Summary of TNF16 and Planning for TNF17

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The TNF16 workshop (International Workshop on Measurement and Computation of Turbulent Flames) was held at Politecnico di Milano on 20-21 July 2024 as one of five co-located satellite workshops of the Combustion Institute International Symposium. Sessions on the first day were held jointly with the Premixed Turbulent Flames (PTF) workshop, such that the agenda included a blend of TNF-style curated sessions and PTF-style individual talks on connected topics. The combined attendance was of over 150.

This summary briefly outlines the scope and history of the TNF series, the contents of the six TNF-lead topical sessions, some key discussion points as expressed in Christian Hasse's summary from the final TNF session, and steps being undertaken to prepare for TNF17 in 2026.

The TNF16 Proceedings and the proceedings from all previous TNF workshops may be downloaded from tnfworkshop.org. Summaries and presentation slides for the TNF16 sessions are included, along with TNF poster abstracts, while the slides and abstracts for the PTF contributed talks are available from the PTF website.

IMPORTANT NOTE: Results presented at the TNF Workshop may represent work in progress. It would be inappropriate to quote or reference unpublished information from the proceedings without first checking with the authors for permission and for the latest information on results and references.

TNF Scope and History

The TNF workshop focuses on fundamental issues of turbulence chemistry interactions in gaseous flames. The objectives are to:

- Establish a library of well-documented flames that advance fundamental scientific understanding of turbulent combustion and are appropriate for testing and extending models for complex combustion systems.
- Provide a framework for collaborative comparisons of refence data from experiments and DNS with modeled results from LES.
- Identify priorities for further experimental and computational research.

One TNF legacy – among others – is the availability of instantaneous and averaged thermochemical states from Raman/Rayleigh experiments that are crucial for turbulent combustion model development and validation. Up to TNF14 in Dublin (2018), a wide range of flames with different modes (premixed, stratified, partially premixed, non-premixed) and regimes (Re, Da, Ka number) were investigated mostly for CH4, with only small excursions to DME and very early (before 2000) also to H_2. TNF sessions evolved around data sets from target flames, and the numerical results from different groups were compared to experimental data. Preliminary and work-in-progress results were submitted. The open workshop atmosphere allowed discussions on the physics of the flames and how the models could be improved. Modeling results usually improved substantially from workshop to workshop, and new experimental configurations were discussed to challenge the models.

In Vancouver (2022), as a practical response to a lower overall attendance due to lingering effects of the COVID pandemic, all sessions were held jointly with the PTF workshop. There were substantially fewer TNF-style discussions on burners and model deficiencies. Interest had decreased for pure hydrocarbon target flames, and there was only one session on the Darmstadt Multi Regime Burner. Despite the large interest in H_2 and NH_3 as carbon-free fuels, experimental data were not yet available; only first DNS data for premixed H_2 flames had been generated. While this did not allow for a TNF-style comparison, the discussion session on modeling was very intense and engaging. That clearly showed the need for new reference data sets.

TNF16 Topical Sessions

A major development between 2022 and 2024 was that several new data sets for flames of carbon-free fuels became available. This allowed a return to one of the central activities of the TNF workshop series – collaborative comparisons of measured and modeled results for selected target flames. Joint TNF/PTF sessions were also part of the TNF16 program, which combined TNF-style curated sessions with PTF-style contributed individual talks on connected topics. The six TNF-lead topical sessions are briefly outlined below.

Fundamentals of Premixed Hydrogen Flames

This was a return topic from the Vancouver workshop that is of great current interest to the turbulent flame community. The session aimed to give a comprehensive review, assembled by Thomas Howarth, of new research on both laminar and turbulent flames that has occurred since the Vancouver TNF/PTF workshop and to highlight some currently unanswered questions. Corresponding references are listed in the session summary. Brief descriptions of available data sets on turbulent lean premixed hydrogen flames, from both DNS and experiments, were also presented.

The review of turbulent H_2 flames and the subsequent discussion were very engaging and identified several open scientific questions especially for lean H_2 flames. These include among others:

- How does the thermo-diffusive instability (TDI) interact with turbulence? Is the interaction synergistic?
- How does the interaction of turbulence and TDI change for high Ka numbers?
- What are the governing parameters? Ze, Ka, Pe and/or others?
- How to model flames under high pressure. Do the observed differences between high- and low-pressure laminar flames carry over to turbulent flames?

This non-exhaustive list clearly demonstrates the need for TNF-style target flames from experiments and DNS to systematically address these scientific questions.

Chemical Kinetics for Ammonia Combustion

Ammonia is a “hot” topic as a potential alternative fuel or hydrogen carrier. However, in spite of the long history of research on the chemical kinetics of ammonia as a NOx reduction additive and, more recently, on ammonia as a fuel, there are still significant areas of disagreement among the numerous kinetic models for ammonia combustion that have been published in recent years. This is especially true for the kinetics of pollutant formation, which is a key challenge for ammonia combustion technologies. This is a relevant topic for the TNF community because it is essential to have reliable kinetic models in order to conduct informative comparisons of measurements and simulations of turbulent flames.

In this session, Peter Lindstedt provided some background on ammonia chemistry and an overview of the current state of kinetic mechanisms, with attention to appropriate criteria for assessing kinetic models and areas of uncertainty. The role of flame data in kinetic model validation and some ways in which the TNF community might collaborate with kinetic modelers were also addressed. The second part of the session, presented by Gaetano Magnotti, examined the potential for TNF-type diagnostic tools to contribute toward the development and validation of kinetic models for ammonia, with the main focus being on multi-scalar experiments in laminar flames, including both published examples and possible future experiments.

Looking forward, there are current uncertainties for some key fundamental reaction sequences and these will need to be addressed by the kinetics community. Thus, chemical mechanisms for DNS and LES are likely to evolve over the next years, and needs to be considered in the planning of the numerical work.

Comparisons on the HYLON Burner

The HYLON burner, which was developed under a large EU project, uses a swirled hydrogen-air injection system within a model gas turbine burner geometry. This session, presented by Thierry Poinsot and Thierry Schuller, introduced this ongoing project to the TNF/PTF audience by reviewing the burner design features and its extensive experimental characterization, and by summarizing comparisons of those measurements with results from twenty-five modeling groups that had computed two selected flame cases operated at 1 bar and featuring different modes of flame stabilization. The next phase of this project will use a new version of the burner (HYLON2) to extend the studies to elevated pressure up to 10 bar, with experimental measurements being carried out at KAUST.

Comparisons on Piloted Ammonia Jet Flames

The objective of the session was to compare recent experimental measurements (from KAUST) and numerical simulations of a series of turbulent partially-premixed $H_2/N_2/NH_3$-air flames stabilized on the Sydney piloted burner. Following the example of the Sandia piloted methane flame series, three cracked-ammonia flames (labeled D, E, F) were measured, with jet Reynolds numbers of 24000, 32000, and 36000, corresponding to 59%, 79%, and 89% of the global blowoff condition. These flames are characterized by varying levels of local extinction and effects of differential diffusion, both of which present challenges to numerical simulations. Nine teams were involved in the simulations, which were preliminary at this stage because the experimental data had been released only a few months before the workshop.

Overall, this dataset was deemed interesting by the TNF community, and the large number of groups involved despite the short time available for the simulation promises that in-depth analysis, conditioned on the type of models used, will be possible. To go further with the analysis, significant improvement of the mixture fraction field will be necessary prior to analyzing the effect of different turbulence-combustion models. Velocity measurements, especially in the near field, would be desirable to help converge to common and more detailed boundary conditions for all the simulations.

AI/ML for Turbulence-Chemistry Interaction

ML for combustion was introduced as a TNF focus topic in 2022. Since then, various ML methods have been adopted and extended by the combustion community to address problems of turbulent combustion modeling and experimental analysis. This session reviewed recent advances with the goal for connecting the broad field of ML to TNF/PTF-related problems. The session was divided into three topics: 1) Background and nomenclature on ML for combustion: 2) Recent developments of ML methods for turbulent combustion modeling: and 3) Applications of ML methods to extract knowledge form experimental data. The presentations included nine contributions from the TNF and PTF community.

The next key challenges involve: data, benchmarks, and metrics; common models, methods, and approaches; and best practice. It was suggested to identify benchmark problems for ML-applications following the TNF approach. This will allow to evaluate ML-based approaches, e.g., for manifold parameterization or combustion modeling in general. There is interest in sharing ML-models through TNF/PTF infrastructure and by this establish best practice guidelines for ML-model selection, ML-training, and ML-evaluation. The need for diverse data sets accessible to the combustion community was also discuss, and the BLASTNet database (https://blastnet.github.io) was offered as a repository for data contributed by workshop participants and the broader combustion community.

Flame-Wall Interaction

Flame-wall interaction (FWI) has been a TNF topic since 2014. Experimental and numerical work initially focused on side wall quenching of laminar and turbulent, premixed CH_4/air flames. The scope was broadened in 2022 to include interaction of flame with cooling air near a wall and FWI within a crevice. This TNF16 session provided and update on experimental and numerical efforts, identified common findings and key challenges from different FWI studies, and outlined next steps for FWI research. There have been significant recent activities involving H_2 and NH_3. With these new fuels, an expanded scope with active walls and safety, and the corresponding new configurations, there is a good opportunity to bring experiments and simulations closer together in the spirit of the TNF tradition. With respect to hydrogen, it was noted that the near-wall chemical kinetics of rich hydrogen flames is a key area to be addressed before TNF17. A detailed summary of the FWI session is included in the proceedings.

Future Target Flames – Experiments and/or DNS

The availability of reference data on carbon-free fuels has substantially improved over the last two years. TNF-style comparisons were presented for the Hylon burner and the KAUST piloted NH_3/H_2 jet flames, and both HYLON2 and the KAUST piloted flame are likely targets for the next workshop. Several more potential target cases were introduced during the workshop, including experimental data sets from Sydney, KAUST, TU Darmstadt, and others, as well as several DNS datasets, mainly for premixed hydrogen flames. This session simply outlined all the potential candidates for collaborative comparison with simulations, while next steps for selecting specific target cases for TNF 17 were addressed in the final discussion session and are outlined below.

Key Points and Decisions

Turbulent H_2 and NH_3 flames at atmospheric and pressurized conditions are still poorly understood, and turbulence chemistry interaction models are still in the early stages. The dynamics of hydrogen flames change substantially under pressure, so the extrapolation of atmospheric results to technically relevant conditions is more challenging than previously for hydrocarbon flames. Experiments and DNS for pressurized flames remain a formidable challenge that needs to be coordinated between TNF16 and TNF17. The increasing availability of high-quality experimental and numerical data sets for hydrogen and ammonia flames will allow for TNF-style comparisons at TNF17, aiming to *first break and then advance the models*.

Flashback and flame-wall interaction continue to be relevant topics in the TNF scope. Effusion cooling and active walls are to be considered in the future. The availability of reliable NH_3 kinetics and H_2 near-wall chemistry remain open issues. The selection of chemical mechanisms for TNF target flames should be coordinated to ensure a consistent comparison at TNF17.

The TNF community expressed its strong commitment to return to the more original TNF format with discussion evolving around target flame data sets. In contrast to previous workshops, this will feature not only experimental but also numerical DNS data sets. It is expected that more target flame sessions will be required for TNF17 compared to TNF15 and TNF16.

Next Steps for TNF17

1. **Provide an overview of experimental target flames and data sets**
   Coordinators: Dreizler, Hasse (TU Darmstadt)

TU Darmstadt will prepare brief descriptions (one-pagers) for their experimental configurations as examples. These will include short descriptions of the setup, the employed diagnostics, and the data. Target flame descriptions can include both available data and future data with an approximate date when it can be shared with the TNF community. Data can also include supporting numerical data, e.g., detailed flow conditions from an inflow-LES.

This description can be used as templates for other groups to describe their target flames. These descriptions will be shared among the TNF participants and eventually be published on the TNF website.

Research Data Management has become an important aspect for most funding schemes and recommended data repositories may vary within the TNF community. It was decided that data will be made available by the individual groups using their preferred platform. The data will be assigned a DOI as a unique identifier. New DOIs will be continuously added to the experimental one-pager and published on the TNF website.

2. Provide an overview of DNS target flames and data sets

Coordinator: Attili (University of Edinburgh)

Similarly to the experimental data, University of Edinburgh will prepare a one-pager for the DNS configurations. Following this template, TNF participants working on DNS are invited to provide the description of their own configurations. The aim is to identify a sequences of DNS configurations with increasing complexity, e.g., flame in a box ➔ flame in a temporally evolving shear layer ➔ shear flame.

Sharing the descriptions and the data will follow the approach outlined above for the experimental data.

3. Aligning experimental/DNS work with modeling/LES between TNF16 and TNF17

Coordinators: Dreizler, Hasse (TU Darmstadt)

The one-pagers for experiments and DNS will be shared with the TNF community interested in model turbulent combustion model development and LES. These groups will indicate which flames they will be working on for TNF17. This information will be helpful for both the experimental and DNS groups to better plan their next steps.

The planning should be available spring 2025 and should be updated towards the end of 2025 around the submission deadline for the 41st Symposium.

4. Chemical kinetics for TNF target flames

Coordinators: Stagni (Politecnico di Milano), Magnotti (KAUST)

The current uncertainty in NH_3 kinetics and near-wall H_2 kinetics is a challenge for a consistent comparison of experiments/DNS and LES. It is expected that mechanisms will improve in the near future and new versions will be released.

NH_3: When comparing to DNS data, the same mechanism should be used in LES. When comparing to experimental TNF data, a few suitable TNF-preferred mechanisms will be identified and suggested for LES use. The suggestions will be shared with the TNF community and be published on the TNF website. The TNF community can also support the mechanism development with thermochemical states from Raman/Rayleigh/LIF in laminar counterflow flames. This can also include data at higher pressures of up to 5 bars at KAUST.

H_2 near-wall: Several TNF participants indicated their interest to discuss the issue with colleagues, e.g. from Material Sciences.

Feedback concerning NH_3 and H_2 near-wall should be given to A. Stagni, who will summarize potential next steps.