SUMMARY

Seventh International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames

22-24 July 2004
Chicago, IL

R. S. Barlow, R. W. Bilger, J.-Y. Chen, A. Dreizler, J. Janicka, A. Kempf, R. P. Lindstedt, A. R. Masri, J. O. Oefelein, H. Pitsch, S. B. Pope, D. Roekaerts

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 combustion. The emphasis is on fundamental issues of turbulence-chemistry interaction in nonpremixed and partially premixed flames, as revealed by comparisons of measured and modeled results for selected flames. Several participating research groups have strong interest in applying this same framework for detailed measurement–model comparisons to the areas of premixed- and stratified premixed combustion. There is also growing interest in the use of detailed simulations to complement experimental benchmarks for model testing and validation. Our goal in these combined efforts is to accelerate the development of advanced combustion models that are soundly based in fundamental science, rigorously tested against experiments, and capable of predicting the behavior of a wide range of turbulent combustion situations.

TNF7 was attended by 80 researchers from 12 countries. Twenty-nine posters were contributed, with abstracts included in the proceedings, and several additional posters were displayed to augment the invited presentations. Discussion sessions addressed several topics, which are listed in order of the agenda:

- Comparison of measured and modeled results on bluff-body-stabilized flames
- Progress on the Sydney swirl flames
- Statistical modeling of extinction and re-ignition
- Update on radiation modeling for TNF target flames
- Measurements and modeling of scalar dissipation
- Progress in LES of Combustion
- Strategies for linking DNS, LES, RANS, and experiments
- Overview of lifted flames
- Status of experimental studies of premixed combustion
- Priorities and planning for future work and TNF8 (Heidelberg, 2006)

For each main topic a session leader (member of the organizing committee or invited speaker) provided an overview, which included the work of others as well as their own, and outlined key issues for discussion and further work. This format has proven effective in maintaining the focus and continuity of the workshop series, while allowing for inclusion of relevant work by people outside the core of active participants in this collaborative process.

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. Readers are encouraged to also consult summaries from previous TNF Workshops because each workshop builds upon what has been done before.

The complete TNF7 Proceedings are available for download in pdf format from the Internet at www.ca.sandia.gov/TNF. The pdf file includes materials from the proceedings notebook that was distributed to workshop participants in Chicago, as well as additional materials (such as PowerPoint slides) contributed after the workshop.

Several papers relevant to the TNF7 topics and target flames were presented at the 30th Combustion Symposium. Most of these papers may be found in the sections on turbulent combustion within the *Proceedings of the Combustion Institute*, Vol. 30.

ACKNOWLEDGMENTS

Arrangements for the TNF7 Workshop were coordinated by Ms. Judy Neilsen of Sandia. Sponsorship by ANSYS, Continuum Lasers, Fluent, General Electric Aircraft Engines, Reaction Engineering International, Rolls-Royce, and the German SFB-568 research program are gratefully acknowledged. These contributions allowed for reduction of the registration fees for university faculty and students. Support for R. Barlow's work in coordinating TNF Workshop activities is provided by Sandia National Laboratories with funding from the US Department of Energy, Office of Basic Energy Sciences. We especially acknowledge the long-term support of this effort by Bill Kirchhoff, who retired from DOE in 2004.

AN IMPORTANT NOTE OF CAUTION

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.

HIGHLIGHTS OF PRESENTATIONS AND DISCUSSIONS

PowerPoint slides or other prepared materials for each of the main presentations are included in the TNF7 Proceedings.

Comparisons on the Sydney Bluff-Body Stabilized Jets and Flames

Andreas Kempf coordinated and presented a comparison of model calculations of selected cases of the Sydney University bluff-body flames. This type of comparison of multiple model calculations with each other and with experimental results on velocity and scalar fields is probably the most important function of the TNF Workshop series. Such broad and detailed comparisons are almost never seen in the archival literature, yet they offer important information on the relative success of various modeling approaches and the adequacy of experimental data sets as benchmarks for model validation.

Numerical data for all five hydrogen-methane bluff-body flames (HM1e, HM1, HM2, HM3e, HM3) were contributed and compared. The results originated from Kuan&Lindstedt (Imperial College), Liu&Pope (Cornell), Naud&Roekaerts (Delft, Zaragoza), Pitsch&Raman (Stanford, CTR) and Kempf&Janicka (Darmstadt), using approaches from URANS with flamelet chemistry (Imperial College) via Hybrid PDF methods (Cornell, Delft/Zaragoza) to LES (Stanford/Darmstadt).

For the first time, results for the flames HM2 and HM3 were submitted. Both Kuan&Lindstedt and Liu&Pope achieved excellent predictions, where Kuan&Lindstedt have even managed to accurately predict the mixture fraction downstream of x/D = 1.0.

The low speed case HM1(e) was considered by the groups from Cornell, Delft/Zaragoza, Stanford, and Darmstadt, having achieved some progress for the flow-field and major improvements for the scalar fields. The RANS simulations (Cornell, Delft/Zaragoza) show balanced data now, whereas the LES has both strong features and discerning problems: Darmstadt is struggling with numerical oscillations at the centerline, and Stanford hardly predicts any turbulence for the outer shear layer at all. All four simulations show reasonable predictions of the mixture-fraction close to the bluff body, but only Stanford can match the experimental results downstream from x/D = 1.0. Based on these observations, a discussion evolved on how the outer shear layer affects the mixture fraction field. So far, no final answer can be given.

To conclude, the results presented are major steps forward from TNF6. The methods applied have matured, their understanding has improved, and their cost has dropped, as indicated by the entry of LES and a single groups' ability to simulate four flames (Cornell).

For the future, it is suggested to present the calculations in mixture fraction space as well, given that the computation of the flow-field can be expected to be on a high level at TNF8. This will require the availability of conditional means, which will be compiled by Masri.

Swirl-Stabilized Jets and Flames

A comprehensive data set now exists for a range of swirling jets and flames stabilized on the Sydney burner. Depending on the swirl number and stream velocities, a range of flame shapes are stabilized all of which are documented. Flow precession and instabilities exist for both reacting and non-reacting flows and are driven by different modes; only some of which are understood. Some data are available for the flow precession. The entire data set is now made available on the web. There was extensive discussion about this flow, which is receiving particular interest from various LES groups particularly at Stanford and Darmstadt. The following points are made:

- Conditional means need to be provided for the data available for these flames, both with and without density weightings.

- A path needs to be provided for modelers as to the order of difficulty of the flames, i.e. (i) symmetric flames without precession and far from blow-off, (ii) symmetric flames without precession but close to blow-off, (iii) precessing flames.

- Detailed boundary conditions are needed, including time series for the velocity in the swirling annulus and temperature of the ceramic face.

Statistical Modeling of Extinction and Re-ignition

This session, led by Steve Pope, expanded on the TNF6 comparison of the IEM, MC, and EMST mixing models. Additional comparisons were presented of results using these mixing models within PDF and PaSR calculations of several TNF flames that include extinction and re-ignition. Highlights were also presented from a recent DNS study by Mitarai, Kosaly & Riley of mixing model performance. The presentation also posed the questions: What is the dimensionality of the accessed composition space in flames with extinction, and what are appropriate conditioning variables? The conclusions on mixing models that are outlined in the TNF6 summary are essential background to the following points.

- Understanding of mixing model performance is improving. Resilience to extinction increases in the order IEM < MC < EMST and also increases with increasing C_ϕ. MC produces more scatter than EMST.

- Good performance of EMST and MC has been achieved through tuning of C_ϕ.

- Little progress has been made toward understanding the coupled behavior of mixing models and chemical mechanism. Progress on this point from TNF6 will require general availability of all the mechanisms in use by various groups.

- Mixing models perform better in the DNS study when mixing interactions occur locally within a filtered subvolume (LES context as opposed to RANS context).

- Recent results by Sutherland et al. from a 2D-DNS of a $CO/H_2/N_2$ jet flame with extinction show that CO_2 is much more effective than χ in reducing the realized composition space to a two-dimensional manifold. This serves to illustrate that progress variable approaches provide natural ways to efficiently parameterize extinction.

- The choice of progress variable is crucial, and further insights on these choices are to be gained from DNS with complex chemistry and from analysis of recent multiscalar measurements.

- A Lagrangian Flamelet model (Matarai et al.) and Multiple Mapping Conditioning (Klimenko and Pope) were described as new modeling approaches.

Update on Radiation

TNF target flames typically have a low radiative heat loss. Consequently, the predictions of computational models for flow field, temperature, and chemical composition do not depend strongly on the radiation model and a simple model, the optically-thin model, can be used. To accurately predict features strongly depending on accuracy of temperature, notably NO formation, more sophisticated radiation modelling is useful, at least when flow and combustion models already give good agreement for main species and mean temperature. The answer corresponding to a detailed radiation model should be somewhere between the limits of the adiabatic calculation and the optically thin model, provided turbulence radiation interaction is properly taken into account.

In the contribution at the workshop an outline was given of what is involved in a detailed radiation model. Reference was made to recent works concerning spectral radiative effects, turbulence/radiation interaction and measurements and calculations of spectral radiation intensities.

It is shown that, when using the Planck mean absorption coefficient, one finds little difference between the optically thin approximation and a full solution of the radiative transfer equation using discrete ordinates method (DOM). This is explained by the fact that the emission term is at least one order of magnitude larger than the absorption term in the RTE when the Planck mean absorption coefficient is used. However, the Planck mean absorption coefficient yields a poor estimation of the absorption term. Using a spectral model (SLW) in combination with the DOM, the absorption is found to be higher and the radiative heat loss is in better agreement with the experimental data at least for Flame D. To address other flames of different power or size, the analysis of Li and Modest on scale up is of interest. (See references on slides.)

Because different authors in the literature used a different mix of models and put emphasis on different aspects, the answer on the question which model is recommended for the TNF flames as next step beyond the optically thin model, is not yet fully clear. But the following statements may set the some restrictions on how to proceed:

- It is important to take into account turbulence-radiation interaction, most importantly the effect of temperature fluctuations on the mean emission.
- The effect of correlation between fluctuations in temperature and absorption coefficient is relatively small, but not negligible.
- Spectral effects seem important in the evaluation of absorption term.
- Explicit confirmation that the 'thin eddy approximation' is valid is needed. This could be tested in line calculations.

During the discussion, suggestions were made to construct a simple model extending the optically thin model with a optically thick treatment of the 4.3 μm band of CO_2 (Bilger) and to treat the absorption term using the modified Planck mean absorption coefficient, depending on both local temperature and temperature of the surroundings (Gore).

Scalar Dissipation, Scalar Variance, and Small-Scale Structure

The modeling of scalar dissipation is central to flamelet and CMC approaches, and direct testing of scalar dissipation models by comparison with measurements in TNF target flames is an important priority. The session on scalar dissipation outlined various models for scalar dissipation as well as progress and some remaining challenges on the experimental side. In addition to material presented and discussed at the workshop, there were several papers on scalar dissipation presented and the 30th Symposium. Some highlights from both are listed:

- Significant progress has been made on measurements of scalar dissipation in the piloted flames and turbulent opposed jet flames, as documented in 30th Symposium papers from Sandia and TU Darmstadt.
- Preliminary comparisons of measured and modeled scalar dissipation in piloted flame D revealed wide variation among the modeled results (see plots in the proceedings). The reasons for such large discrepancies are not clear and will require further investigation.
- We are not yet able to accurately quantify the experimental uncertainty in scalar dissipation measurements. This is because experimental errors depend in a complicated way on spatial averaging effects, noise contributions to the measured scalar gradient, and bias inherent in

measurements of a 3D quantity using 1D or 2D diagnostics. Some information on these effects is included in the proceedings.

- New insights on effects of spatial averaging, noise contributions, and 1D–2D bias in measurements of scalar dissipation and scalar variance are also provided in 30th Symposium papers by Barlow, Karpetis, Wang & Clemens, Wang & Tong, and Geyer et al. Work is in progress by these groups to better understand these issues, and it is hoped that we will know enough to assign quantitative uncertainty intervals to the measurements before TNF8 and begin to really discriminate among the various models for scalar dissipation.

- Careful attention needs to be given to comparisons of results on the mean and variance of mixture fraction and temperature, in addition to scalar dissipation. Criteria for consistent comparison of measured and modeled results must also be defined and must account for the issues listed above.

- Issues of spatial resolution and noise were shown to be well under control in the new measurements of scalar variance on piloted flames, such that quantitative comparison with models may be carried out with confidence.

- The 30th Symposium paper by Geyer et al. includes analysis that interprets the effect of experimental noise in scalar dissipation measurements by adding noise to mixture fraction results from LES. This is an important illustration of the potential benefits of close coupling of experiments and detailed simulations. More work along this line is expected and encouraged.

- There is great potential for future comparison of doubly conditioned statistics, where the second conditioning variable might be something other than scalar dissipation.

LES of Combustion

Johannes Janicka was separately invited to lead the TNF7 discussion on LES and present a topical review at the 30th Symposium. This gives us the benefit of access to a fully documented review of the state of combustion LES in addition to the overview slides in the TNF7 Proceedings. Discussion of LES was also prompted by the presentation from Luc Vervisch, and some of those discussion points are included here.

Current practice with respect to LES was discussed at length. The following is suggested as the current state-of-play:

- Almost all LES calculations that are currently made do not perform grid independence studies. Users simply make a judicious choice of the filter width based on what they know about the flames or flows in question and proceed with their calculations.

- How much of the energy containing eddies are resolved during LES depends very much on the choice of the filter width and on the nature of the problem. Users seem to claim that they resolve most of these and use a figure of about 80%.

There was discussion about what constitutes "**good LES**", and the following criteria were proposed and accepted as NECESSARY, except for the third criterion which was thought to be problem specific and hence desirable rather than necessary.

1. Provide relevant estimates of the filter size. A standard method of achieving this is to plot estimates of the integral length scale, L_I, the Kolmogorov length scale, L_K, and the Gibson scale, L_G. The filter width can then be set on this plot. Here reference may be made to Figure 1 of Pitsch and Duchamp de Lageneste (*Proc. Combust. Inst*. 29:2001-2008, 2002) where a regime diagram for LES is presented.

2. Vary the filter size and check if the basic flame properties are preserved. The statistical, time averaged properties of the total signal (resolved plus SGS) should NOT depend on the filter size. The procedure to do this may be explicit or implicit filtering.

3. When there is no sub-grid turbulence, the SGS closure should reproduce the filtered laminar flame solution. This was argued to be possible only for premixed combustion and was thought to be not needed in some flow configurations or indeed not possible in diffusion flames. Hence it was deemed to be only a desirable criterion.

Linking DNS, LES, RANS, and Experiments

The overview presentation on this cross-cutting theme included examples from nonpremixed flames, premixed flames, and regimes in between. A clear message is that detailed simulations (both LES and DNS) are increasingly being used as tools to understand fundamental phenomena in turbulent combustion and also to interpret or augment experiments. Results from various groups were discussed: Sandia, Cambridge, NAL, Darmstadt, University of Washington, INSA-CORIA.

1. Some projections on the future of DNS were made, and it was suggested that turbulent Reynolds number of about 1500 will be a possible target within the next ten years using reduced chemistry.
2. So far, DNS of turbulent flames can be organized into three groups:
    a. DNS of a fully synthetic problem, as a planar flame (premixed, partially-premixed or diffusion) interacting with a freely decaying turbulence.
    b. DNS of a laboratory flame configuration, but after a serious scale-down. Typically, the ratio between premixed characteristic flame thickness and turbulent integral length scale is about ten times smaller in the DNS than it is in the experiment.
    c. DNS of a laboratory flame, but considering only a small portion of the flow, as it is done in the lifted flame simulation by the NAL group (Mizobuchi et al.).

    Various chemistry and transport properties have been used for all those simulations: Single-step, reduced, tabulated or detailed chemistry, combined with fixed or variable Lewis and Schmidt number or even complex transport.

There was a large consensus on the weakness of the estimation of prediction capabilities of SGS closures from DNS. Because of the lack of large scales in DNS, it can only be viewed as a very first step, which cannot be considered as fully conclusive. However, DNS results are very useful as a complement to experiments, to better select the underlying physical assumptions that may be used in SGS modeling. An example of this was given from DNS of flames stabilized on evaporating droplets, where DNS is combined with OH measurements to elucidate complex flame structures that will appear at the SGS level.

Update on Lifted Flames

A brief update was given on recent progress in current understanding of lifted flames stabilized in cold or vitiated co-flows. Submissions were received from the following research groups and presented at the meeting:

- Mastorakos at Cambridge: Experiments in flames auto-igniting in heated air
- Pope at Cornell: PDF calculations of lifted flames in vitiated co-flow
- Chen at Berkeley: PDF calculations of lifted flames in vitiated co-flow
- Mansour at Cairo: Lifted, partially premixed flames, PIV-LIF
- Lyons at North Carolina State: LIF imaging and PIV in lifted flames in cold co-flow

The following observations are made:

- Lifted flames in cold co-flows are receiving little current attention from the modeling community, and there is not yet a comprehensive data set for well-characterized flames where full flow, mixing, and composition field data are available at the stabilization base. The closest to that is the data set provided by Lyons et al.

- Lifted flames in vitiated co-flows are receiving attention with a particular focus on auto-ignition as a stabilization mechanism. The Cabra configuration with a large, hot co-flow seems to have (i) lifted modes where stabilization occurs by premixed flame propagation; and (ii) auto-ignition modes where the flame is dominated by convection and reaction only. Investigations are continuing to further unravel the mysteries of such flames.

- A new and interesting configuration is devised by Mastorakos where pulses of fuel issuing in heated air auto-ignite in a distinct way and with a popping or crackling noise. The noise is qualitatively very similar to the Cabra flame when it is believed to be in auto-ignition mode.

Chemical Mechanisms

Peter Lindstedt pointed out deficiencies in some current mechanisms of methane especially with reference to low temperature combustion relevant to auto-ignition. A near-term priority is to make available a reliable methane mechanism for broad applications including low-temperature combustion and auto-ignition.

Turbulent Premixed Flames

Several groups that are actively involved in the TNF Workshop series are also conducting research on turbulent premixed combustion and are interested in applying the same process of collaborative comparisons of measured and modeled results to selected premixed target flames. Andreas Dreizler presented an overview of the current state of premixed combustion experiments. Key discussion points from this session are:

- Turbulent premixed combustion processes will be addressed in future TNF workshops.

- An emphasis on chemistry and turbulence-chemistry interaction will be maintained.

- Several potential target flames were discussed; advantages and disadvantages of the configurations are not addressed here.
    - Piloted jet flame, data set from Chen et al., Combust. Flame 107 (1996) 223. Data available.
    - Low swirling flame, initial reference Bédat & Cheng, Combust. Flame 100 (1995) 485. Different designs of the burner are circulating. Before deciding for a specific configuration some agreement within the TNF community should be achieved. Collaborative experiments are planned by TU Darmstadt and Lund University (Mark Linne).
    - Strong swirling flame, information on data and design to be published soon (Schneider & Dreizler), data on flow field and turbulence structure available, detailed information on inflow boundary conditions available, scalar field work-in-progress. GT-relevant nozzle configuration.
    - V-flame and bluff-body flame, data available from F. Dinkelacker
    - Confined premixed swirl burner (Sandia), so far no detailed data available.
    - Premixed burner in vitiated co-flow (Sydney). This is in development as a simple extension of the vitiated-coflow burner from Berkeley. High shear rates are generated between jet and coflow.
    - Stratified-premixed burners are also in development by Erlangen and Darmstadt

Challenges of Sharing and Mining Large Experimental and Computational Data Sets

The first several TNF Workshops focused on comparison of single-point statistics of velocity and scalars in relatively simple flame geometries. Such data sets are easy to distribute, and the generation of collective comparison plots can be reasonably managed by one or two people. Collaborative comparisons in the future will have to address new challenges.

- Rigorous comparison of measured and modeled results is becoming increasingly difficult as we move to more complex flames. Complex flow fields must be documented before detailed consideration of finite-rate chemistry can be carried out in composition space. In the future, it may be desirable to develop automated tools for collecting and comparing results. Any interface that is developed must be simple, or it will not be used.

- In a similar context, it would be useful to collect and preserve results from various calculations of TNF flames, particularly once the calculations are published in the archival literature and especially if the results are “good”. In many cases, the details of a calculation are lost when the graduate student finishes. This restricts our ability as a community to really understand whether we are making progress.

- The very large DNS of the lifted H_2 jet flame by Mizobuchi and coworkers confronts the combustion community with a challenge to develop efficient methods to mine and share very large data sets. Large LES calculations of a few million nodes present similar challenges. Even the relatively small data sets from recent multi-scalar line imaging experiments at Sandia are more difficult to share than the simple point statistics that have been the main basis of TNF flame comparisons until now. PLIF and PIV imaging data present their own challenges. Work is clearly needed to find efficient methods for data sharing, so that we can explore increasingly complex science without becoming bogged down in the mechanics for data handling.

ORGANIZATION OF TNF8

Location and Dates: The TNF8 Workshop will be held in or near the Heidelberg, Germany around the time of the 31st Combustion Symposium. The schedule is likely to mimic that of TNF7.

Possible Focus Topics: Focus topics for TNF8 will be defined more specifically during the year before the workshop. However, it seems likely that some the following will receive attention:

- Progress in LES: It is anticipated that rapid advances in combustion LES, including increased resolution as well as advances in combustion submodels, will offer interesting opportunities for comparison with experiments and for extraction of new physical insights.

- Scalar Dissipation: More detailed comparisons on measured and modeled results for scalar dissipation and related quantities in the piloted CH_4/air flames are anticipated. In order to do this well, we will need to compare more than just scalar variance and scalar dissipation. Comparisons should extent to back to aspects of the turbulent velocity and scalar fields, such that the reasons for the wide differences among predicted scalar dissipation profiles seen at TNF7 may be understood. In addition, work must be completed to quantify the combined effect of noise, spatial averaging, and angle bias in the measurements of scalar dissipation, such that realistic uncertainty estimates may be provided.

- Mixing Models: It would be interesting to carry forward work on the performance of mixing models in combination with chemical mechanisms, as advocated at TNF6. This will require general availability of all the chemical mechanisms used by various groups.

- Sydney Bluff-Body and Swirl Flames: Further comparisons on the Sydney bluff-body and swirl flames should address details of turbulence-chemistry interaction by including comparisons in mixture fraction coordinates. This is expected to require conditioning on specific spatial locations, as opposed to inclusion of data from complete radial profiles (as was done for simple and piloted jet flames).

- Premixed Flames: TNF-style comparisons involving premixed combustion are awaiting the availability of at least one appropriate data set that includes measurements of velocity and scalar fields and are based on well defined boundary conditions that are computationally friendly. Premixed combustion activity at TNF8 will depend on the pace experimental progress and the adoption by modelers of one or more target cases.

- Lifted Flames: More activity on lifted flames, including the vitiated co-flow flames, can be expected, and this may expand to address the lifted CH_4 flame cases from Berkeley.