

Workshop

Summary

The 15th TNF Workshop (International Workshop on Measurement and Computation of Turbulent Flames) and the 17th PTF (Premixed Turbulent Flames) Workshop were held as a combined event on July 22-23, 2022 at the Coast Cole Harbor Hotel in Vancouver, Canada. Traditionally, TNF and PTF have used different formats, with PFT consisting of relatively short, contributed presentations and TNF consisting of longer "curated" sessions on pre-selected focus topics. Overall participation (roughly 80) was lower than expected, due to lingering effects of the corona virus pandemic. This prompted the organizers to combine and blend the programs and presentation styles of the normally-separate workshops. Feedback on this combined approach was generally very favorable, and the PTF and TNF Organizers have discussed the possibility of using a similar approach for at least a part of 2024 workshops in Milan. Italy. These Proceedings follow the format for past TNF Workshops but include information and presentations from the full TNF/PTF program. Slides from PTF contributors are also available from the <u>PTF web site</u>.

A key part of each TNF Workshop has been to present collaborative comparisons of experimental and computational results for selected target flames that are intended to challenge the state-of-the-art in turbulent combustion simulations, while sticking to relatively simple burner geometries and fuels. For 2022, the comparisons were coordinated by Benoit Fiorina and targeted selected cases from the Darmstadt multi-regime burner (MRB). There were also TNF-style sessions on: modeling challenges associated with combustion of hydrogen; combustion of ammonia as an energy/hydrogen carrier; flame-wall interaction; combustion machine learning; and compressible/supersonic combustion. Contributed PTF talks on topics related to these TNF sessions were grouped accordingly in the agenda, while PTF contributions on other topic were grouped into separate PTF-style sessions.

A summary of each TNF-style session (except supersonic combustion) is included in the Proceedings, along with presentation slides. Only a few points from those summaries are listed here.

- **Hydrogen Flames**: Present combustion models do not capture the effects of thermo-diffusive instabilities in turbulent H₂ flames. Predictive and validated models are required in view of the transition toward sustainable fuels. Currently available DNS and experimental databases, as well as needs for new cases, were discussed, and it was proposed that all those interested in collaborating hydrogen combustion should contact Heinz Pitsch (h.pitsch@itv.rwth-aachen.de) to be added to the e-mail list.
- Ammonia Combustion: There is growing interest in ammonia as carbon-free energy carrier, but there are many open questions regarding its deployment in combustion devices, including challenges related to flame stability and pollutant formation. Recent DNS results from SINTEF, Sandia, and KAUST on turbulent combustion of pure or partially-cracked ammonia were reviewed, with emphasis on the importance of thermo-diffusive instabilities in NH₃/H₂/N₂ flames, sensitivity to equivalence ratio of the formation of NO_x and N₂O, the need for accurate chemical kinetic mechanisms for use in DNS and LES, and pressure effects on NH₃/H₂/N₂ flames. Progress on diagnostic developments for ammonia flames, experiments on the resilience to blowout of laminar and turbulent premixed flames of partially cracked ammonia, and initial comparisons of measured and simulated results on turbulent non-premixed jet

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flames of partially cracked ammonia at 5-bar pressure was outlined. Three potential test cases for were proposed for measurement campaigns at KAUST to provide datasets for TNF16.

- **Multi-Regime Combustion**: The session consisted of a brief overview of the Darmstadt multiregime burner (MRB) and available experimental data, a brief review of the Gradient Free Regime Identification (GFRI) approach as applied to experimental data and LES data, and collaborative comparisons of simulation results on selected MRB cases from ten contributing groups. The objective of the joined numerical study is to give a state-of-the-art of turbulent combustion modeling community. Causes of significant differences among predictions of CO were discuss, and possibilities for new target cases emphasizing stratified or multi-regime combustion hydrogen were discussed.
- Flame-Wall Interaction: Flame-wall interaction (FWI) has been a TNF topic since 2014. This session provided updates on recent numerical progress (six contributing groups) and experimental progress (four contributing groups), conclusions regarding common challenges and findings from the different FWI studies, and recommendations on future research needs and priorities.
- **Combustion Machine Learning**: This session was organized to provide the TNF community with an overview of ML techniques and their application to TNF/PTF-related problems in combustion. To this end, this session solicited and reviewed contributions from the TNF/PTF research community, resulting in a total of eleven contributions. The discussion session evolved around four main topics: i) data and how TNF/PTF existing database can be leveraged for CombML applications; ii) the integration of ML into TNF and PTF workshops; iii) pathways for establishing ML-models, best practice, and benchmarks for ML training and ML evaluation; and iv) the integration of domain knowledge into CombML.

The workshop concluded with a **panel discussion** and general discussion on **"Key Points, Opportunities, and Priorities."** Excerpts from the summary of that discussion session (written by K. Ahmed, A. Dreizler, C. Hasse (chair), M. Ihme, and H. Im) are included below.

In the final discussion, we took up the key points of the two days. The challenges for the future are especially new fuels for CO_2 -neutral/ CO_2 -free combustion (H₂, NH₃, and blends, MeOH, EtOH, OME, DMC, SAF). Secondly, physical phenomena or conditions of turbulent flames, including high Ka, high pressure, turbulent flames close to the stability limit, and flame wall interactions are of particular interest. As a starting point for the discussion, three possible targets for the next 2 years were formulated:

- 1. Consolidated chemistry for NH_3 use in DNS and LES
- 2. Transport processes/differential diffusion in turbulent flames (esp. new fuels)
- 3. Experimental and DNS configurations that build on TNF heritage

The key outcomes of the discussion were:

There is a great need for NH₃ kinetics, so kinetics experts from our community should be integrated into the workshop. The goal is to have a common mechanism for DNS and LES.

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Reference configurations for the new fuels will be defined, with two possible options:

- Some blends can probably be investigated in known reference burners. For this purpose, planning is currently underway at the various locations, including Darmstadt and KAUST. The big advantage for the modeling is that simulation setups are available, and several groups worldwide have experience regarding the specifics of the respective configurations. From previous TNF workshops there is extensive knowledge regarding the comparison of the simulations.
- 2. New burners, e.g. for pure H₂ or NH₃/H₂ mixtures, are currently under development. These can be either a new design or a modification of previous configurations. One example is the stratified/steam diluted H₂ burner (CORIA, EM2C) as a further evolution of the previous burner from T. Schuler. Depending on the funding opportunities in the respective countries, several new configurations are expected to become available in the next few years.

Regarding the quantities to be quantified experimentally, the discussion participants emphasized that NO is a crucial quantity for the validation of the model. This should be measured locally in laminar and turbulent flames.

DNS should be integrated into the investigations from the beginning and provide further information that the experiments and LES cannot deliver. As far as possible, phenomena such as flame stabilization and ignition should also be investigated. LES of the DNS configuration could become a part of the model comparisons like the reference experiments.

The participants in the discussion were in favor of having a TNF 15.5 in about a year's time, in preparation for TNF16 in Milan.

Thanks to all who contributed.

TNF15 Organizing Committee:

Robert Barlow, Andreas Dreizler, Benoit Fiorina, Christian Hasse, Matthias Ihme, Andreas Kempf, Peter Lindstedt, Gaetano Magnotti, Assaad Masri, Joseph Oefelein, Heinz Pitsch, Zhuyin Ren, Luc Vervisch

PTF17 Organizing Committee: Andy Aspden, Aaron Skiba, Sina Kheirkhah