SUMMARY

Sixth International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames

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INTRODUCTION

The series of workshops on Measurement and Computation of Turbulent Nonpremixed Flames (TNF) is intended to facilitate collaboration and information exchange among experimental and computational researchers in the field of turbulent nonpremixed (and partially premixed) combustion. The emphasis is on fundamental issues of turbulence-chemistry interaction, as revealed by comparisons of measured and modeled results for selected flames.

TNF6 was attended by 64 researchers from 12 countries. Thirty-five posters were contributed and abstracts are included in the proceedings. The main agenda for the discussion sessions was divided roughly into four parts:

1. Presentations and discussion on specific submodels (mixing, chemistry, radiation, and scalar dissipation) mainly in the context of piloted jet flames
2. Comparison of measured and modeled results on bluff-body-stabilized and swirl-stabilized jets and flames
3. New experimental work, including new measurements on TNF target flames and experimental techniques directed at LES validation.
4. Proposals, priorities, and planning for future work and TNF7 (Chicago, 2004).

The complete TNF6 Proceedings are available for download in pdf format from the Internet at www.ca.sandia.gov/tdf/Workshop. The pdf file includes materials from the proceedings notebook that was distributed to workshop participants in Sapporo, as well as additional materials (such as vugraph copies) contributed after the workshop. This summary briefly outlines highlights from presentations and discussions on these topics. 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.

Results in this and other TNF Workshop proceedings are contributed in the spirit of open scientific collaboration. Some results represent completed work, while others are from work in progress. Readers should keep this in mind when reviewing these materials. It may be inappropriate to quote or reference specific results from these proceedings without first checking with the individual authors for permission and for their latest information on results and references. It should also be noted that several papers relevant to the target flames were presented at the 29th Combustion Symposium, and these papers contain more detailed descriptions and comparisons than are included here.

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HIGHLIGHTS OF TECHNICAL DISCUSSIONS

Mixing Models and Piloted Jet Flame Calculations

Parametric evaluation of mixing models for pdf calculations was a major focus topic for this workshop. S. Pope (see full Proceedings) presented comparisons of the properties and results of three mixing models: modified Curl, EMST, and IEM. Highlights are outlined below in the context of the piloted methane flames.

At TNF4 and TNF5 calculations of the Barlow & Frank flames, *D*, *E* and *F* were presented by several groups. But for flame *F*, which exhibits substantial local extinction, there were only four sets of calculations, all using PDF methods. These were from the groups at Berkeley, Cornell, Darmstadt, and Imperial College. At TNF6 further PDF calculations were contributed by the Imperial College and Cornell/Fluent groups, and predictions of extinction/re-ignition in the *D-E-F* flame series was demonstrated using ODT (Echekki et al. poster). From all of these calculations the following conclusions can be drawn, and suggestions made.

- The model calculations have a first order dependence on both the mixing model and chemical mechanism used.
- Increasing the mixing rate (through the constant C_ϕ) decreases the calculated extent of local extinction.
- Calculations in good agreement with the data for flame *F* have been obtained with two approaches:
    1. with the modified Curl model (C_ϕ =2.3) and the Lindstedt mechanism (Imperial College)
    2. with the EMST model (C_ϕ = 1.5) and the augmented reduced mechanism (Cornell University).
- Flame *F*, being close to global extinction, is sensitive to small changes in boundary conditions and model constants. Hence it is more reliable to study the behavior of models as a function of jet velocity (from flame *D* to *E* to *F*), rather than just at one fixed condition.
- All current mixing models have unsatisfactory aspects.
- The fuel used by Barlow & Frank (methane/air in volume ratio 1:3) has a stoichiometric mixture fraction of $\xi_s \approx 0.35$, which makes the flame easier to model than a flame of pure methane ($\xi_s \approx 0.05$). Hence it would be valuable in future experiments to vary the fuel mixture (and hence ξ_s), as well as for modelers to consider the older data, which is available for a range of fuels.
- A systematic study of different mixing models *and* chemistry mechanisms is still needed. To this end, the different mixing models and mechanisms are to be made available on the web.

In addition to the calculations noted above, Lindstedt and Louloudi presented a paper at the 29th Combustion Symposium that is directly relevant to this TNF6 discussion topic. They performed pdf calculations on a series of four piloted methanol flames (ξ_s = 0.135) and achieved reasonable agreement with measured trends in local extinction by using the same mixing model parameters as for their methane flame calculations. They also include some discussion of the effects of changing C_ϕ, and note that re-ignition may be more sensitive than extinction.

Chemical Mechanisms

For methane/air flame studies, the principal mechanisms in use by TNF Workshop participants are GRI 2.11, GRI 3.0, Lindstedt's mechanism, and reduced versions of these same mechanisms (with 12 or more steps and 16-20 species, including NO). Differences among these mechanisms are considered small with regard to predictions of major species. However, flames approaching blowoff are recognized as sensitive to small differences in various parameters. Therefore, broad availability of mechanisms will facilitate further parametric studies on the coupled influence of submodels and their parameters on computed results.

Work was begun immediately after TNF6 to make several relevant mechanisms available in Chemkin format. The following reduced mechanisms will be made available for download from the TNF web site:

- Methanol – reduced mechanism from Lindstedt with Chemkin translation by J-Y Chen
- Methane – reduced versions of GRI 2.11 and GRI 3.0 from Chen and coworkers, including ARM2 as used by the Cornell group.
- $CO/H_2/N_2$ – reduced mechanism from Chen (tested only for the Sandia flame mixture)
- H_2 – 5-step reduced mechanism from Chen (already on the web)

The relative performance of various mechanisms in predicting NO formation in laminar CH_4/air flames was a major topic at TNF5 (Delft 2000). Further direct comparisons are needed and would be facilitated by availability of mechanisms in a common format. However, the tentative conclusion from TNF5 remains that the Lindstedt methane mechanism and GRI 2.11, as well as reduced versions, yield NO results in reasonable agreement with measurements in laminar CH_4/air flames having the same degree of partial premixing as the piloted jet flames (75% air, 25% CH_4).

It appears that the relative performance of mechanisms in predicting NO in methane flames depends on the degree of partial premixing. In the context of future TNF comparisons of NO results in the Sydney bluff-body and swirl flames (CH_4, 1:2 CH_4/air, and 1:1 CH_4/H_2), it would be useful to test various mechanisms against measurements from laminar flames with these same fuel mixtures.

Radiation

The main effect of flame radiation in calculations of the piloted jet flames is to reduce the predicted level of NO; the influence of radiation on major species mass fractions is not significant in the calculations. Therefore, the main question facing TNF participants is whether the recommended radiation model, which assumes the optically thin limit, is adequate for assessment of NO predictions in the target flames. Unfortunately, we have yet to reach a clear conclusion on this because there appear to be contradictions among calculated results for total radiant fraction, which is the most reliable experimental indicator of the integrated effect of radiation. Values (from past workshops) of the predicted total radiant fraction from piloted flame D range from about 6% to about 12%, even though the radiation model is supposed to be the same and the predicted scalar and velocity fields are similar. The measured radiant fraction is 5.1%, so some calculations suggest the optically thin model is about right, while others suggest that it over predicts radiation by more than a factor of two. Reasons for the differences in the predictions are still unclear, and careful comparisons of model implementations might be useful.

A detailed study of several radiation models applied to flame D was presented on a poster by Coelho et al. Their results suggest that the optically thin model is not accurate for flame D and that a more sophisticated radiation model is needed for agreement with the measured radiant fraction. Unfortunately, the authors were unable to attend the workshop, so this work was not fully discussed. Detailed radiation calculations are computationally expensive, and the consensus among modelers present at TNF6 was to continue using the optically thin model for now.

For calculations that include NO formation, modelers are still encouraged to run both adiabatic and radiative cases to represent upper and lower bounds on the predicted NO levels.

New spectral radiation data are available on several of the TNF jet flames (see the contribution by Zheng et al.). Such data can be used to evaluate the relative importance of absorption of the strong CO_2 band within the flame.

Scalar Dissipation

The scalar dissipation, χ, is an important quantity in most modeling approaches to non-premixed turbulent combustion. The statistics of primary interest are its PDF, its variance, and its conditional mean. In spite of their importance, model predictions of scalar dissipation statistics are seldom reported. It would be profitable now for modelers to pay more attention to scalar dissipation. What do different models imply for scalar-dissipation statistics? How do these compare to the available experimental data?

Overviews of issues relevant to the modeling and measurement of scalar dissipation were presented by R. Bilger and R. Barlow, respectively. The main conclusion from both is that more work is needed. Good progress is being made on the experimental side, as represented by the contributions from Karpetis & Barlow and Frank et al. Details of both experiments are presented in 29th Combustion Symposium papers. However, we are not yet at the point of fully understanding the limitations and accuracy of these measurements, so it is still premature to conduct quantitative comparisons with models.

Another 29th Symposium paper that is very relevant to this topic is from H. Pitsch and presents a LES/unsteady-flamelet calculation of flame D that achieves improved agreement on CO, H_2, and NO by accounting for the effect of resolved scalar dissipation rate fluctuations. This result suggests that the over prediction of reaction progress in fuel-rich conditions observed in other flamelet-based calculations and in CMC results for flame D may also be corrected by improved modeling of scalar dissipation.

Scalar dissipation is expected to be a major topic for the next workshop. An important issue to be addressed by experimentalists and modelers in collaboration is how best to compare 1D and 2D results from experiments with models representing scalar dissipation in the 3D field. Issues of spatial resolution in the measurements will also require careful attention.

Bluff Body Flow and Flame Comparisons

For the non-reacting case, two submissions were made: an LES calculation from TU Darmstadt (Kempf and Janicka) and a standard RANS(k-e) calculation by McDermott Technology (Sayre). For the reacting case HM1, there were a range of submissions from three groups: Pope's at Cornell using the PDF approach, Lindstedt's at Imperial College using unsteady RANS and PDF, and Roerkaerts' at TU-Delft using RANS (and computing case HM1E instead of HM1). In his PDF calculations, Lindstedt used a 20 species detailed mechanism that included NO. All other calculations assumed either flamelets or equilibrium chemistry.

Generally, calculations are in much better agreement with the measurements and this is a substantial advance made since the last workshop. The LES calculations for the non-reacting cases are very promising and should be extended to the reacting cases. Improved numerical methods used with Pope's PDF approach have resulted in significant improvements, since TNF5. It appears that the discrepancy, which remains between the measurements and the calculations at downstream locations in the jets and flames, may be due to vortex shedding on the outer surface of the bluff-body. Lindstedt's transient calculations support this argument, since they show better agreement at downstream locations. It is worth noting here that vortex shedding was imaged in these flames and reported in 1998 (Masri at al., *Proc. Comb. Inst*. 27:1031-1038, 1998). It is of interest, therefore, to compare approaches based on steady RANS, unsteady RANS (axi-symmetric and 3*D*) and LES.

While using the fast chemistry assumption (or flamelets) may be adequate to compute the mean temperature and compositional structure in the recirculation zone of flame HM1, calculations further downstream are more likely to require detailed chemical kinetics due to the occurrence of some localized extinction. The computations of Lindstedt, which use 20 species, are adequate for temperature, major species and NO but not for CO and OH, which still show significant deviations. It should be noted that the flame considered here (HM1) does not exhibit large finite-rate chemistry effects. For TNF7, the series HM1, HM2 and HM3 should be target flames, so as to test the models' abilities to represent local extinction and other finite-rate chemistry phenomena. For these flames the comparisons should be expanded beyond spatial profiles to include such things as scatter plots, conditional means, and the burning index for select scalars.

Swirl Flow and Flame Comparisons

It is a natural progression for the TNF program to tackle increasingly complex flows, which are more relevant to practical combustors. The swirl burner, developed at the University of Sydney and introduced in TNF5, provides such a flow, which has the added complexity of swirl and flow recirculation, while maintaining simple boundary conditions. Depending on the swirl number and stream velocities, this flow displays a rich variety of qualitatively different flow patterns. In many cases there appears to be large-scale unsteadiness, including the precession of the jet. A range of swirling jets and flames, for which an extensive database is made available on the web, are now target problems for TNF workshops.

For TNF6, two non-reacting jets and two flames were selected for calculations. The jets (N16S159 and N29S054) have swirl numbers of 0.5 and 1.6 and a jet velocity of 66m/s. The first flame is (SMH1) which uses a mixture of methane-hydrogen (1/1 by vol.), has a swirl number of 0.37, a fuel jet velocity of 140.8m/s and is at 53% of the blow off velocity. The second flame is (SMA2) with a methane-air mixture (1/2 by vol.), a swirl number of 1.59, a fuel jet velocity of 66.3m/s. Flame SMA2 is at 31% of the blow off velocity.

Only a few calculations of these new target cases were presented. The University of Sydney submitted results using full 3D, transient RANS calculations for the non-reacting jets and 2D axisymmetric calculations for the flame. The computed velocities for the non-reacting jets are very close to the measurements for the low swirl number case (N29S054) but deviations are more significant at high swirl numbers (N16S159). The 2D axisymmetric results for the flames are less encouraging implying that full 3D transient calculations are necessary. It should be noted that vortex breakdown and jet precession are computed for the non-reacting cases and these must be verified against experimental data. Pitsch from Stanford performed LES calculations for the high swirl case of the nonreacting flow and showed encouraging results (vugraphs added to the final proceedings).

It is noted that an improved set of boundary conditions is necessary and this will be provided in time for TNF7.

New Experiments on TNF Flames and Experiments Directed at LES Validation

Nearly all comparisons of measured and modeled results for TNF target flames have been based on single point statistics of scalars and velocity. Such comparisons are relatively easy to perform and interpret, and they are expected to remain the primary means for quantitative evaluation of turbulent combustion models. However, it will be necessary to expand comparisons to include quantities that represent the spatial structure and flow dynamics of target flames, such as the bluff-body and swirl flames, which may be strongly affected by large-scale unsteadiness. The definition of procedures and criteria for such comparisons will be an important area for collaboration between experimental and computational researchers.

These two sessions in the TNF6 agenda were intended to: i) raise awareness concerning experimental techniques and types of data that may be useful for future comparisons with models, ii) promote discussion to identify specific data needs of modelers, particularly with regard to LES validation, and iii) promote discussion of specific criteria for comparing measured and modeled results on spatial structure and flame dynamics.

Several new experiments were conducted on various TNF Workshop flames over the past two years, and the majority of these involved imaging techniques or time series measurements of spatial structure or dynamics. New experiments included various measurements in the Darmstadt turbulent opposed jet burner, measurements of scalar dissipation in piloted flame D, combined PIV and multi-frame OH-PLIF imaging in the DLR $CH_4/H_2/N_2$ jet flame, and OH time series measurements in the Darmstadt "H3" hydrogen jet flame. In addition, A. Dreizler presented an overview of techniques and issues related to experimental validation of LES models.

Discussions of specific data needs and criteria for comparison were limited, reflecting the fact that this is new ground. Continued discussion of these issues is strongly encouraged because the high costs of relevant experiments and large-scale calculations will limit our opportunities for meaningful, quantitative comparisons.

State of LES

A significant advance in TNF6 was the presentation of LES calculations of several of the target flames. In order for LES to be a reliable predictive tool, care must be taken (a) to ensure that the grid is sufficiently fine to resolve the bulk of the energy and stress (b) to have an appropriate means to specify time-dependent turbulent inflow conditions, and (c) to model the subgrid turbulence/chemistry interactions.

It is clear from the LES calculations presented that a wide variety of grid resolutions are being employed. This disparity is primarily due to limited computational resources and the long turn-around times required when one uses denser (but preferable) grids. As research progresses, it will become imperative that grid resolution issues be addressed in a systematic way to establish the appropriate performance metrics and better separate numerical errors from modeling errors.

The issue of boundary conditions was also addressed to some degree and will be an issue of high priority in future workshops. LES requires the specification of both mean flow quantities and the higher time evolving moments at respective inflow boundaries. Well-defined pressure conditions must be provided at out-flow boundaries of bounded domains with subsonic flow. This is especially important for recirculating swirl flows in confined geometries. Unbounded domains pose analogous requirements. It will be important in future studies to understand the influence of various boundary condition treatments on interior flow characteristics.

The appropriate specification of boundary conditions is inherently coupled to the specification of grid resolution requirements and the related sensitivities. Ideally, future studies should address both issues simultaneously. Detailed analysis of the accuracy and sensitivities associated with LES subgrid-scale models, particularly those associated with turbulence/chemistry interactions, can only occur after we have a high level of confidence in our ability to simulate the geometrically dominated turbulent fluid dynamic processes associated with the various target flames.

Because combustion occurs at the smallest scales, it will become more and more important to study subgrid turbulence/chemistry interactions with minimal ambiguities associated with both the experiments and companion calculations. To achieve this goal in the systematic manner described above it is imperative that the target flame descriptions include simultaneous velocity-scalar measurements with well documented boundary conditions. Good progress has been made, and it will become more and more important to establish high-fidelity benchmarks that systematically focus on the three key areas outlined above.

Other Topics

While the TNF Workshop is mainly focused on fundamental issues, many participants are separately involved in research more directly related to applications and, in particular, gas turbine combustors. In the interest of promoting collaboration and information exchange in this area of common interest, time was allotted for several people to give brief overviews of research activities related to combustion in gas turbines, including both premixed and nonpremixed combustion. Details are not included in the proceedings, but expanded collaborations in this area are expected.

L. Rahn (see poster abstract) described US DOE supported work to develop network tools for data sharing. One current project that may be directly useful to TNF participants is the development of web-based tools for automatic translation of chemical mechanisms across different formats. This could facilitate parametric comparison of chemical mechanisms in combination with other submodels. Formatting and sharing of large data sets from imaging experiments and from LES calculations is another area of anticipated future need. We will be following progress in both areas.

AREAS FOR FURTHER WORK

During the closing discussion, several areas for further work related to the main target flames were identified and are listed below with the hope that progress can be made in these areas before the next workshop. In addition to these listed topics there is ongoing work by several groups on other TNF target flames and other topics closely related to the workshop objectives. This includes work on such things as chemical mechanisms for TNF use, radiation modeling, turbulence modeling, development of LES for combustion, measurement and calculation of other TNF flames, and development of experimental methods.

Piloted Jet Flames

- Systematic evaluation of mixing models and chemical mechanisms (in combination), with particular attention to the sensitivity of local extinction and re-ignition to changes in these submodels.

- Further experiments in which parameters are varied (e.g., the fuel composition). There is particular interest in cases with a lower stoichiometric value of the mixture fraction.

- Calculations and evaluation of older Sydney/Sandia data sets with other fuels. There may be greater errors in some species results from these older experiments, but information on local extinction trends should be very useful for the combined evaluation of mixing models and chemical mechanisms.

- Continued experiments on scalar dissipation and related quantities, combined with collaborative work to define appropriate ways of comparing measured and modeled results.

Bluff Body Flames and Swirl Flames

- Examination of turbulence/chemistry interactions in the series of bluff-body flames HM1, HM2, and HM3. Model calculations that achieve good agreement with measured velocity and scalar fields in a complex, recirculating flow and also track the trends of localized extinction and re-ignition would represent a major step forward.

- Measurements of velocity profiles upstream of the burner exit and inside the annulus of the swirl burner were specifically requested by LES modelers because bulk velocities and profiles downstream of the exit are not sufficient for good specification of the model problem.

- More calculations of the Sydney bluff-body swirl burner using LES, PDF, and 3D-transient RANS.

- Examination of large-scale, unsteady motions via LES and/or unsteady RANS.

- Examination of flames of other fuels such as methanol and H_2/CO.

- Consideration of existing data and future needs for experimental results on the spatial structure and dynamics of the bluff-body and swirl cases.

PROPOSALS FOR NEW TNF TARGET FLAMES

TNF Workshop has approached the model validation process by selecting target flames that cover a progression in complexity, with respect to both fluid dynamics and chemical kinetics. This has made it easier to isolate specific submodels and understand their capabilities and limitations. In adding new target flames it is desirable to select cases that test the robustness of specific submodels or include new combustion processes that must be mastered on the way to developing predictive capabilities for practical combustion systems. It is also important to avoid cases that are too far beyond present modeling capabilities or cannot be characterized with the accuracy and completeness needed for useful comparisons with models.

Three types of flames were proposed. Inclusion of these flames as formal workshop targets will depend upon the level of interest from modelers and upon the quality and completeness of the available measurements.

Lifted Jet Flames

Flame stabilization in a non-uniformly mixed flow is a challenging model problem. Most turbulent burners are operated so that the flame is not in direct contact with hardware (i.e. lifted). The nonpremixed swirl flames being studied at DLR and at Stanford as simple analogues of gas turbine combustors are both lifted. Furthermore, in many of the Sydney Bluff-Body and Swirl cases the reaction zone at the outer edge of the recirculation zone is lifted above the corner of the bluff body. The lifted jet flame is an appropriate starting point for investigation of models that must eventually predict the flame stabilization details of more complicated burners.

Lifted flames have received a lot of attention in the experimental literature. Therefore, existing experimental data on lifted flames should be considered before new experiments are undertaken. There is also a need for some discussion regarding the types of experimental data that will be most useful. Because lifted flames can be sensitive to coflow conditions, the coflow needs to be carefully controlled and characterized. The same is true for all boundary conditions. Experimental parameters, such as coflow velocity and jet velocity, and fuel composition, should be varied in order to test models' abilities to reproduce trends.

Vitiated Coflow Flames

Data for a possible model flame investigated at UC Berkeley by Dibble and Cabra are available (see Cabra et al. poster abstract). The Berkeley flames are lifted flames stabilized in a vitiated coflow. Practical burners use recirculation of combustion products to promote flame stabilization, and the Berkeley burner was designed to examine flame stabilization in combustion products without the complexity of flow recirculation.

Dally at Adelaide has also a possible data set for a range of flames stabilized on a FLOX burner, which has reduced O_2 and elevated temperature in the coflow. (see Dally et al. poster abstract).

Spray Flames

Masri's group at the University of Sydney is developing a data set for spray flames with well-defined boundary conditions and dilute loadings.

ORGANIZATION OF TNF7

Location and Dates – The TNF7 Workshop will be held in the Chicago area near the time of the 30th Combustion Symposium (probably just before).

Target Problems – We can expect TNF7 to include work on piloted, bluff-body, and swirl flames as outlined above in AREAS FOR FUTURE WORK. Additional target flames or focus topics will be added as appropriate, based on research progress and the interests of the organizers and participants.