material:

- Book of Abstracts
- List of attendees

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The Flame Chemistry Workshop (FCWS), held biennially prior to the International Symposium on Combustion, has become a focal point for identifying these cross-cutting challenges and fostering collaborative solutions. The 7th FCWS, convened in Milan in 2024, emphasized the importance of moving beyond isolated advances toward an integrated framework for addressing both fundamental and application-driven questions. Discussions were organized into five main topics. *Topic 1 – Sustainable fuels combustion* underscored the need to incorporate new data and theory into models for hydrogen, ammonia, and sustainable aviation fuels, particularly under extreme conditions (e.g. high pressure), while reconciling detailed mechanistic and reduced engineering approaches. *Topic 2 – Advanced diagnostics for combustion measurements* highlighted persistent difficulties in extracting reliable targets for validation, the need for improved access and reporting of raw data, and closer integration with theory and simulation. *Topic 3 – Plasma combustion: experiments and modeling* identified the absence of standardized experimental protocols and solvers, as well as open questions about the treatment of excited states in kinetic mechanisms. *Topic 4 – AI, Automation, Benchmarking and knowledge transfer in ab initio transition state theory-based master equation techniques* reflected the growing reliance on automated model generation and theoretical calculations, while stressing the lack of agreed-upon standards for data management, implementation of theory outputs, and uncertainty quantification. Finally, *Topic 5 – Kinetics mechanism development: progress in accuracy and details* focused on the integration of new experimental speciation data, treatment of non-Boltzmann intermediates, and the challenge of balancing accuracy with usability in predictive models.

This perspective documents the major outcomes of the Milan workshop and articulates current high-priority challenges for the combustion kinetics community. By framing the key challenges in these five domains and outlining strategies for addressing them, the FCWS aims to build a sustained, collaborative platform for advancing the science of combustion chemistry and accelerating the development of next-generation combustion and energy conversion technologies. The sections that follow provide topic-by-topic summaries of the identified challenges, offering a coherent basis for future collective progress.

2. Perspectives, challenges, advances, and community priorities

2.1. Topic 1 – sustainable fuels combustion (Chair: liming CAI)

Currently, the global energy system is accelerating its transition toward low-carbon, clean, and diversified sources. For industrial and transportation sectors, where full electrification still remains challenging, sustainable biofuels derived from biomass or e-fuels synthesized with renewable electricity are of ultimate importance, by offering advantages, such as high energy density and infrastructure compatibility [1,2]. Hydrogen and ammonia as non-carbon-based e-fuels attracted most research attention from the combustion community in recent years [3,4]. However, their industrial application is still limited by their combustion characteristics, which are strongly different from conventional petroleum fuels. Their blending with other hydrocarbon or sustainable fuels provide potential solutions to these limitations [5,6], which, however, simultaneously increases the complexity of combustion behaviors and reaction kinetics. Sustainable aviation fuels (SAFs) play an important role in attaining carbon neutrality goals for the aviation industry [7]. Concerning the production routes and resources, the chemical compositions of SAFs can differ strongly in components and their blending ratios. This leads consequently to different combustion characteristics and kinetics of various SAFs [8,9], which remain largely unexplored. The application of sustainable fuels with advanced combustion techniques, such as flameless/MILD (moderate or intense low-oxygen dilution) combustion [10] and plasma-assisted combustion [11], is seen as a promising way to achieve increased efficiency and reduced pollution in practical combustion systems. Nevertheless, this joint consideration and optimization increases inevitably the research

complexity of sustainable fuel combustion in terms of various perspectives, including fuel design [12], combustion reactivity [13], pollutant emission [8], reaction chemistry [14], and model development [15].

This session on sustainable fuels combustion started with a keynote by Kai Moshhammer (*Physikalisch-Technische Bundesanstalt*) with focuses on the combustion of the aforementioned hydrogen, ammonia, and SAFs. Short invited talks from Sven Eckart (*TU Bergakademie Freiberg*), Yuyang Li (*Shanghai Jiao Tong University*), and Rodger E. Cornell (*US Army DEVCOM – Army Research Laboratory, Colorado School of Mines*) followed.

Moshhammer gave a comprehensive overview of recent achievements in fundamental combustion research of hydrogen, ammonia, and SAF and highlighted chemical aspects associated with these sustainable fuels. This keynote also covered various aspects of combustion studies, such as the application of artificial intelligence, the interaction chemistry of fuel blends, measurement techniques, and combustion targets for model validation highlighting progresses in researching new fuels through both innovative and conventional approaches.

The invited talk of Eckart reported various experimental observations on the impact of hydrogen addition on oxy-methane combustion. Both premixed [16] and non-premixed oxy-flames [17] were investigated and the influence of hydrogen addition on flame structure, temperature, and species distributions was evaluated. While the flame temperatures and structures are slightly affected by the hydrogen addition up to a blending ratio of 35 vol.-%, notable impacts were observed at higher ratios, indicating the difficulties of flame stabilization. These findings are of high importance for the application of hydrogen in large-scale industrial devices.

Li proposed fuel modification [18,19] and oxygen enrichment [20,21] strategies in his talk for a clean and efficient combustion of ammonia in gas turbine applications. As known, ammonia combustion is associated with low reactivity and high pollutant emissions. Co-firing of more reactive fuels and ammonia pre-cracking were shown to enhance the combustion of ammonia significantly, while nitrogen oxide emission from the laminar and swirl flames of ammonia can be reduced considerably by oxygen enrichment.

Modeling of sustainable fuel combustion remains an enduring challenge in the combustion community, which was discussed extensively in Topic 5. Here, Cornell talked specifically about the chemical model of ammonia. An accurate model was developed with the MultiScale Informatics (MSI) approach [22] by simultaneously taking experimental data and high-level theoretical kinetics calculations into account in the optimization.

The open discussion highlighted additional interesting themes:

- **Fuel design:** due to the urgent definition of future fuels, fast fuel screening and design [23,24] become of increasing interest, especially in terms of the optimization of sustainable aviation fuel compositions and the application of multi-fuel technology involving hydrogen or ammonia.
- **Chemical kinetics:** with respect to the understanding of sustainable fuels combustion, hydrogen and ammonia present complex kinetic behaviors, which have not yet been captured well by current chemical models. Reaction kinetics of certain interesting SAF components remain unexplored. Fuel interactions in multi-fuel applications and between SAF components are poorly characterized [25,26].
- **Combustion targets:** in addition to macrokinetic targets such as ignition delay times and flame speeds, the definition of robust validation targets must begin with an assessment of the availability and uncertainty of fundamental microkinetic data, including theoretically calculated rate constants and excited-state reactivity, which should be incorporated into mechanism development and validation. Validation experiments representative of the high-pressure and high-temperature conditions of advanced combustion devices are highly valuable but remain scarce in the literature.

- **Combustion chemistry models:** the disconnect between mechanistic and reduced engineering models (e.g. skeletal and reduced kinetic models for multidimensional reactors, engines and flames simulations) is exacerbated by a lack of strategy for convergence; systematic consideration of uncertainties is essential to guide model reduction and optimization approaches and to ensure consistency across modeling levels.

In summary, this session provided a comprehensive update on the investigation of sustainable fuel combustion, while also raising numerous questions regarding the future application and research of sustainable fuels, especially in terms of fuel design for particular devices, underlying kinetics of hydrogen/ammonia blends and SAFs, and tailor-made combustion targets for model validation at application-relevant conditions.

2.2. Topic 2 – advanced diagnostics for combustion measurements (Chair: Andrea Comandini)

The development of predictive chemical kinetic models depends critically on experimental techniques that probe combustion chemistry across different scales of time, conditions, and complexity. Diagnostics provide global parameters such as ignition delay times and laminar flame speeds, as well as detailed reaction rate measurements and speciation data. Current models reproduce many of these observables with remarkable fidelity, but further progress requires new diagnostics capable of providing additional mechanistic targets and improved accuracy. This is particularly challenging given the physical and chemical complexity of combustion, where processes depend on concentrations, dilutions, temperatures, pressures, and timescales. The need is even more acute for emerging fuels—such as hydrogen, ammonia, and biomass-derived species—that differ significantly from traditional hydrocarbons, and for unconventional operating modes like oxy-fuel, MILD, and low-temperature combustion. In these cases, conventional methods often cannot probe the chemistry with sufficient detail. A combination of complementary diagnostics, sometimes enabled by synchrotron light sources, is increasingly essential for comprehensive characterization.

The session on advanced diagnostics showcased recent state-of-the-art developments through a keynote and a series of invited talks. *Alison Ferris* (Princeton University, USA), in collaboration with Ron Hanson (Stanford University, USA), presented new optical diagnostics coupled to shock tubes: laser-based multi-speciation applied to NH_3 oxidation [27] and high-temperature laminar flame speed measurements behind reflected shock waves, with and without pre-ignition chemistry [28–30]. These studies address urgent needs for time-resolved, detailed data to reconcile discrepancies between NH_3 kinetic models [6] and measured combustion properties under relevant conditions not attainable in conventional setups.

Following this, *Robert Tranter* (Argonne National Laboratory, USA) and *Wenhao Yuan* (Shanghai Jiao Tong University, China) presented advances in synchrotron-based techniques applied to shock tubes and flow reactors, respectively. A miniature high-repetition-rate shock tube facility coupled to time-of-flight mass spectrometry at the Advanced Light Source (Lawrence Berkeley National Laboratory, USA) [31–33], as well as experiments at Synchrotron SOLEIL (France) using double imaging photoion-photoelectron coincidence (PEPICO) spectroscopy in collaboration with *Nabiha Chaumeix* and *Andrea Comandini* (CNRS, France) [34,35] was described. These approaches allow speciation at high pressures and the identification of complex isomeric mixtures. Yuan highlighted results from synchrotron vacuum ultraviolet photoionization mass spectrometry in laminar flow reactors [36–39] and micro flow reactors [40], performed in collaboration with Zhongyue Zhou, Fei Qi (Shanghai Jiao Tong University, China), and Jiuzhong Yang (University of Science and Technology of China, China). He demonstrated how species profile measurements and isomer identification, combined with

ab initio theory, provide detailed mechanistic insight into fuel oxidation pathways.

Olivier Herbinet (University of Lorraine and CNRS, France) then presented diagnostics coupled to jet-stirred reactors, including cavity ring-down spectroscopy for H_2O_2 detection [41,42], fluorescence assay by gas expansion (FAGE) for OH and HO_2 radicals [43,44], and time-of-flight mass spectrometry with synchrotron vacuum ultraviolet ionization for hydroperoxide detection [45,46]. These tools provide access to intermediates critical for low-temperature oxidation chemistry.

Next, *Nabiha Chaumeix* (CNRS, France) discussed spherical reactor studies of laminar and turbulent flame propagation, with emphasis on facility dimensions [47,48], turbulence homogeneity and isotropy [49], and the use of the new FAIRS (Fast Absolute InfraRed Sensor) instrument for absolute, real-time radiation measurements [50]. Her talk underscored how facility design and diagnostic innovation can be jointly used to improve measurements effectiveness.

Finally, *Rémy Mével* (Zhejiang University, China) presented on detonation-wave kinetics. He described techniques including soot foils, schlieren visualization, Rayleigh scattering, and NO-PLIF [51–54], and highlighted strategies to incorporate chemistry of increasing complexity into detonation simulations. These ranged from global models for macroscopic dynamics [55] to reduced and detailed mechanisms enabling direct comparison with two-dimensional planar experiments [56].

The open discussion emphasized several recurring themes:

- **New validation targets:** novel intermediates and measurements at relevant conditions must be defined for different fuel classes (conventional, heavy, nitrogen-based), requiring new diagnostics and facilities. Complementarity among diagnostics is essential, especially given varying sensitivities. Targets must also be generated and transferred in sufficient quantities for detection.
- **Experimental uncertainties:** quantification remains inadequate. Comparisons across facilities often show discrepancies larger than reported errors, particularly for speciation. High-fidelity model (i.e., chemistry and reactors) simulations were suggested to probe non-idealities and their impacts. Examples highlighted in the presentations include critical aspects related to laminar flame speed measurements (i.e., radiation effects and size of the flames in expanding configuration) or the dynamics inside small-bore shock tubes.
- **Raw data access:** providing raw datasets could enable re-interpretation with improved knowledge or simulations. For instance, laminar flame speed measurements in spherical reactors, now reported as functions of equivalence ratio, could later be analyzed with 2D simulations to extract additional insights.
- **Data needs for emerging diagnostics:** methods such as synchrotron-based mass spectrometry require accurate photoionization cross-sections and photoelectron spectra. While available for many small species, data are scarce for PAHs and other recent targets, with theory remaining computationally demanding.
- **Databases and reporting standards:** repositories such as ReSpecTh [57], SciExpeM [58], the Photoelectron-Photoion Spectral Compendium [59], and the Photonization Cross Section Database [60] are invaluable, but require better data reporting and standard formats to ensure usability and maintenance.
- **Conditions and extended validation:** broadening the range of temperatures, pressures, and timescales probed experimentally is critical for comprehensive model validation.
- **Experiment-modeling synergy:** high-fidelity simulations can guide experimental design and reduce uncertainties, but require closer collaboration between experimentalists and modelers.

Together, the session illustrated both the impressive recent advances in diagnostics and the pressing need for systematic coordination across techniques, data standards, and modeling integration to ensure that the

next generation of kinetic models is robust, comprehensive, and predictive.

2.3. Topic 3 – plasma combustion: experiments and modeling (Chair: Bin Yang)

Plasma-assisted combustion (PAC) is an increasingly important area at the intersection of plasma physics and combustion science, offering promising strategies to enhance ignition, flame stability, and pollutant control, while also opening new pathways for sustainable energy conversion. Unlike conventional approaches that rely exclusively on thermal energy, PAC leverages the unique reactivity of non-equilibrium plasmas, where energetic electrons, ions, and excited species can selectively accelerate chemical steps, broaden lean-burn limits, stabilize flames, enable in-situ fuel reforming, and influence processes as diverse as ozone synthesis, flow control, and even space propulsion [61–66]. Despite these advances, a comprehensive understanding of the coupling between plasma and combustion remains a central scientific challenge, particularly in terms of characterizing plasma under reactive conditions, quantifying electron–molecule interactions, developing validated kinetic mechanisms with excited species, and integrating non-thermal processes into predictive models of real combustion systems.

The session opened with a keynote by *Ramses Snoeckx (Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland)*, who provided a broad overview of challenges, advances, and opportunities in PAC research. This was followed by presentations from *Xingqian Mao (Tianjin University, China)* on plasma-assisted ignition and NO_x formation in NH₃/air mixtures, *Yong Tang (Beijing Institute of Technology, China)* on microwave plasma ignition of ionic liquid and metal fuels, *Wenting Sun (Georgia Institute of Technology, USA)* on plasma-assisted ammonia combustion, and *Quentin Malé (ETH Zürich, Switzerland)* on the integration of plasma effects into modeling of real combustors.

Snoeckx emphasized that while PAC applications are rapidly expanding, fundamental gaps remain in understanding physicochemical processes. The strong influence of balance gases in plasma discharges (e.g., Penning reactions, fast gas heating) [67,68] was noted and the challenges of accurately measuring and controlling the reduced electric field (E/N), a key parameter for electron-driven chemistry [69], were discussed. From a modeling perspective, three major data deficits persist: (i) cross-section data for electron collisions, especially for larger molecules and even for basic species such as O₂ [70]; (ii) chemical kinetic data for low- to mid-temperatures, where HO₂ chemistry is still uncertain even in H₂/O₂ systems [67,71]; and (iii) reaction data for excited species, including temperature-dependent information and quenching rates with larger molecules. Opportunities for synergy between high-temperature combustion and low-temperature plasma communities, advocating for standardized experimental setups, mechanism development, and computational data generation were outlined.

The talk by Mao focused on plasma-assisted low-temperature ignition and NO_x formation in NH₃/air mixtures using a repetitively pulsed nanosecond discharge at atmospheric pressure and an experimentally validated kinetic model [72]. Plasmas were shown to shorten ignition delay times by 2–5 orders of magnitude via production of excited species and radicals such as NH₂, NH, H, and O, which enhance OH formation and accelerate NH₃ oxidation. The non-monotonic dependence of ignition delay time on E/N was presented, with an optimum demonstrated for around 250 Td. At lower E/N, gas heating dominates; at higher E/N, ignition inhibition can occur despite high radical generation. Plasmas were also more effective under fuel-lean conditions, due to accelerated O(¹D) and O production from air, which promotes NH₃ oxidation, while NO_x formation was found to further enhance ignition.

Tang introduced a novel microwave plasma actuator (2.45 GHz compact torch) with a rotational temperature of ~2000 K and a vibrational temperature of ~4800 K [73,74]. This device enabled reliable multi-start ignition of ionic liquid propellants by rapid thermal decomposition, with copper atoms from electrode erosion acting as catalytic

promoters. For aluminum powder fuels, plasmas overcame the high ignition barrier by disrupting the oxide shell, reducing ignition delay, and promoting flame stability. At higher particle densities, a shift to group combustion was observed. Ignition of aluminum with a CO₂ plasma torch was also illustrated, pointing to negative-carbon applications when integrated with carbon capture.

Sun addressed plasma-assisted ammonia combustion, situating ammonia not merely as a hydrogen carrier but as a unique fuel with narrow flammability limits, low laminar flame speeds, and high NO_x emissions. He emphasized that PAC is more established for hydrocarbons, with its role in NH₃ combustion remaining underexplored, especially in relation to NO_x. Early numerical [75,76] and experimental [65] studies indicate that plasmas can enhance flame propagation and lean blow-off while potentially reducing NO_x. Remaining challenges include identifying plasma–ammonia interaction pathways (especially in NH₃/H₂ mixtures), improving models of ammonia kinetics [77], advancing diagnostics (e.g. scarce NH/NH₂ detection, NO-LIF difficulties [78]), and addressing transport-property changes due to plasma-produced H₂. Additionally, the need for PAC studies under high-pressure conditions relevant to engines was stressed.

Malé presented the integration of PAC into combustor simulations, a key step toward practical applications. He described the high computational cost of coupling plasmas (electric fields, electron transport) with reactive CFD and reviewed simplified models such as Castela et al. [79], which reproduce non-equilibrium plasma (NEP) effects like rapid heating and O₂ dissociation from electronically excited N₂, and slower vibrationally induced heat release. These models have been applied in direct numerical simulations (DNS) [80] and large-eddy simulations (LES) [81] for turbulent flame ignition. The PACMIND model [82] extends these capabilities to predict NO_x in CH₄/air, while adaptations for NH₃/air mixtures are emerging [83]. Challenges in modeling pulse-to-pulse effects in nanosecond repetitively pulsed discharges [84], uncontrolled discharge locations in turbulent flows (addressed with empirical models [85]), high-pressure plasma effects, where spark-type discharges may dominate, and the lack of validated kinetic data [73] were emphasized.

The open discussion, strongly promoted by Nils Hansen (Sandia National Laboratories), Yiguang Ju (Princeton University), and others, highlighted key recurring themes.

- **Data gaps for mechanism development:** lack of validated electron–molecule cross-sections (especially beyond C₄), missing rate constants for ions and excited species, and scarce high-pressure plasma kinetics.
- **Experimental standardization:** need for well-defined reactors covering broad T, p, and discharge conditions, with reproducible “typical systems” and standardized diagnostics for the reduced electric field (E/N, the ratio of the electric field E to the gas number density N), electron density, electron temperature, and plasma–flame parameters.
- **Modeling and theory tools:** urgent need for calculated cross-sections, automated mechanism generation (akin to RMG [86]), and robust plasma solvers linking experimental observables to modeling variables.
- **Core mechanism development:** unlike thermal combustion, PAC lacks validated core mechanisms; establishing such a core first requires a systematic assessment of available plasma-kinetic data and their associated uncertainties, with key challenges arising from low-temperature oxidation chemistry (HO₂/RO₂) and the consistent treatment of excited states.
- **Emerging applications:** PAC in CO₂ conversion and NH₃/H₂ mixtures presents both opportunities (e.g., in-situ H₂ production) and complexities (e.g., altered transport, NO_x pathways).

Overall, consensus was reached on the urgent need for standardized experiments, simplified apparatuses to isolate chemistry, validated data

for kinetic models, and coordinated mechanism development. Only through these collective steps can PAC transition from a promising technique to a predictive, deployable tool for advanced combustion systems.

2.4. Topic 4 – AI, automation, benchmarking and knowledge transfer in *ab initio* transition state theory-based master equation techniques (Chair: Feng Zhang)

The predictive capability of combustion modeling depends fundamentally on accurate kinetic parameters—network of reactions, rate coefficients, and thermochemistry—that govern fuel transformations across diverse conditions. Historically, these quantities have been obtained manually through compilation of experiments and quantum chemical calculations, with additional analogy rules, and expert-driven assembly of mechanisms. With the growing chemical complexity of modern fuels and the demands for models spanning broad temperature, pressure, and compositional ranges, manual approaches are increasingly insufficient. Over the past decade, advances in computational chemistry, algorithm development, and high-performance computing have accelerated a shift toward automation. Automated tools now allow one to discover reaction pathways, explore potential energy surfaces (PESs), compute rate constants using transition state theory and master equation (TST-ME) methods, and assemble kinetic models [87–93]. In parallel, artificial intelligence (AI) and machine learning (ML) approaches are emerging to speed up calculations, predict kinetic data, and analyze the massive datasets generated by these workflows [94–99]. Together, these advances define the growing field of AI-TST-ME, which promises to increase efficiency and accuracy while enabling systematic knowledge transfer.

The session on AI-TST-ME at the 7th FCWS brought together leading voices in this emerging space. A keynote by *Luna Pratali Maffei (Politecnico di Milano, Italy)* was followed by short invited talks from *Sarah Elliott (Argonne National Laboratory, USA; presented by Stephen J. Klippenstein)*, *Kai Leonhard (RWTH Aachen University, Germany)*, *Judit Zádor (Sandia National Laboratories, USA)*, *Emilio Martínez-Núñez (Universidade de Santiago de Compostela, Spain)*, and *Lili Ye (Dalian University of Technology, China)*. Collectively, the talks illustrated how automation and AI are reshaping theoretical kinetics, while raising shared challenges in reproducibility, uncertainty quantification, and data infrastructure.

Pratali Maffei opened with a comprehensive overview of automation in theoretical kinetics and the urgent need for systematic knowledge transfer. Automated approaches to reaction path discovery and PES exploration, from mechanistic implementations such as KinBot [89] and Arkane/RMG [96], to molecular dynamics-based tools like AutoMeKin [100] and ChemTraYzer [93], and hybrid workflows combining conformer sampling with transition state searches [98] were highlighted. Codes like AutoMech [90] and EStokTP [88] enable high-accuracy rate constant calculations for defined pathways, but remain system-dependent and require expert oversight. Critical gaps in current automation, including the treatment of roaming mechanisms, intersystem crossing, stereochemistry, and non-thermal effects [91,101,102] were identified. Thermochemistry predictions have advanced further—especially for enthalpies of formation at 298 K using bond additivity corrections and connectivity schemes [99,103]—yet challenges remain for PAHs, transition states, and anharmonic corrections. Rate constant codes likewise fail to capture the full suite of combustion-relevant effects, such as anharmonic vibrations and collisional energy transfer. Examples of application of AI/ML for PESs and rate constants were also discussed, noting their promise for large systems but cautioning that training data quality and benchmarking are critical. The need for implementation of big-data practices—standardized storage, open databases, and reproducible workflows—emerged clearly, warning that, without infrastructure, much of the value of automation is at risk of being lost.

Elliott and Klippenstein demonstrated the power of automated

workflows through a case study of n-butane oxidation, built using AutoMech [90]. The reaction network included >180 elementary steps, explicitly accounting for stereoisomerism. Stereochemical effects altered barrier heights by up to 4 kcal/mol and rate constants by factors of 2–4, directly influencing ignition delay times. The workflow also enabled systematic uncertainty quantification [100], identifying which approximations (e.g. vibrational scaling, 1D rotor models) most affected predictions. Results emphasized that automation should not only accelerate mechanism building but also provide feedback for refining methodologies.

Leonhard then discussed about data management and findability, accessibility, interoperability and reusability principles (FAIR) [104] warning that automated workflows generate massive datasets for intermediates—geometries, energies, metadata—that are often discarded once reduced mechanisms are built, representing a major lost opportunity. ChemTraYzer [93] was presented as an example of a tool that now automatically archives quantum chemistry data, enabling provenance tracking and repository integration (e.g. NOMAD, Zenodo), pointing at the need for community standards for metadata, transparency, and vocabulary to prevent “black box” automation and ensure reproducibility.

Zádor presented advances in neural network PESs (NNPESs), showing how ML potentials trained from KinBot-sampled stationary points can reproduce DFT energetics for C₈–C₈ hydrocarbons at a fraction of the cost [89,105,106]. This approach uncovered new benzyl radical pathways and was extended to barrierless reactions using VRC-TST. Limitations for high-temperature rate accuracy introduced by errors in harmonic frequencies and partition functions were noted, as well as the uncertainty in transferability of ML potentials across systems. An ongoing debate was directly addressed: should ML be used for direct k(T,p) prediction, or to accelerate PES evaluations that then feed into TST-ME frameworks to determine k(T,p)?

Martínez-Núñez described the evolution of AutoMeKin, which combines molecular dynamics, graph algorithms, and kinetics simulations for automated reaction discovery [97]. Recent advances include rare-event acceleration, heuristics-guided PES exploration, and visualization via the amk-tools library [107]. While AutoMeKin can generate vast reaction networks, accessibility is key: interactive dashboards, repositories, and graph-based tools are needed to make outputs usable by non-specialists.

Finally, Ye presented a graph neural network (GNN) approach for directly predicting rate constants from molecular features [108]. Using OH abstraction reactions across alkenes, cycloalkenes, and larger systems, her ML models achieved strong accuracy with inputs as simple as SMILES strings. This work suggests a path to large-scale rate predictions without costly calculations, proposing an online platform for ML-predicted rate constants, supported by benchmark datasets.

The open discussion highlighted cross-cutting themes:

- **Automation vs expertise:** workflows still require supervision; accessibility to non-specialists remains limited.
- **Accuracy vs throughput:** debate over refining details (anharmonicity, stereochemistry) versus enabling high-throughput scans; consensus leaned toward a hybrid strategy.
- **Knowledge transfer:** theory outputs must integrate smoothly into simulation codes (CHEMKIN, Cantera), but users often lack the expertise to implement advanced findings correctly.
- **FAIR data and metadata:** urgent need for standardized archiving of QM data, PESs, and rate constants.
- **Machine learning strategies:** direct k(T,p) prediction and ML-accelerated PES evaluation both hold promise; benchmarking will clarify trade-offs.
- **Uncertainty quantification:** propagating uncertainties in energies, frequencies, and correlations remains a key gap.
- **PES exploration completeness:** defining when an automated search is “complete” is still unresolved.

- **Experiment–theory connection:** theory now often exceeds experimental resolution; models must remain grounded in observables.
- **User-friendliness:** poor documentation and lack of standards for usability remain barriers to adoption.

The session converged on a vision of a more predictive, transparent, and collaborative discipline. Achieving this will require community standards for metadata and UQ, shared databases for PESs and rate constants, hybrid AI–automation strategies, stronger experiment–theory links, and improved usability and training. As emphasized in Milan, automation is not the end-goal, but a pathway to collective progress, ensuring that AI-TST-ME fulfills its promise: delivering predictive, transferable, and scalable kinetic models for the combustion community.

2.5. Topic 5 – kinetics mechanism development: progress in details and accuracy (Chair: Brandon Rotavera)

The construction of chemical kinetics mechanisms has traditionally followed two approaches. The first emphasizes detailed mechanistic rigor, incorporating all conceivable, relevant reactions and species with rate parameters and thermochemical properties obtained from experiments or high-level quantum chemistry. These mechanisms are often aimed at answering fundamental physical chemistry questions and evolve gradually toward application. The second approach, more common in engineering contexts, relies on reaction classes [109], empirically derived parameters, and simplifications to deliver reduced, skeletal, or lumped mechanisms compatible with computational fluid dynamics (CFD) codes [110–112]. Both approaches are valuable but face growing demands: detailed speciation measurements now capture numerous constitutional isomers, stereoisomers, and conformers; new intermediates are discovered in low-temperature chemistry; and non-Boltzmann energy distributions are increasingly recognized as important in explaining product channels. As experimental targets become more stringent, mechanisms must balance accuracy, detail, and usability while incorporating advances in theory, optimization, and uncertainty quantification.

The session on kinetics mechanism development reflected this tension, beginning with a keynote by *Jérémy Bourgalais (Institut de Physique de Rennes, France)* on isomer-resolved measurements for mechanism development. This was followed by discussions from *Fabien Goulay (West Virginia University, USA)* on OH radical reactions with conjugated hydrocarbons, *Xuefei Xu (Tsinghua University, China)* on ROO radical kinetics, *Leonid Sheps (Sandia National Laboratories, USA)* on synchrotron-based speciation in high-pressure reactors, *Malte Döntgen (RWTH Aachen University, Germany)* on quantum-chemistry-based thermochemistry, and *Shijun Dong (Huazhong University of Science and Technology, China)* on the C3MechV3.3 detailed mechanism for surrogate fuel blends.

Bourgalais introduced synchrotron-based vacuum ultraviolet photoionization mass spectrometry (SVUV-PIMS) for isomer-resolved detection, where mass-selected photoionization efficiency (ms-PIE) curves allow discrimination of isomers by vibronic structure. For near-degenerate ionization energies, SVUV-PEPICO (photoelectron–photoion coincidence spectroscopy) provides higher selectivity through analysis of photoelectron spectra. Measurements using the PEPICO spectrometer on the DESIRS beamline at Synchrotron SOLEIL were compared with quantum-chemistry-based Boltzmann-weighted threshold PESs [113]. Challenges in mass resolution, sensitivity, and quantification, all of which limit mechanism accuracy, were also detailed.

Goulay focused on OH reactions with conjugated hydrocarbons such as cyclopentanone, cyclopent-2-en-1-one, and methyl-substituted derivatives. These systems feature competition between OH-addition and H-abstraction, both yielding resonance-stabilized radicals implicated in aromatic ring formation [114] and soot precursor growth [115]. Results

from multiplexed photoionization mass spectrometry (MPIMS) experiments up to 500 K at 4 Torr were described showing that temperature-dependent branching produces rate coefficients with minima, and that the transition temperature depends on unsaturation and substituents [116]. The roles of barrierless van der Waals complex formation, stabilization of OH-adducts by resonance, and competitive back-dissociation were also emphasized. The data highlighted the importance of resonance-stabilized radicals with reduced reactivity toward O₂-addition [117,118].

Xu examined organic peroxy radicals (ROO), central intermediates in low-temperature combustion and volatile organic carbon (VOC) oxidation focusing on ROO → QOOH isomerization, which drives autoignition and chain-branching. Challenges include multireference character in PESs [119], requiring high-level multi-reference methods; torsional anharmonicity [120–122]; and tunneling contributions with pressure dependence. Uncertainties in ROO· kinetics that propagate directly to ignition predictions were also highlighted.

Sheps presented a high-pressure flash photolysis reactor with SVUV-PIMS detection at Sandia [123]. This setup enables time- and isomer-resolved, multiplexed detection of many intermediates in a 0D reactor in order to target specific classes of reactions, such as ROO reactivity, at low temperatures [124–128]. Quantification requires photoionization cross-sections, and global carbon balance analysis allows estimation for species lacking reference spectra [128]. The key role of simultaneous, quantitative detection of multiple intermediates for constraining mechanisms was also discussed.

Döntgen described progress in computing thermodynamic properties from quantum chemistry [99] and compared results with group additivity methods [129–131], highlighting difficulties in assigning uncertainties for entropy and heat capacity, in NASA polynomial fitting, and in treating intermediates with non-Boltzmann distributions. Despite the essential role of quantum-chemistry-based datasets, more consistent uncertainties must be quantified for streamlining kinetic model integration.

Dong closed the session with updates on C3MechV3.3, a detailed mechanism for hydrocarbon and biofuel surrogates developed by the Computational Chemistry Consortium (C3) [132], highlighting efforts to capture interaction chemistry among blend components, including alkanes, alkenes, alcohols, and aldehydes, as well as ammonia/*n*-heptane [133] and NO_x/TPRF. The work emphasizes the radical-pool-mediated cross-chemistry that dominates blend behavior, along with direct interactions in some systems. Dong underscored the challenge of simultaneously describing NO_x, PAHs, and surrogate blend interactions in a single framework, jointly developed by leading groups in kinetic modelling, currently constituting a virtuous example for the entire community.

The open discussion emphasized several recurring themes:

- **Ionization-based speciation:** synchrotron experiments rely on accurate photoionization cross-sections and PESs for isomer discrimination. Limited ability to resolve species due to hindrance from similarity in onset energy or in spectral features, lack of pure samples of high-value species, such as ketohydroperoxides for calibration spectra, and computational uncertainties collectively complicate assignments.
- **Conformer effects:** temperature-dependent conformer populations can bias quantification in photoelectron/ionization experiments, particularly for large species with long relaxation times.
- **Elementary reaction rates:** accurate OH, HOO, and other radical reactions remain critical, as branching fractions from the initiation step control ignition delay times and species profiles [58].
- **Resonance-stabilized radicals:** may act as third-body colliders influencing radical pools and flame dynamics, but this role is poorly understood and not properly accounted for in models.

- **Thermochemical uncertainties:** embedding species- and condition-specific uncertainties into models is increasingly important.
- **Chemistry of blends:** cross-over reactions in multicomponent fuels [134–139] are a major source of uncertainty; radical recycling and scavenging effects complicate mechanistic understanding.
- **Novel reactions and rules:** prompt reactions [140,141] and new mixture rules [142–144] require standardized implementation strategies for inclusion in mechanisms.

The session thus underscored that mechanism development is entering an era of unprecedented detail, where accurate measurements, theory, and modeling must converge. Progress depends not only on capturing new species and reactions, but also on embedding uncertainty, cross-chemistry, and standardization into community-accepted frameworks.

3. Summary

To begin addressing the challenges identified across the five thematic areas of the 7th Flame Chemistry Workshop, we propose a set of tasks that align with the objectives of dedicated working groups whose structuring, coordination, and management will be defined during the 8th FCWS (Kyoto, 2026). These tasks are designed to foster collaboration, ensure reproducibility, and accelerate progress toward predictive chemical kinetic models for combustion and plasma systems.

3.1. Topic 1 – sustainable fuels combustion

1. Select and define reference fuels (H_2 , NH_3 , SAF or mixtures) as community benchmarks, ensuring both scientific insight and industrial relevance.
2. Assemble and maintain “best available” kinetic models, integrating experimental data (micro- and macrokinetic) with theoretical findings (excited states, collisional efficiencies).
3. Perform validation under realistic conditions, including extreme temperature and pressure regimes and multi-fuel interactions, and use discrepancies to guide data re-analysis and new experimental priorities.

3.2. Topic 2 – advanced diagnostics for combustion measurements

1. Establish a shared data framework for reporting speciation, flame speeds, ignition delays, and diagnostic metadata, using standardized formats compatible with major databases.
2. Coordinate benchmark experiments across facilities, leveraging complementary diagnostics to assess reproducibility and quantify uncertainties.
3. Define a roadmap for new validation targets, jointly with modelers, to prioritize intermediates and measurement conditions most critical for emerging fuels.

3.3. Topic 3 – plasma combustion: experiments and modeling

1. Standardize discharge configurations and diagnostics (e.g., E/N, electron density, plasma–flame coupling) using agreed benchmark reactor designs to improve reproducibility and streamline design of experiments.
2. Develop a community core mechanism for CH_4/Ar , CH_4/O_2 , $CH_4/CO_2/Ar$, and $CH_4/CO_2/He$ mixtures, combining experiments with theory-derived cross sections and excited-species kinetics.
3. Promote solver and tool development for plasma–combustion coupling, including simplified reduced models suitable for CFD applications.

3.4. Topic 4 – AI, automation, benchmarking, and knowledge transfer

1. Define community standards for uncertainty quantification (UQ) in automated TST-ME workflows, including treatment of anharmonicity, tunneling, and variational effects.
2. Create benchmark datasets and repositories (PESs, rate constants, metadata) under FAIR principles to enable reproducibility and machine learning applications.
3. Establish best practices for model integration, ensuring theory outputs are implemented correctly and consistently in combustion kinetic models and simulation codes.

3.5. Topic 5 – kinetics mechanism development: accuracy and detail

1. With expertise and chemical insight on combustion continuing to rise, chemical kinetics mechanisms must enter into a period of convergence, where a decreasing number of mechanisms are utilized and subsequently refined as new data is produced. This is an imperative for the sake of consolidating the vast amount of progress developed over the decades and for efficiently incorporating new reaction-related details to accomplish the oft-stated aim of chemical kinetics mechanisms being reliable for simulating practical combustion applications.
2. Embedding uncertainties in rate parameters and thermochemical properties into all mechanism releases is needed to move beyond validation-by-fit toward quantified predictive confidence.
3. Cross-section measurements of high-priority species is an essential component of experimental approaches where species detection and quantification are paramount. The inability to routinely quantify ketohydroperoxides, alkylhydroperoxides, and others, presents a major barrier to reliable predictions of radical populations and species produced from subsequent reactions of such intermediates. Machine learning approaches may aid species identification and theoretical methods are required for quantification.

A dedicated discussion aimed at coordinating and identifying strategies to address the above challenges will follow at the 8th Flame Chemistry Workshop (Kyoto, 2026).

CRedit authorship contribution statement

B. Rotavera: Writing – review & editing, Writing – original draft, Formal analysis, Conceptualization. **L. Cai:** Writing – review & editing, Writing – original draft, Formal analysis, Conceptualization. **F. Zhang:** Writing – review & editing, Writing – original draft, Formal analysis, Conceptualization. **A. Comandini:** Writing – review & editing, Writing – original draft, Formal analysis, Conceptualization. **N. Hansen:** Writing – review & editing, Conceptualization. **S.J. Klippenstein:** Writing – review & editing, Conceptualization. **B. Yang:** Writing – review & editing, Writing – original draft, Formal analysis, Conceptualization. **M. Pelucchi:** Writing – review & editing, Writing – original draft, Supervision, Formal analysis, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

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