SUMMARY

Tenth International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames (TNF10)

29-31 July 2010
Beijing, China

R.S. Barlow, J.-Y. Chen, A. Dreizler, M.J. Dunn, J.H. Frank, R. Gordon, S. Hochgreb, J. Janicka, A. Kempf, E.W. Knudsen, A. Kronenburg, R.P. Lindstedt, A.R. Masri, H. Pitsch, S.B. Pope, E.S. Richardson, D. Roekaerts

INTRODUCTION

The series of workshops on Measurement and Computation of Turbulent Nonpremixed Flames (TNF) facilitates 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 flames that are relatively simple in terms of both geometry and chemistry. The TNF Workshop series was initiated to address validation of RANS based models for turbulent nonpremixed flames, as well as partially premixed flames where combustion occurs mainly in a diffusion flame mode. Although the title has not changed, our scope is expanding, and the TNF10 agenda emphasized recent progress toward addressing three challenges that were elaborated at TNF9 in Montreal (2008). These challenges are:

- Development and validation of modeling approaches which are accurate over a broad range of combustion modes and regimes (nonpremixed, partially premixed, stratified, and 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 and utilization of approaches which extract knowledge and understanding from comparisons of detailed experimental measurements with detailed simulations.

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 had 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. 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 turbulent combustion modes and regimes.

During the two years between workshops, we have made greatest progress on the first of the three challenges, as demonstrated by the inclusion of model comparisons on two new target burners for premixed and stratified combustion.

TNF10 was attended by 93 researchers from 13 countries. The main sessions topics included:

- Overview and recent progress on lifted flames in hot coflow
- Model comparisons on the Sydney Piloted Premixed Jet Burner (PPJB)
- Overview of stratified combustion experiments
- Overview of modeling approaches for partially premixed and stratified combustion
- Model comparisons on the Darmstadt stratified flames
- Progress on kinetics and diagnostics for "new" fuels
- Best practice in LES

This summary briefly outlines the presentations and discussions. 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 TNF10 Proceedings and also the Proceedings of previous TNF Workshops, because each workshop builds upon what has been done before.

The complete 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 the presentations, presentation slides, and two-page abstracts of 39 contributed posters.

ACKNOWLEDGMENTS

Local arrangements for the TNF10 Workshop were coordinated by Profs. WU Yuxin and ZHANG Hai. Sponsorship by the German SFB-568 research program, General Electric, Edgewave, The Leverhulme Trust, La Vision, Numeca, Continuum Lasers, Princeton Instruments, and Sirah Lasers is gratefully acknowledged. These contributions allowed for reduction of the registration fees for university faculty and students. Support for Rob Barlow in coordinating TNF10 and past Workshop activities has been provided by the U. S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences. Sandia National Laboratories is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94-AL85000.

IMPORTANT NOTE ON USE OF THIS MATERIAL

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 would be inappropriate to quote or reference specific results from these proceedings without first checking with the individual author(s) for permission and for the latest information on results and references.

HIGHLIGHTS OF PRESENTATIONS AND DISCUSSIONS

Lifted Flames in Hot Coflow

The coordinators of this session, Rob Gordon and Dirk Roekaerts, provided a detailed review of the state of knowledge on lifted flames in hot coflow, including recent progress and recommendations for future work. Development of their contribution into a published review article is very much encouraged. The session provided a review of the existing experimental and numerical work that has been conducted on burner configurations of a non- or partially premixed jet in a hot coflow. In most cases, the hot coflow is provided from post-combustion gases of lean flames and hence is reduced in oxygen level compared to air (vitiated). This design permits the investigation of conditions in the combustion zone similar to those arising by entrainment of recirculated flue gas occurring in industrial combustion devices but with the advantage that the flow pattern is much simpler, and the chemistry of the coflow is decoupled from the combustion products. This allows the focus of the investigations to be on turbulence-chemistry interaction and flame stabilization mechanisms. In the presentation by the coordinators, characteristics of the available experimental databases and past and recent modeling efforts were reviewed, as well as near future research plans. Planned new experiments considerably extending the scope of the past experiments (high Reynolds number, high pressure, other fuels) were also discussed.

The coordinators would like to highlight the following key results:

- The CO-LIF data collected for the Cabra CH_4/Air case is known to be high compared to the Raman CO data. This has been identified as a systematic error in the original data processing, and division by a factor of 2.11 corrects the data well.
- New experimental databases are available from experiments in the Delft (Oldenhof et al.) and Lund (Duwig et al.) burners.
- A comparison of LES of the Cabra burner CH_4/air case, closed with either tabulation of auto-ignition (AI) and premixed flamelets (AI-PF-FPI) or unsteady diffusion flamelet based progress variable (FPV) was made, highlighting some differences in predictions of standard deviation of temperature and CO.
- 1-D Linear Eddy Model computation of autoignition has been undertaken to investigate the role of differential diffusion (Sauer et al.).
- DNS data were used to validate some LES modeling assumptions, with a key result that LES prediction with only diffusion flamelets over predicts liftoff height (LH) and only AI under predicts LH (Knudsen and Pitsch, poster).
- Liftoff height sensitivity to time step choices in the transported PDF modeling due to fractional step methods was pointed out (Naud, poster).
- Unsteady tabulated non-premixed flamelets methods are developed for simulating these flames (Ihme, contribution to presentation; Vicquelin et al., poster)

The need for parametric variation in experiments and for evaluating model development based on ability to match parametric response was re-emphasized. The presently available databases do represent such parameter variation, and this should be followed in modeling efforts.

Piloted Premixed Jet Burner (PPJB) Comparisons

The aim of the PPJB session, coordinated by Matt Dunn, was to compare some recent numerical computations of the PPJB with the experimental measurements. There were contributions from four modeling groups, two using RANS based PDF methods and two using LES methods. The PPJB features a small diameter jet from which a lean methane-air mixture issues at high velocity. Surrounding the central jet is a stoichiometric pilot, which ensures initial ignition of the central jet. Both the central jet and pilot are surrounded by a large hot coflow of hydrogen-air combustion products, ensuring that the central jet combustion process is not diluted or quenched by ambient air. By varying the central jet velocity and keeping all other parameters constant, a parametric flame series of four flames (PM1-50, PM1-100, PM1-150, and PM1-200) with increasing degrees of finite-rate chemistry effects has been investigated. The flame structure in the series varies from being thin and flamelet like in the lowest velocity flame (PM1-50) to broad and partially extinguished in the higher velocity cases. Flames PM1-150 and PM1-200 exhibit an initial ignition region close to the jet exit, followed by an extinction region, then a re-ignition region further downstream as the turbulence intensity decays. The PPJB experimental measurement database includes single point velocity measurements, planar imaging of temperature, OH and CH_2O, as well as 1D line imaging using the Raman/Rayleigh/CO LIF technique combined with crossed PLIF of OH.

The modeling results from the Sydney group (*Dunn and Masri*) utilized a transported thermo-chemistry PDF model coupled with a RANS turbulence model. Generally it was found that the predictive capability of the RANS turbulence model was not optimal, even in the non-reactive case of a variable density jet. By increasing the value of time scale ratio C_φ, the degree of the predicted finite-rate effects increased, although correspondingly the error in scalar variance and flame length increased, making the generality of such an increase in C_φ difficult to justify. Generally the mean flame length was predicted to be too short and this correlated with the predicted reaction rates being too high compared to the experiments. No significant differences in the predicted results were found between the modified Curl, EMST and IEM micro-mixing models.

The Cornell group (*Rowinski and Pope*) utilized a joint velocity-turbulence frequency-composition PDF model. Generally the mean and rms mixing fields were simulated well for all flames. The reaction progress in the calculations of the flame with the lowest jet velocity, PM1-50, is in reasonable agreement with the measurements. However, as the jet velocity increases, the reaction progress is increasingly overpredicted. An exhaustive parameter sensitivity study was conducted and the primary source of error was concluded to be the modeling of the conditional diffusion term (the micro-mixing model). The importance of the jet to pilot velocity ratio on the variation of jet-pilot and jet-coflow interaction, hence finite-rate chemistry effects through the flame series was raised as an important parameter, experiments keeping this ratio constant were proposed to examine this effect.

Although one of the strengths of the PDF method is the ability to implement complex chemical mechanisms, a question was raised as to whether kinetic mechanisms (such as GRI 3.0) are suitably accurate for the mode of combustion in the PPJB where fresh methane-air mixes with hydrogen-air combustion products. The accurate prediction of the turbulent burning velocity in a premixed flame is a challenge for PDF models, and in particular there is a high sensitivity to the micro-mixing model. The fact that the use of different mixing models was shown to have such little impact on the predicted flame structure indicates that the sensitivity of the flame structure to the predicted turbulent burning velocity is low in the PPJB flame series. This is quite different to the high sensitivity to the turbulent burning velocity experienced in more traditional turbulent premixed flames. One of the conclusions from the PDF calculations was the need for further calculations (DNS or highly resolved LES) and potentially experimental measurements of conditional diffusion to gain a better understanding of the performance of mixing models in highly turbulent premixed combustion for the regimes experienced in the PPJB. This is in the hope that such studies may provide further insight that leads to the formulation of improved or new mixing models. In PDF methods, although models for variable values of C_φ seem well justified, it was shown that for the flames examined varying the value of C_φ does not have a significant influence on improving the numerical predictions for the PPJB.

The Stanford group (*Mittal, Pitsch and Knudsen*) utilized an LES flamelet model combined with a level set G-Equation approach. A systematic investigation and validation of the mesh quality was presented using the velocity measurements from four non-reacting cases, which correspond to the bulk flow velocities of the four reacting cases. In addition, it was shown that a correct inflow generation method for the jet and correct modeling of the chamfer on the pilot shroud were important to obtain good velocity field predictions. Using the non-reacting case to validate the code, the mesh and boundary condition treatment was shown to be an important test to gain confidence in these parameters for the reacting cases. Preliminary results for all four reacting case results were presented. Results for the mixing fields were encouraging. However, in general the mean flame length was predicted to be too short, indicating an over prediction of the reaction rate. Future developments of this modeling methodology will include an enhanced ability to incorporate finite-rate chemistry effects.

The Lund/Haldor Topsøe/ Hong Kong Polytechnic group (*Duwig, Nogenmyr and Chan*) presented an LES model termed integrated LES (ILES), where transport equations for all reactive species are solved and the reaction rates are determined directly from the filtered species mass fractions and temperature. The results of a grid and chemical mechanism sensitivity study were presented for the PM1-100 flame. The results for the mixing fields, minor species (CO and OH) and temperature profiles for the PM1-50 and PM1-100 flames indicated that ILES is capable of good results for all of these measures in regions where the mesh is sufficiently fine ($x/D<20$). Preliminary results for the PM1-150 flame indicated that the ILES method is capable of closely capturing the initial ignition and subsequent extinction region of this flame. Further simulations will be required to see if the ILES method can capture the downstream re-ignition region of the PM1-150 flame and the PM1-200 flame in general. It was proposed that part of the success of this methodology to problems with strong finite-rate chemistry effects is that the characteristic chemistry progress variables are not neglected. It was shown that an important parameter for successful ILES simulations is that sufficient grid resolution must be used to resolve both the flame-front and the flow-fields. Because the ratio of the jet diameter to the flame-front thickness is relatively small for the PPJB, an ILES PPJB simulation requires only a relatively moderate (in terms of LES) computational cost for successful ILES results (e.g., $D/40$ mesh resolution). Quantitative measures that determine when the ILES approach will be valid were presented as a work in progress and are under further development.

A general finding for the simulations of the PPJB flame series was that for the PDF calculations (Cornell and Sydney) and the Stanford LES calculations similar findings were found; for the low velocity cases an acceptable predictive capability for the reaction progress field was found, whilst for the higher velocity cases the predictive capability of the reaction progress field decreased (especially for the 200m/s case). The RANS PDF modeling results presented were close to their final form and further improvements in the RANS PDF models predictive capabilities will most probably require the development of a revised or new micro-mixing model. Both of the LES results presented were preliminary results in that issues with boundary conditions, model development, and simulating the entire flames series (and flame length) are currently being resolved and may deliver further improvement in the results compared to those presented at TNF10.

If significant new progress is made on the PPJB predictions before TNF11, it would be appropriate to have another PPJB session at TNF11. Any new individuals or groups interested in contributing simulations of the PPJB for TNF11 should contact Matthew Dunn (mjdunn@sandia.gov) to obtain the experimental database.

Overview of Stratified Combustion Experiments

Given that stratified combustion is a new area for the TNF series, the objective of this session was to provide an overview of experimental information on the effects of mixture stratification on flame structure, including published work as well as work in progress. The session was split into two parts, with Simone Hochgreb covering the broad overview and Andreas Dreizler providing details of experiments on the TU Darmstadt Stratified Burner, which was a target for model comparisons at this workshop.

Most of the published experimental research on the structure of stratified flames deals with fuel-lean combustion in laminar or mildly turbulent flows (u'/S_L not much higher than 1). The mildly turbulent cases include rod stabilized V-flame and expanding, spark-ignited flames in grid-generated turbulence. From this work there is reasonably consistent evidence on the following. Local flame structure and propagation speed are affected by the gradient in equivalence ratio ϕ, and the effects depend on the magnitude and sign of the gradient in ϕ. When a flame propagates through a fuel-lean mixture with decreasing equivalence ratio, it is described as a back supported flame, meaning that the products immediately behind the flame have higher temperature and higher radical concentrations than the corresponding homogeneous flame at the same equivalence ratio. This back-supported structure enhances the local burning rate and extends the lean flammability limit. In mildly turbulent cases, experiments have shown that stratified flames have broader and more symmetric curvature pdfs and increased flame surface density compared to homogeneous premixed flames. There is also evidence that flame thickness is less sensitive to ϕ in stratified cases.

Detailed velocity and scalar data sets from burners with higher turbulence levels and well defined boundary conditions are needed for model validation. Two burners have been developed for this purpose. The TU Darmstadt Stratified Burner has a co-annular design with a central premixed pilot flame. The inner and outer annular flows can have the same or different equivalence ratios, and they have long development lengths to yield fully developed turbulent flow at the burner exit. This burner was designed to isolate the effects of mixture stratification in statistically stationary flames without the modeling complications of swirling or recirculating flows. Turbulence levels (u'/S_L) can exceed 20 in this configuration. Velocity measurements have been published and scalar experiments are in progress. A second burner for stratified flames was developed jointly by Cambridge and Sandia, and it was designed to be a next potential modeling target after the Darmstadt burner. It adopts the co-annular concept of the Darmstadt burner, but uses a central bluff body for flame stabilization and allows for variable swirl in the outer annular flow, yielding greater complexity of the overall flow field. Examples of scalar and velocity measurements are included in the Hochgreb presentation.

Modeling Approaches for Stratified and Partially Premixed Combustion

The goal of this session, which was coordinated by Ed Richardson and Ed Knudsen, was to review the current of state of stratified, partially premixed, and mixed regime turbulent combustion models, and to suggest directions for future work that will help to advance the fidelity of model performance in these challenging conditions.

The first half of the presentation reviewed the combustion physics that characterize mixed-regime burning, and that must be accounted for by any relevant modeling approach. So-called `front-supported' and `back-supported' premixed flames were used as example cases that motivate this discussion. In these flames, the equivalence ratio of a co-flow is set as either farther from stoichiometric (front-supported) or closer to stoichiometric (back-supported) than a central jet stream. Newly available DNS data was referenced to demonstrate how these different configurations change the premixed flame's structure and burning speed. Once the possible effects of stratification are understood, it becomes important to understand the conditions under which these effects are expected to appear. Therefore, in an effort to more rigorously distinguish between stratified combustion and purely premixed combustion, the controlling variables that might appear in a regime diagram for stratification were discussed. These include the ratio of the maximum possible change in burning speed to the mean burning speed, the ratio of the Kolmogorov length scale and the mean flame thickness, and the mixing timescale associated with the local fuel concentration.

In the second half of this presentation, several of the most widely used LES combustion models were discussed with respect to how they handle multi-regime burning. The approaches considered were the flamelet model, the thickened flame model, filtered density function approaches, and the linear eddy model. Each of these approaches was noted to have some particular advantages and particular disadvantages in the context of partially premixed combustion. For example, the flamelet model is expected to predict flame structure very accurately in both the non-premixed and premixed limits, but the extent to which descriptions of these asymptotic regimes can be combined to describe a mixed mode flame structure remains unclear.

Finally, several approaches to locally distinguishing between premixed and non-premixed regimes in an LES were discussed. The simplest of these approaches is the flame index, but more detailed approaches that rely on coordinate transformations that explicitly distinguish regimes were also discussed. These approaches are now being actively applied in LES, and are the subject of ongoing model development efforts.

One point that was raised throughout the workshop was the particular challenge that premixed combustion presented, and how this challenge was distinct from the non-premixed modeling challenge. Because stratified and partially premixed combustion inherently have premixed-like behavior, models for premixed flame propagation and flame structure are essential for any predictive multi-regime approach.

Comments on Future Work:

- A continuing need exists for the improvement of regime distinguishing indicators. These indicators will be needed in most combustion models that involve tabulated chemistry, but have only begun to be developed.
- Beyond the need for regime indicators to be used within models, a broad framework (e.g. regime diagrams) for classifying and comparing different partially premixed flows – and

the resultant combustion physics – will be helpful. Further study of the stratified and partially-premixed data sets presented at this workshop may help determine the relevant effects of various equivalence ratio and equivalence ratio length-scale distributions.

Darmstadt Stratified Flames: Model Comparisons

The Darmstadt Stratified Flames were presented as a new test case for the TNF 10 workshop. These flames were developed at the Technical University of Darmstadt and have been investigated by Seffrin, Fuest, Geyer and Dreizler. Model comparisons were coordinated and presented by Andreas Kempf.

Preliminary experimental data for temperature (Rayleigh, Raman-Rayleigh), mixture fraction and CO_2 mass fraction (Raman) were also made available and presented at the workshop in comparison to the numerical simulations. (These preliminary experimental scalar data were only made available for presentation at TNF10. They will not be distributed further, as improved data will become available soon.)

A set of flames was chosen as preferred target for the comparisons, and contributors were encouraged to simulate at least the non-reactive case TSFAi2 and the basic stratified case TSFAr. Only the Stanford group submitted further data for case TSFG.

Cases in descending order of priority:

1. TSFAi2 (isothermic) 2. TSFAr (stratified, no shear)
3. TSFGr (not stratified, no shear) 4. TSFCr (stratified, shear)
5. TSFEr (not stratified, shear)

All groups performed Large-Eddy Simlations, using (i) a sub-grid pdf/stochastic fields method in combination with the static Smagorinsky model (Imperial, Jones' Boffin-LES code), (ii) a flamelet model combined with the G-Equation and the Germano model (Stanford, NGA-3DA), (iii)premixed flamelet generated manifolds with local flame thickening and the Germano model (Darmstadt, FASTEST) and (iv) Fureby's flame surface density model with the static Smagorinsky model (Imperial, Kempf's PsiPhi code).

Two approaches were taken to represent the computational domain: Darmstadt and Stanford simulated the flow upstream, using one large domain with local refinement (Darmstadt) and a cascade of precursor simulations (Stanford). Both groups obtained results that were in good agreement with the experimental velocity data. Both groups from Imperial used a more compact computational domain, starting simulations at the outlet of the inner nozzle, prescribing the experimental velocity data.

Overall, all groups achieved good predictions of the data, particularly considering that a new TNF case was simulated. As the scalar data (temperature, mixture fraction and CO_2 mass fraction) only became available very late, the predictions of these quantities can be considered as 'blind'; modellers had no opportunity to tune their simulations to match the data. The features of the flames that were found to be most challenging were the intricate geometry of the flame holder, the chamfer on the nozzle exits, and the relatively low co-flow velocity of only 0.1 m/s, which makes a long simulation time necessary.

For TNF11, it is recommended that the Darmstadt stratified flame series be considered as a test case. The lessons learned for TNF10 should enable all groups to accurately predict the flow and mixing, so that the focus can be shifted towards the effect of stratification on flame-turbulence interaction. It is hoped that groups will be able to start the TNF11 simulations earlier in the cycle than was the case for TNF10, thus allowing sufficient time for detailed simulations to be completed and potentially interesting comparisons to be made.

Any groups interested to contribute simulations of these flames for TNF11 should contact Andreas Kempf (a.kempf@imperial.ac.uk) to be included in the mailing list.

Progress on Kinetics and Diagnostics for "New" Fuels

Extending validation work to fuels more complex than methane was one of the challenges outlined at TNF9. DME and ethanol were identified as relatively simple fuels which have very different properties and are of practical interest. For example, ethanol has a RON of 129, while DME has a cetane number in the range 55-60. Furthermore, molecular transport properties of the two fuels are very similar and, accordingly, differences in fuel behaviour can be directly related to chemistry effects. Peter Lindstedt and J-Y Chen coordinated a session to review progress on kinetics and diagnostics for these "new" fuels. The topics included an assessment of the need to (i) provide a systematic determination of high quality thermodynamic data, (ii) the derivation and testing of alternative detailed reaction mechanisms using data related to flame structures and ignition related properties. (iii) The need to identify critical reaction pathways and assess the impact of uncertainties in key kinetic rate parameters on model predictions, (iv) the reduction of the resulting mechanisms to an acceptable size and, finally, progress in the efforts to procure high quality experimental data in a "friendly" burner configuration (c.f. Sandia A-F series).

Reaction mechanisms have been published for ethanol by UCSD, LLNL and Dryer's group, and for DME by the LLNL and Dryer groups. Presentation slides form Berkeley and Imperial College included comparisons of predicted ignition delay characteristics across a range of conditions for both fuels, as well as comparisons of predictions from these mechanisms against published experimental data on low pressure flame profiles, laminar flame speed, and ignition delay times. Substantial differences in ignition delay times between the different mechanisms were shown using a Cabra type burner configuration. The differences were such that one ethanol mechanism was found to ignite more readily than the DME variant from another group. Sensitivity analyses were presented that show a strong impact of the thermal dissociation of DME and the need for accurate rate determinations was identified for a number of reactions. It was further shown that in a HCCI type environment temperature changes of up to 30 K were required in order to bring similarity in behaviour between alternative mechanisms. Such differences in temperature should be contrasted with the strong sensitivity to boundary conditions experienced in, for example, the Cabra configuration and as reported by the groups at Berkeley, Cornell and Imperial College among others. On the positive side, a systematically reduced 28-species mechanism from Berkeley, based on the Dryer mechanism, was shown to be in very close agreement with the parent mechanism across a broad range of conditions. Furthermore, work to identify critical reaction pathways in order to select, or determine, appropriate reaction rate parameters was also summarized with examples shown using laminar flame configurations.

Progress at TU Darmstadt and Sandia to extend quantitative Raman/Rayleigh scattering methods to DME flames was also reviewed. Here the main point was that hydrocarbon intermediates in DME flames are much more important for Raman/Rayleigh data interpretation than in methane flames. Raman/Rayleigh signals from DME flames cannot be interpreted usefully unless these intermediates are accounted for, and a method for doing this, based on information from laminar flame calculations was introduced. Preliminary results for a series of piloted, partially premixed DME/air jet flames were also presented.

Other Highlights

Jonathan Frank and Andreas Kronenburg organized a session to highlight other recent work of direct or potential relevance to the TNF Workshop process. This included:

- Pros and cons of turbulent counterflow flames as potential TNF targets. Bruno Coriton presented work performed at Yale, Sandia, and Imperial College on two different counterflow burners. The Yale burner was shown to produce turbulence Reynolds numbers up to roughly 1000 and methods for separating out low frequency contributions using techniques formulated at Yale and Imperial College were discussed.
- Development of a piloted jet flame burner for sooty fuels (by Shaddix and coworkers at Sandia), along with an overview of experiments using simultaneous OH/PAH PLIF and PLII, laser extinction, 3-color extinction/emission, local radiant emissions, and PIV.
- Results from Raman/Rayleigh/CO-LIF measurements on the Cambridge Swirl Burner showing that preferential transport can significantly alter the mean atom balance across a turbulent premixed flames.
- Slides from Luc Vervisch an coworkers (presented by Kronenburg) describing a multi-scale convergence methodology for DNS, where the meshes of Large-Eddy-Simulations are repeatedly refined until the smallest scales are sufficiently resolved. The target experiment is a premixed swirl flame reported by Meier et al.

Best Practice in LES

The session on best practices for LES was organized by Heinz Pitsch and Johannes Janicka, who solicited and compiled input from many colleagues to lead off the discussion. Some studies on the topic were presented, and some of the open questions were raised first. This was followed by an open discussion.

The presented material includes examples of criteria for mesh refinement, discussions of the effect of numerical schemes on modeled quantities, and sensitivity studies. As an example, an extensive sensitivity study by Janicka was shown, where the Sydney bluff-body flame was computed and results were compared with experimental data. Then variations of grid, boundary conditions, SGS model, combustion model, and several parameters and modeling assumptions included in the combustion model were performed to study the sensitivity of the solution of these parameters. For this validation study, several other configurations were further considered.

Several recommendations for best practices were made:

1. One of the most important issues is the numerical mesh, which typically also defines the LES filter. Mesh refinement studies should be performed. However,
    a. It is not sufficient to simply do a global refinement. Mesh refinement should be performed using refinement criteria, since also mesh distribution is important. The local resolution should be reported. This can be done in terms of spectra, fractional sub-filter energies, or relevant length scales. It is important that a distribution is shown, not just a few points.

b. If the mesh resolution is too fine, the model is not tested. Further, a very high mesh resolution that might be achievable in simple canonical cases cannot be used in the application of models to realistic systems for which the models are ultimately developed.
c. While the mesh is a numerical parameter, the filter size is a model parameter. The question was discussed whether it is important in changing the mesh, to separate the effect of model from numerics, which is not easily possible.

2. Sensitivity studies for uncertain parameters should be performed. These parameters could include, for example, grid, boundary conditions, models, model parameters, and modeling assumptions. However, there is a large space of uncertain parameters and there is no general guideline for which parametric uncertainty should be investigated.
3. The simulations should be documented in all details. This should include a description of the mesh, boundary conditions, numerical algorithms, and all models and model parameters.
4. Report about length scales and length scale ratios (integral scales, filter size, Kolmogorov scales)

Recommendations to experimentalists (most of these are obvious and already considered in most experiments):

1. Boundary conditions need to be specified in as much detail as possible.
2. Experimental uncertainties need to be well characterized and reported.
3. Error bars should be provided.
4. Series of experimental data sets should include ‘easy’ cases and cold flow.

Priorities and Planning for TNF11

TNF11 Workshop will be held in Darmstadt, Germany just prior to the 34th Combustion Symposium (Warsaw, August, 2012) and will be hosted by the Technical University of Darmstadt. Andreas Dreizler and Andreas Kempf will be the Program Co-Chairs. Darmstadt is convenient to Frankfurt airport, which is a major international hub.

It is anticipated that more expensive model comparisons will be carried out for the Sydney Piloted Premixed Jet Burner and the Darmstadt Stratified Burner. Interested modeler should contact Matt Dunn or Andreas Kempf, as indicated in their respective summary sections. It is possible that other target flames will be added, and such announcements will be made as early as possible. Those interested in modeling other flames that are relevant to the TNF process are encouraged to contact the authors of work on those specific flames.

We also expect to continue work toward developing a more complete framework for combustion LES validation. Progress and challenges in areas of LES quality assessment, parameter variation, and uncertainty quantification are likely to be on the agenda. Development of better methods for quantitative comparison of experiments and LES will also be a priority for the next workshop.