SUMMARY

Thirteenth Workshop on Measurement and Computation of Turbulent Flames (TNF13)

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INTRODUCTION

The TNF Workshop series was initiated in 1996 to address validation of RANS based models for turbulent nonpremixed flames and partially-premixed flames where combustion occurs mainly in a diffusion flame mode. The emphasis has been on fundamental issues of turbulence-chemistry interactions in flames that are relatively simple in terms of both geometry and chemistry. Although the TNF acronym has been retained, the word *nonpremixed* has been dropped from the title, and our scope has expanded (since TNF9 Montreal, 2008) to address three challenges:

- Development and validation of modeling approaches which are accurate over a broad range of combustion modes and regimes (nonpremixed, partially-premixed, stratified, and fully premixed).
- Extension of quantitative validation work to include more complex fuels (beyond CH_4) and fuel mixtures that are of practical interest.
- Establishment of a more complete framework for verification and validation of combustion LES, including quality assessment of calculations, as well as development of approaches for quantitative comparisons of multidimensional and time-resolved data from experiments and simulations.

Our overall goal is to accelerate the development of advanced combustion models that are soundly based in fundamental science, rigorously tested against experiments, and capable of predicting flame behavior over a wide range of conditions. One of the most useful functions of this workshop series has been to provide a framework for collaborative comparisons of measured and modeled results. Such comparisons are most informative when multiple modeling approaches are represented and when there has been early communication and cooperation regarding how the calculations should be carried out and what results should be compared. Experience has shown that comparisons on new target flames can generate significant new insights, but also many new questions. These questions motivate further research, both computational and experimental, and subsequent rounds of model comparisons. Another important function of the workshop series is to provide overviews of new work on established target cases, as well as new burner configurations and emerging topics that are relevant to our overall goals and may attract a critical mass of people interested in collaboratively investigating the new burner or research topic.

Previous workshops were held in Naples, Italy (1996), Heppenheim, Germany (1997), Boulder, Colorado (1998), Darmstadt, Germany (1999), Delft, The Netherlands (2000), Sapporo, Japan (2002), Chicago, Illinois (2004), Heidelberg, Germany (2006), Montreal, Canada (2008), Beijing, China (2010), Darmstadt, Germany (2012), and Pleasanton, California (2014). Proceedings and summaries of all the workshops are available at http://www.sandia.gov/TNF.

TNF12 was attended by 101 researchers from 13 countries. The main sessions topics were:

- Update on Stratified Flames
- Sydney Partially-Premixed Jet Flame Comparisons
- Progress Variable and Regime Indicators in Partially-Premixed Flames
- Update on DME Flames
- Counterflow Flames
- Flame-Wall Interaction
- New Burners and Flames
- Experiments and Simulations at Elevated Pressure

The complete TNF13 Proceedings are available for download in pdf format from www.sandia.gov/TNF. The pdf file includes the list of participants, workshop agenda, summary abstracts of technical sessions, presentation slides, and two-page abstracts of the 41 contributed posters.

The sections that follow briefly outline the presentations and key points of discussion. Comments and conclusions given here are based on the perspectives of the authors and do not necessarily represent consensus opinions of the workshop participants. This summary does not attempt to address all topics discussed at the workshop or to define all the terms, acronyms, or references. Readers are encouraged to consult the complete TNF13 Proceedings and also the Proceedings of previous TNF Workshops, because each workshop builds upon what has been done before.

PLANNING

The 2018 TNF Workshop will be held in Dublin, Ireland prior to the 37th Combustion Symposium. It is likely that the schedules of the TNF, ISF, and PTF Workshops will overlap on July 27-28, 2018 (Friday and Saturday). The respective organizers are coordinating on venue and agendas to minimize conflicts and complications for the participants.

Key challenges and research priorities to be addressed before TNF14 are outlined at the end of this summary. Early coordination to select target cases, define ground rules for model comparisons, and establish priorities for collaborative experimental and computational work is strongly encouraged. Regular communication among members of the organizing committee and key contributors is also strongly encouraged. Suggestions for new topics should be communicated to the TNF Organizing Committee.

ACKNOWLEDGMENTS

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HIGHLIGHTS OF PRESENTATIONS AND DISCUSSIONS

Each section that follows was condensed from a session summary in the complete proceedings.

Update on Stratified Flames

Coordinators: Andreas Kempf, Fabian Proch

This was the fourth TNF Workshop to consider stratified combustion as a focus topic. The objective of the session was an update on new simulation results and new experimental data for the stratified burners investigated at Darmstadt University and Cambridge University (with Sandia National Laboratories). Both are co-annular burners with relatively simple geometries, and both sets of experiments were designed to isolate effects of mixture stratification of on turbulent methane flame structure and provide test cases for combustion models. The session included an overview of the geometry and experimental conditions for these two burners, a review of previous comparisons, and results from new simulations completed since the comparisons at the 2014 workshop.

A broad conclusion regarding these flames is that good predictions are achieved by combustion models that treat the stratified flame as an ensemble of homogeneous premixed flames of different mixture fractions. This was not necessarily expected at the outset. The important conclusion that mildly stratified flames can be modeled as premixed flames was also supported by the recently published conditional analysis of the Cambridge flames. Although effects of stratification are present in the experimental results and can be isolated by multiple conditioning methods, the effects on overall scalar structure and flame propagation are minor.

Sydney Partially-Premixed Flame Comparisons

Coordinator: Benoît Fiorina

The objective of the session was to compare recent simulations of the Sydney piloted burner. The burner geometry consists of two concentric tubes surrounded by a pilot annulus. It is centered in a wind tunnel supplying a co-flowing air stream. A set of experimental data has been provided by Sydney University and Sandia. In the configuration studied in the workshop, the central tube is fed with fuel whereas air is flowing through the outer tube. The air co-flow velocity is fixed at 15 m/s. The central pipe can be recessed upstream of the burner exit plane, varying therefore the mixing between fuel and air. For sufficiently large recession distance (Lr) of the inner tube with respect to the burner exit plane, the mixture is nearly homogeneous at the burner exit, while intermediate recession distances lead to equivalence-ratio inhomogeneities. This experimental configuration, conducive to multiple flame structures, is extremely interesting for model validation. It is indeed representative of practical combustion chambers, which may exhibit strong equivalence ratio heterogeneities, promoting the development of mixed combustion regimes. The Sydney burner constitutes a challenging target for turbulent combustion models, which have in general their own flame affinity.

This session provided: 1) An overview of the burner configuration and flame features; 2) An overview of the modeling approaches and simulation parameters used by the different groups; 3) A discussion of specifications for the inflow boundary conditions, including information on precalculated inflows from nonreacting LES by the Princeton group; 4) Comparison of measured and predicted mean and rms profiles of velocity and selected scalars; and 5) Preliminary observations regarding tendencies of different flamelet modeling approaches. Results from a comprehensive parametric experimental study of the effects of pilot flame parameters on the stability of piloted turbulent CNG and LPG jet flames on the Sydney inhomogeneous burner were also presented.

Except for the first radial profiles close to the burner exit, significant differences are observed between simulations and experiments. In particular, most of the computations do not capture the mixing between fuel and air, which makes the analysis of the combustion model difficult. A very large scattering is observed for CO, for which the production rate is very sensitive to the combustion regime. Analysis and conclusions have to be conducted with great care as most of numerical data are preliminary. This exercise is however very promising, mainly for two reasons. First, the configuration is challenging and should break the models, especially regarding the prediction of CO formation. Second, as many groups are involved in the comparison, results can be conditioned by the type of model. For instance, it is possible to verify if several simulations conducted with turbulent combustion model dedicated to premixed flames will draw similar conclusions.

To go further into the analysis, most of the numerical results have to be consolidated. In particular, an improvement of the mixture fraction field is mandatory prior analyzing the turbulent combustion model impact. Ideally, mesh independency studies for mixing and velocity under non-reactive conditions should be conducted. To limit differences between computational set-up, groups should use the same prescription of boundary conditions. Complimentary velocity and mixture fraction measurements on cold configurations would be, in this context, very useful.

Progress Variable and Regime Indicators in Partially Premixed Flames

Coordinators: Robert Barlow, Christian Hasse, Matthias Ihme

This session consisted of three parts, all related progress variable definitions, combustion regime indicators, and the connections between experiments and modeling on these topics. The first part considered alternative definitions of progress variable in the context of Raman/Rayleigh experiments in partially-premixed methane flames. Results on the joint statistics of progress variable and mixture fraction in the Sydney piloted jet flames were presented as examples of a possible additional basis for comparing measured and modeled result in the future.

The second part introduced a novel approach to extract information on the local combustion regime, chemical explosive mode, and heat release rate from 1D Raman/Rayleigh measurements. An important point is that this approach avoids the need to measure 3D gradients, which are used in most definitions of regime indicators in the computational literature.

The third part considered progress variable definitions in the context of modeling. The possibility to optimize a progress variable definition to maximize signal to noise ratio in results Raman/Rayleigh experiments was also introduced. Various combustion regime indicators from the literature were reviewed. A combustion model compliance indicator was introduced, with an example application of flamelet model assignment in LES of the Sydney piloted flame.

Update on DME Flames

Coordinator: Andreas Kronenburg

A series of piloted partially-premixed jet flames of dimethyl ether (25 volume percent DME in air) was introduced at TNF11 to extend experiment/model comparisons to more complex fuels than methane. This session reviewed the available experimental data on these flames and key points from modelling contributions at TNF12. Results from three new modeling contributions were presented, including RANS/multi-environment-PDF of flame DME-F, LES/PDF of flame DME-D, and LES/MMC of flames DME-D and DME-F. New measurements have now extended the parameter range of the original flame series: DME flame G’ has a reduced pilot velocity to increase localized extinction.

New auto-ignition DME experiments of the Sydney group are now available. The fuel jet consists of DME/air mixtures varying from pure DME to a DME-to-air ratio of 1:7. The jet is surrounded by a hot co-flow with temperatures ranging from 1200K to 1500K. The experimental campaign includes lift-off height graphs, simultaneous OH and CH_2O PLIF, temporal evolution and statistics of the flame base and ignition kernels, and simultaneous acoustic and chemiluminescence data. First RANS-PDF computations show strong dependencies on the chemical mechanism during ignition events.

Goals for TNF14 should comprise computations of the entire piloted jet flame series (Sandia DME D-G’) with focus on the accurate prediction of the degree of localized extinction, in particular in flames G and potentially G’. We should also seek clarification of the predictions’ dependencies on the chemical mechanisms. This may include the need for a quantitative comparison of formaldehyde as this is the measured species with the most pronounced differences for all flame and flow conditions.

Counterflow Flames

Coordinator: Jonathan Frank

The session on turbulent counterflow flames extended experimental and computational studies from TNF12 using the two burner designs from Yale University and Darmstadt/Imperial College. New work addressed several issues identified at TNF12. LES (Sandia) of internal flow dynamics in the Yale burner addressed the need for detailed treatment of boundary conditions. LES/PDF parametric studies (Cornell) of partially-premixed methane flames showed excellent agreement with experiments.

Influences of chemistry on combustion regime transitions were investigated (Imperial College) by varying the fuel (CH_4, DME, ETOH) and upper nozzle equivalence ratio (0.2-1.0). Fuel chemistry effects influenced the conditional velocity statistics, and the impact of fuel chemistry on fluid state probabilities indicated an approximate scaling with Da number. Simulations (Duisburg-Essen) of lean premixed CH_4 counterflow flames (Φ=0.8, 0.9) in the reactant-vs-reactant configuration of the Darmstadt/Imperial College burner were extended from TNF12 using both LES/FDF calculations and moment methods.

Goals for TNF14 should include more contributors with different modeling approaches, testing models across different modes of combustion using the counterflow geometry, and using simulations of internal flow to specify boundary conditions at the nozzle exits. A comparison of the two existing internal flow simulations of the Yale burner geometry would be useful. Goals should also include more detailed analysis of conditional statistics using experiments and high-fidelity simulations that focus on the inter-nozzle region. This effort could include additional fuels and flame conditions and sufficiently long simulation times to study the temporal evolution of localized extinction and re-ignition.

Flame Wall Interaction

Coordinators: Andreas Dreizler, Johannes Janicka

Flame-wall interaction (FWI) has been identified as a highly relevant process. However, FWI has received comparatively little attention within the scientific community. Based on issues discussed at TNF12, the objective of the FWI-session at TNF13 was twofold: to introduce a new benchmark configuration that is available as a TNF target flame; and to show the progress made in simulating the physical processes associated with near-wall reactive flows and identify important shortcomings of modeling flame-wall interactions to steer future efforts.

The new target case is a side-wall quenching (SWQ) configuration. Recent measurements regarding the thermochemical state, reaction rates, and velocity boundary layers were presented. For the example of stoichiometric methane-air flames, by comparison with most recent DNS data, it could be shown that diffusion rather than low temperature reactions cause significant deviations within the thermochemical state compared to unbounded flames.

Simulations of FWI by several groups were presented, including works of SINTEF (Trondheim, A. Gruber), UMich (Michigan, V. Raman), EM2C (Paris, O. Gicquel), UniBW (Munich, M. Pfitzner) and TUD (Darmstadt, J. Janicka).

New Burners and Flames

Coordinator: *Wolfgang Meier*

Two burners were presented in this session: The first one was a dual swirl gas turbine model combustor for partially premixed flames that was developed by KIT and DLR within the collaborative research center SFB606. This dual swirl burner was operated with methane and air at thermal powers of typically 25 kW. Raman multispecies and temperature measurements as well as PIV velocity measurements have been performed for two cases: (1) A stable flame with P_{th} = 22.5 kW, φ = 0.63 and air split ratio between outer and inner swirler of 1.6; (2) an oscillating flame with P_{th} = 25.0 kW, φ = 0.70 and air split ratio of 1.6. The second burner was the industrial gas turbine swirl burner G30 DLE from the Siemens SGT-100 turbine that was investigated in a high-pressure test rig and included here as part of the introduction to the challenges of experiments and simulations at elevated pressure. Experimental data on this burner is currently available only to cooperation partners of Siemens.

Experiments and Simulations at Elevated Pressure

Coordinator: *Bill Roberts, Hong Im, Joe Oefelein*

The intent of this session was to introduce key issues and challenges associated with model validation efforts for combustion at elevated pressure. The session started with an overview of a few existing high pressure facilities designed for studying canonical flames, followed by the description of the new KAUST facilities that will be available for international collaboration. An overview of challenges and opportunities for temperature and major species measurements in high pressure flames at the KAUST facility was also presented. To guide the experimental effort, large eddy simulations (LES) capabilities have been developed by the KAUST group in collaboration with University of Rome, and initial simulations at various pressure conditions have been conducted. Based on scaling, increasing Re with pressure, while maintaining Da approximately constant, is proposed as a first set of parametric studies for the TNF community.

The Sandia group focused on challenges and progress in modeling turbulent combustion processes at elevated pressure, including simulation of multiphase and supercritical fuel injection and mixing with real-fluid thermodynamics and transport, use of UQ methods to optimize chemical models for simulations, and simulation of auto-ignition dynamics. Recent developments in quantitative imaging of turbulent mixing dynamics in high-pressure fuel injection systems were also reviewed.

KEY CHALLENGES AND PRIORITIES

In the area of stratified combustion it would be desirable to develop a burner configuration that achieves higher levels of stratification (higher local mixture fraction gradients) and higher levels of turbulence than in the TU Darmstadt and Cambridge/Sandia cases considered so far.

An important related challenge is to extend work that has been done in measurement and modeling of highly turbulent premixed flames (e.g., Sydney PPJB). High-turbulence and high-Ka premixed flames were prominent on the agenda of the Premixed Turbulent Flames (PTF) Workshop, so the topic was dropped from TNF13 to avoid conflicts. Coordination with the PTF organizers may facilitate a broader community effort in this area.

The Sydney piloted inhomogeneous jet flames attracted many modeling efforts, but because most of the computational results were preliminary, more work will be needed to allow for detailed comparisons. On the experimental side, velocity measurements (nonreacting and reacting) are needed at flow conditions matching those of the scalar experiments. On the simulation side, there are needs to consolidate the treatment of boundary conditions, improve mixture fraction predictions, demonstrate mesh independence, and improve CO predictions. Application of conditional averaging should also be done in a coordinated way to achieve better physical understanding.

Regime identification and regime-independent modeling will be important topics for TNF14. Further work on development of regime indicators for simulations and experiments should prove beneficial for understanding of multi-regime combustion.

Development of target cases that combine features of high turbulence, high mixture-fraction gradients, and regime crossing should be considered. Important objectives in this context would be to avoid high sensitivity to boundary conditions (such as with piloted flames near blowoff) and include features relevant to practical combustors, while keeping geometric complexity within the reach of most academic codes.

It is important to continue working with fuels more complex than methane. Goals for TNF14 should comprise computations of the entire piloted DME jet flame series (Sandia DME D-G') with focus on the accurate prediction of the degree of localized extinction. We should also seek clarification of the predictions' dependencies on the chemical mechanisms. This may include the need for a quantitative comparison of formaldehyde, as this is the measured species with the most pronounced differences for all flame and flow conditions. Quantitative LIF of formaldehyde remains a challenge. Direct measurements of intermediate species by Raman scattering have proven difficult, but important progress has been made, and such data may still allow for more detailed comparisons. Modeling of recently measured DME jet flames in hot coflow (Sydney) should be considered as possible focus topics for TNF14.

For counterflow flames the goals for TNF14 should include more contributors with different modeling approaches, testing models across different modes of combustion using the counterflow geometry, and using simulations of internal flow to specify boundary conditions at the nozzle exits. A comparison of the two existing internal flow simulations of the Yale burner geometry would be useful. Goals should also include more detailed analysis of conditional statistics using experiments and high-fidelity simulations that focus on the inter-nozzle region. This effort could include additional fuels and flame conditions and sufficiently long simulation times to study the temporal evolution of localized extinction and re-ignition.

The side-wall-quench (SWQ) flame is proposed as a future TNF target configuration. Priorities for experimental work are to measure more scalars, measure wall temperature and heat transfer, and conduct parametric variation of such things as wall temperature, surface coatings, fuel, and effusion cooling.

Other challenging topics that are important for the overall TNF goals but were not included as main topics at TNF13 are: quality metrics and uncertainty quantification in LES; analysis and comparison of multi-dimensional data from experiments and simulations; and hot coflow flames, specifically cases where the mechanism of stabilization transitions between auto-ignition and flame propagation.