SUMMARY

Eleventh International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames (TNF11)

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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 1st TNF Workshop was held in Naples, Italy in July 1996. Its objectives were to select experimental data sets for testing combustion models and to establish guidelines for collaborative comparisons of measured and modeled results on those target flames. Subsequent workshops were held in Heppenheim, Germany (1997), Boulder, Colorado (1998), Darmstadt, Germany (1999), Delft, The Netherlands (2000), Sapporo, Japan (2002), Chicago, Illinois (2004), Heidelberg, Germany (2006), Montreal, Canada (2008), and Beijing, China (2010). Proceedings and summaries are available at http://www.sandia.gov/TNF.

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 has expanded since TNF9 (Montreal, 2008) to address three challenges:

- Development and validation of modeling approaches which are accurate over a broad range of combustion modes and regimes (nonpremixed, partially premixed, stratified, and 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.

TNF11 was attended by 84 researchers from 13 countries. The main sessions topics included:

- Turbulent stratified flames and model comparisons
- Differential diffusion effects in turbulent premixed flames
- Lifted flames in vitiated coflow

- Model comparisons on the Sydney Piloted Premixed Jet Burner (PPJB)
- Progress on DME flames and chemistry
- Oxy-fuel and MILD combustion
- Interpretation and utilization of temporally resolved data
- LES/DNS quality and best practice
- Turbulent opposed jet flames

This summary briefly outlines the presentations and key discussions points. 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 TNF11 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 technical sessions, presentation slides, and two-page abstracts of the 34 contributed posters.

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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

Turbulent Stratified Flames and Model Comparisons

Coordinators: Andreas Kempf and Benoit Fiorina

The objective of the session was to compare recent simulations of turbulent stratified flames against experimental data. Burner configurations from TU-Darmstadt and Cambridge University provided the target cases, both burning methane. Five groups were involved in the simulations: the Technische Universität Darmstadt (TUD), the Institute for Combustion Technology (ITV, Aachen), Lund University (LUND), the

EM2C laboratory at Ecole Centrale Paris (EM2C), and a team from Imperial College London and Duisburg-Essen University (IC-UDE).

All groups performed Large Eddy Simulations using Low Mach Number solvers. TUD applied a premixed flamelet tabulation with local flame thickening, ITV used a flamelet progress variable approach also based on premixed flamelet tabulation, LUND described the combustion chemistry through a 4-steps mechanism combined with Implicit LES, EM2C applied the model F-TACLES that is based on filtered premixed flamelet tabulation, and finally IC-UDE used a flame surface density approach. All modeling strategies were designed to predict a flame propagation speed equal to a laminar flame speed when the flame wrinkling is fully resolved on the LES grid. However different assumptions regarding the species transport description have been made. The TUD and ITV models assume that the flame front structure is similar to a 1-D premixed flamelet computed under unity Lewis assumption when subgrid scale flame wrinkling vanishes. At the opposite end, LUND and IC-UDE assumed that the flame front has the same structure as a 1-D premixed flamelet for which differential diffusion phenomena are considered. These assumptions regarding the multi-component transport properties affect the value of the effective laminar flame front propagation speed. EM2C proposed two model formulations with and without differential diffusion effects on the laminar flame speed.

The *Darmstadt stratified burner* consists of three 5-mm-staged concentric tubes placed in a 0.1 m/s coflow. Burnt gases exit from the central tube (pilot) to stabilize the flame. Different approaches have been taken to represent the computational domain: TUD computed the entire flow upstream within slot1, slot2 and the pilot tube; EM2C restricted the flow upstream computation to slot1 and slot2; LUND, IC-UDE and ITV used a more compact computational domain, starting simulations at the outlet of the inner nozzle, prescribing the measured velocity data. All groups performed simulations of the TSF-A reactive case. Also, ITV computed the TSF-Cr configuration, EM2C and IC-UDE the TSF-Ai (inert) case, and ICUDE the TSF-G (reactive) case.

Both adiabatic and isothermal assumptions have been considered to set up the pilot burner wall boundary conditions. To estimate the burner wall temperature, TUD developed an analytical analysis to model heat exchange between the pilot tube and stream 1, while EM2C performed a RANS 2D-axisymmetric computation of the fluid flow inside the burner coupled with conductive heat transfer within the burner wall. Both studies estimate a wall temperature for the pilot tube of around 700K. For the TSF-A case, an extensive comparison of simulation and experimental data was presented for the mean and RMS field of velocity, temperature, mixture fraction, and major species mass fractions. In general, good agreement has been observed between the numerical predictions and the measurements. All adiabatic computations predicted a flame anchoring at the burner lips, while the non-adiabatic simulations predicted a lift-off of the flame of half a pilot diameter. The comparison of the mean temperature field and the species formation/consumption against the experimental data provides evidence that accounting for heat losses improves the prediction of the flame position. However, the impact of heat losses on the combustion chemistry remains only one possible explanation of the flame lift-off. Other phenomena like an incomplete burning of the pilot gases could also explain this observation. Further measurements are needed to conclude on the effective stabilization mechanism.

It has been also observed that multi-component transport assumptions significantly affect the mean flame position. Accounting for differential diffusion phenomena in the direction normal to the flame front seems to improve the quality of the prediction. Another conclusion from numerical data analysis is that the effect of stratification on the flame front propagation remains weak for the TSF-A case. For future work on the Darmstadt burner, the focus should be shifted towards more stratified cases where the modeling of subgrid scale mixture fraction heterogeneities will be more challenging and influential.

The *Cambridge/Sandia burner* also consists of three concentric tubes in a laminar coflow, but the center tube is sealed with a ceramic cap, and the flame is stabilized by recirculation of combustion products downstream of this central bluff body. Computations were performed by EM2C and IC-UDE, both groups included the last part of the burner into the computational domain. Three non-swirling cases were considered: an isothermal reference case (SwBc), a homogeneous case with an equivalence ratio of 0.75 within both annular tubes (SwB1), and a stratified case with equivalence ratio of 1.0 in the inner and 0.5 in the outer tube (SwB5).

For the case SwBc, comparisons of mean and rms profiles for the axial and radial velocity component with PIV measurements were presented for various downstream locations. Both groups achieved good agreement with the measured flow field. For the reactive cases SwB1 and SwB5, comparisons of mean and rms profiles for the axial and radial velocity-component with PIV measurements and for temperature and equivalence ratio have been presented at various downstream locations. In general, good agreement between experiment and simulation was observed. However, significant deviations were observed within the recirculation zone: on the one hand, the predicted recirculation zone has a lower negative axial velocity magnitude and is shorter than the measured one, which is more visible with the modelling approach chosen by UDE-IC. One possible explanation could be that the real flame is lifted, in contrast to the anchored flame predicted by the adiabatic simulations. This theory is also supported by the temperature profiles for the stratified case SwB5, where the peak value is about 125 K lower than the one predicted by both simulations. As the maximum temperature is about 300 K higher compared to the homogeneous case SwB1, conduction and flame lift-off are likely to become more important. On the other hand, the measurement predicts a peak of the equivalence ratio profiles within the bluff body region, which is not visible in the simulation results. It could be assumed that this is caused by differential diffusion effects, as discussed in the next section, which are not taken into account with either model. More detailed investigation of the influence of mass and heat transfer near the bluff body could be an interesting topic for future studies. It was agreed that surface temperatures of the ceramic pilot tube of the TUD burner and the ceramic bluff body cap of the Cambridge burner would be measured using thermographic phosphor techniques at TU Darmstadt.

Differential Diffusion Effects in Turbulent Premixed Flames

Coordinators: Simone Hochgreb and Luc Vervisch

This session was devoted to understanding differential diffusion in turbulent premixed flames. Specifically, the focus was on bluff-body stabilised turbulent flames, and the role of the recirculation zone in enhancing the effect of differential diffusion.

Recent experiments involving premixed and stratified turbulent flames ($Re{\sim}10^4$) stabilized on an annular burner with a central bluff body (the Cambridge/Sandia burner and a simpler single slot burner) showed that the carbon–hydrogen balance is not conserved across the flame in the region adjacent to the recirculation zone. Instantaneous and averaged measurements of equivalence ratio and the C/H atom ratio calculated from major species at a distance of 10 mm above the bluff body surface show a jump across the flame zone, unlike measurements made on laminar premixed flames or turbulent flames without a recirculation zone. The CO_2 mass fraction is higher than expected in the products, while the O_2 mass fraction is lower. This behavior has been attributed to the differential transport (diffusion and convection) among species. Near the flame stabilization point at the edge of the recirculation zone, there is strong shear due to the velocity difference between the reactant stream and products within the recirculation zone. In this region, the shear layer thickness is of the same order as the flame thickness. Diffusion acts across this layer to transport oxygen and fuel from the reactants toward products and CO_2, H_2O, CO and H_2 from products back toward reactants. As in a planar flame with no shear (1D calculation), diffusion of CO_2 from products to reactants is slower than that of hydrogen containing species, hydrogen and water. In the bluff body case, however, the boundary conditions are affected by the presence of intense convection on the reactant side, and recirculating convection on the product side. The H-rich mixture on the reactant side is convected away (downstream), whilst the C-rich mixture on the product side is recirculated. In retrospect it appears that there was evidence of this same effect in published Raman/Rayleigh measurements on the TECFLAM premixed swirl burner.

Laminar and turbulent simulation results for a similar bluff body burner were presented by Vish Katta. These simulations included full transport and chemistry (GRI Mech 3.0). Results for state profiles across the flame (scalars vs. temperature) agree well with measurements, confirming that the effects of differential transport, including differential diffusion and shear near the bluff body, are responsible for the observed behavior.

This issue creates additional difficulties for modellers attempting to use such a database for validation, as differential diffusion is typically not accounted for in many LES models using mixture fraction and progress of reaction as scalar variables. Luc Vervisch considered the problem in the context of flamelet models, and whether it is possible to find an approximate source term to take care of differential transport. The differential transport effect arises due to the difference in velocities across the reacting shear layer. The effect of differential diffusion can be estimated from the difference in residence time along the burner, and estimates from LES calculations without differential diffusion predict a difference of around 7% in mixture fraction. Further, it is possible to incorporate the differences in mixture fraction (defined either from the major species or minor species) by using a source term, defined as the remainder after the reaction and average diffusion term are subtracted from the calculations. LES results using this simple approach showed significant improvement in comparison with measurements from the Cambridge burner.

Key questions raised during discussion where how relevant differential diffusion may be as the level of turbulence is increased, as well as its role in energy transport.

Lifted Flames in Vitiated Coflow

Coordinators: Matthias Ihme and Ed Richardson

The focus of this presentation was threefold:

- Review and characterize relevant ignition and flame-stabilization scenarios in lifted and vitiated flames.
- Provide a comprehensive overview of recent research progress on the modeling of lifted flames, with specific focus on the modeling of jet-in-hot-coflow (JHC) burners from Adelaide and Delft and simulating the vitiated coflow burner (VCB) or "Cabra" burner. An overview of other related experimental configurations, new measurement-data, and consideration of additional operating conditions was given.
- Discuss the utilization of DNS-databases on lifted flames for analysis and model-development.

Three different flame-ignition mechanisms were identified and characterized:

- *Autoignition-mode:* The ignition and transition from unburned to burned states depends on the condition of the local scalar dissipation rate. This ignition mode requires that the local dissipation rate reduces below the so-called ignition-dissipation rate. If this condition is reached, onset of ignition occurs, in which radical-production and heat-release exceed the diffusion rate, promoting transition to a burning flame-structure. Conditions for the occurrence of the ignition location dependent on turbulent flow-field structure and duration over which the dissipation-rate remains below the ignition-dissipation rate.
- *Gradual/continuous transition:* This ignition mode pertains to the MILD combustion regime. In MILD combustion, the S-shape curve degenerates so that the notional ignition and quenching dissipation conditions merge into a single point. Under this condition, the S-shape curve has a single inflection point, promoting the transition between unburned and burning flame-states along the monotonically increasing S-shape curve.
- *Secondary ignition-mechanism:* This ignition mechanism is observed under conditions that promote transport of heat/radicals into the flame-region. Examples for this are strong flow recirculations, swirling flows, and cross-flow conditions. Under these conditions, the ignition onset is controlled by the flame-environment, and external heat/radical entrainment into the flame promotes ignition. Characterizing this ignition mode in terms of the S-shape curve shows up as direct crossing of unstable flamelet-branch, which is not feasible from fundamental 1D-flamelet arguments.

Vitiated coflow burner (VCB, "Cabra" burner): Since the last TNF-workshop, a number of groups have performed RANS and LES computations of the "Cabra" vitiated coflow burner, considering H_2- or CH_4-fuels. Recent RANS computations include DQMOM-computations by Lee, Park, and Kim of the H_2-VCB, and ADF-PCM computations by Collin & Michel. Several LES-computations on this burner have been reported, including conditional moment closure (Navarro-Martinez et al.), multiple mapping conditioning (Sundaram et al.), unsteady flamelet/progress variable model (Ihme & See), and flow-controlled chemistry tabulation (Enjalbert et al.). The presentation contains a discussion of all contributions, including a brief overview about the model-formulation, details regarding the numerical method and computational setup, and comparisons of model-results and experiments. Since all modelling efforts employed different discretization-schemes, gridresolutions, SGS-models, and temporal integration methods, only comparisons of individual modelling-results against experiments were discussions. An objective comparison of all models is not meaningful, and no quantitative conclusions about best model-practice or relative model-performance are given.

Adelaide jet-in-hot-coflow (AJHC) burner: The jet-in-hot-coflow (JHC) burner was developed at the University of Adelaide with the objective to investigate oxygen-diluted and three-stream combustion. Measurements in this burner include speciation, temperature, and mixture fraction for three operating conditions of decreasing oxygen-concentration (9%, 6%, and 3% O_2) in the coflow-stream. Recent studies by Medwell and Dally extended the measurements to other fuels and a wider range of operating conditions (including changing jet-exit Reynolds number, coflow temperature, and oxygen-concentration). The focus of recent measurements was on effects of operating conditions on the apparent lift-off height. For this, a combination of visualization, chemiluminescence, and long-exposure flame-photographs were used to characterize trends in lift-off heights as function of jet Reynolds number, coflow temperature and oxygen-level. It was concluded that the apparent "lift-off" is not a monotonic function of coflow-temperature, and also depends on the O_2-level and Reynolds-number.

In the AJHC-burner the oxygen-diluted coflow is provided through a secondary burner, resulting in inhomogeneous and transient scalar inflow conditions in the coflow stream. Effects of variations in scalar inflow conditions on the flame structure have been investigated by Ihme et al. (2011, 2012), and it was concluded that the effects of inflow inhomogeneities extend throughout the entire flame region. This was attributed to the low-Damköhler number combustion regime. These findings could also have implications for other vitiated burner configurations in which one or more oxidizer streams is generated from a secondary burner. Further measurements of temperature, velocity, and species (or a subset thereof) would be most useful to provide boundary conditions for model-inputs. Apart from mean data, it was discussed that measurements of second moment statistics (rms of temperature and species) and temporal correlations would be of direct relevance to modellers.

Delft jet-in-hot-coflow (DJHC) burner: The Delft-group has reported comprehensive measurements on a JHC-burner (Oldenhof, 2010, 2011, 2012) that is similar in design to the AJHC. Several operating conditions, fuel mixtures, and oxygen-dilution ratios (mostly at the upper limit of the MILD-regime) are considered, further extending the JHC-experimental database. Point-wise measurements for velocity and temperature have been reported. Of interest to modellers, these experiments also include PIV measurements, and enable comparisons with predictions of the velocity field. Oldenhof reported joint OH-PLIF-PIV measurements and analysed the velocity-statistics as a function of distance from the OH-layer. Comparisons with simulations have not been performed and can be subject of subsequent investigations.

Three groups provided contributions from recent modelling efforts. De et al. and Sarras et al. performed RANS computations using EDC and transported PDF-methods (JCPDF, JVPDF). These investigations considered the cases DJHC-I and DJHC-X, which correspond to oxygen mass fractions of 7.6% and 10.9% and Re_{jet} between 4100 and 8800. Analysis of model results and comparisons with experiments indicate that the ignition behaviour depends on consideration of molecular transport, PDF-method, and micro-mixing model. Similar to the findings in the context of the AJHC, it was observed that the prescription of inflow conditions is crucial for predicting the outer flame region; heat-losses to the burner wall and inhomogeneities in the secondary burner are not quantified and require further consideration in the model-formulation. Kulkarni & Polifke performed Fluent-LES computations of the DJHC-I and DJHC-X configurations using a stochastic fields approach. Predictions for velocity are in good agreement, but over predictions of temperature suggest higher predicted reactivities of the model compared to experiments. Similar observations have been made by other groups and require further investigations.

Insights and challenges from DNS: The preceding comparison of different modelling approaches for lifted flames in vitiated coflow is impaired by the high sensitivity of the model predictions to uncertain or unknown experimental boundary conditions, and to uncertain chemical kinetic models. Direct Numerical Simulation of turbulent lifted flames provides validation data with precisely known boundary conditions and physical models. The potential use of such DNS data for model development was raised as a topic for discussion at the workshop. A set of new DNS computations involving lifted flame stabilization has been contributed by the group of J.H. Chen. These include a parametric study of the effect of co-flow temperature on lifted hydrogen jet flames (Yoo et al) and parametric investigation of jet in cross flow flame stabilisation with various fuel compositions and jet nozzle geometries (Grout et al.). It was noted that the parametric variation between these flames causes transition between auto-ignitive, propagative, and secondary stabilization processes, as defined above.

Models have previously been compared in terms of ensemble- (conditionally-) averaged profiles, with respect to predictions of the mean lift-off height. Given complete knowledge of the spatio-temporal evolution of all flow and chemical quantities from DNS, however, there is scope for more detailed and more quantitative comparison between the DNS and turbulent reacting flow model. The question of which flame features to consider when evaluating predictive model performance was discussed. The use of DNS data for a posteriori model validation for lifted flames in vitiated coflow was also discussed, taking the work of Knudsen et al. as a case study. Due to the relatively moderate Reynolds numbers which characterize current state-of-the-art DNS, conclusions about LES model performance must be drawn with care. The modeller should be careful to distinguish whether the model has been validated in the context of ‘high fidelity’ LES or ‘energy resolved’ LES, as discussed by Pope and Vervisch during presentations on LES quality at this meeting. The study by Knudsen et al. reveals certain advantages to working with DNS data as opposed to experimental data. The first advantage, as noted above, is exact knowledge of the boundary conditions and physical models. Second, the resulting three-dimensional turbulent solution is known completely. The third advantage, which was realized by Knudsen et al. when their initial attempts at modelling the flame were only partially successful, is that the DNS data provides very detailed information about why particular models do or do not work. By interrogating the DNS data, they were able to identify – and remedy – deficiencies in their modelling of scalar dissipation rate and molecular transport, achieving greatly improved agreement. It was noted during discussion that, while use of DNS data removes some layers of uncertainty from model comparison, implicitly filtered LES models (which are used predominantly) combine the effects of the modelling with the numerical method. This is a feature of most current LES methods which affects comparisons with both laboratory measurements and DNS, and which should be considered further.

Discussion points and future directions: Main discussion points and further research directions that came up during the workshop presentation were:

- Wall heat-losses in the secondary burner is of great importance in vitiated flames. Measurements of wall-temperature would provide valuable information for model comparisons.
- Information about spatial and/or temporal correlations could be used to further interrogate and scrutinize LES combustion models. High-speed laser-diagnostics could provide an accessible approach to evaluate temporal correlations, and spatial correlations could be evaluated from planar measurements.
- A major source of uncertainties is the specification of inflow-conditions. Measurements of exit profiles for temperature, species, and velocity could further assist model validation and reduce ambiguities in specifying boundary conditions. This issue becomes increasingly relevant for low-oxygen and low-Damköhler number combustion regimes and for configuration that supply reactants from secondary burners or mixing systems.
- Different metrics have been considered experimentally to quantify the lift-off height in vitiated flame. While most of them have been developed from experimental considerations, only few of them can be evaluated in simulations. Examples are chemiluminescence measurements or photographs with exposure times of the order of seconds cannot be considered in LES for the reason that these computations are often only conducted over a fraction of this period. Another reason is that excited species, such as OH*, CH*, CH2* are not included in skeletal and some of the detailed mechanisms (such as GRI). Inclusion of such species is feasible, but will increase the computation time.
- Some valuable DNS-LES comparisons have been reported, and DNS researchers are encouraged to facilitate comparison with their data by providing full details of initial/boundary conditions and physical models, and, where possible, by providing access to the code used to implement the physical models and to generate the initial/boundary conditions. The data required for LES validation are, in the first instance, similar to those reported for laboratory flames, and DNS researchers are encouraged to provide profiles of single-point statistics of scalars and velocities as a minimum.

Piloted Premixed Jet Burner

Coordinators: Matthew Dunn, Assaad Masri, and Heinz Pitsch

The purpose of the session on the piloted premixed jet burner (PPJB) was to evaluate developments in large eddy simulation of the PPJB since TNF10. Four groups were involved in the simulations: Stanford/Aachen, Imperial College London/Sydney, University of Michigan, and Lund University. The PPJB was introduced as a modelling target flame at TNF10, with PDF and preliminary LES results reported. The LES results presented at TNF11 represent a significant step forward from the LES results presented at TNF10.

The Stanford/Aachen simulations utilised a steady premixed flamelet model, with a 4D tabulated chemistry table. The chemistry tabulation incorporated the rms mixture fraction, two mean mixture fraction variables, and reaction progress as parameterization coordinates so as to accommodate for mixing with the coflow and pilot. They reported essentially negligible difference in results between 4 and 9 million grid cell meshes. The University of Michigan results employed a steady nonpremixed flamelet based tabulation combustion model approach with two mixture fractions to account for the variation between pilot and coflow streams mixing with the jet.

The Lund simulations employed an ILES model, which allowed the incorporation of complex chemistry (19 transported species). As the ILES model is dependent on the mesh size and quality, model quality measures were developed, and it was shown for the PM1-150 flame good results were obtained up to and including x/D=15 with an unstructured hexahedral grid of 2 million cells. The Imperial College London/Sydney simulations employed a stochastic field LES model with eight stochastic fields. The stochastic field model utilized a complex chemistry approach (15 transported species) over a 4.8 million cell grid. Interestingly, the stochastic field approach results for the PM1- 200 flame, whilst predicting a flame too short, produced the best results in terms of mean and rms profiles for this flame thus far. However, there is still greater improvement need before successful prediction can be claimed for this flame. Both of the LES methods that incorporated complex chemistry were able to predict some degree extinction and re-ignition for the PM1-150 flame. However the degree of extinction was typically much smaller than measured.

The four groups presented very promising results for the two low-velocity flames PM1-50 and PM1-100. However all groups predict an insufficient degree of extinction in the high velocity flames (PM1-150 and PM1-200) and thus predicted a flame length too short. All four groups presented good results in terms of the mean and rms scalar profiles close to the burner. The success of the tabulated LES flamelet models (Michigan and Stanford/Aachen) for the low velocity PM1-50 flame is somewhat to be expected due to the correlation of the flame structure observed from experiments to the fundamental flame structure assumptions of these models. Therefore, the success of the PM1-50 simulation results can be viewed as a validation for these models assumptions. However, the success of these tabulated chemistry models for the PM1-100 flame and the PM1-150 flame (in the near nozzle region up to and including x/D=15) that have a significant degree of turbulence chemistry interaction is somewhat unexpected due to the assumptions of the models. It was discussed and proposed that if the tabulated chemistry approaches were to have greater success for the PM1-150 and PM1-200 flames in the future, the composition space accessed during extinction must be incorporated in some manner, e.g., through an additional tabulation dimension.

In 2010 at TNF10 the RANS based PDF calculations were presented, showing good results for the low velocity flames and under prediction of the degree of extinction in the high velocity flames. In order to further improve the PDF models, experiments exploring the role of the pilot to jet heat release ratio and the micro mixing model were proposed to be necessary. Such modelling progress also needed additional experiments to be conducted. These experiments were also discussed at TNF11 and were considered to be of relevance to the development and validation of the LES results presented at TNF11.

As always for LES, the sensitivity to boundary conditions was emphasised by all participants. A strong consensus was that accurate profiles closer to the nozzle for temperature and velocity would be very beneficial, particularly near the pilot exit and the pilot-coflow interface. No model has yet been able to show a convincing predictive capability for the entire PM1-150 and PM1-200 flames, which feature significant extinction and reignition. Attempting to solve this challenge will hopefully motivate future developments in combustion models and corresponding experiments, which will utilize the TNF workshop as a forum to drive such progression and collaboration.

Chemistry, Complex fuels, and New Combustion Modes

Coordinators: Peter Lindstedt and Dirk Roekaerts

This session was organized in two parts. The first part covered alternative fuels, with emphasis on recent work on dimethyl ether (DME). The second part was devoted to oxy-fuel combustion and fuel composition effects in MILD combustion.

Progress on alternative fuels: There has been a long-standing ambition for the TNF community to consider alternative fuels. At TNF10, a number of options were discussed, and it was decided to consider alternative fuels by including increasingly comprehensive data sets for DME and ethanol. This combination is particularly attractive as DME is a potential fuel for Diesel engines, while ethanol is already used extensively as a bio-derived fuel additive for gasoline. Furthermore, both fuels are comparatively simple, have the same molecular weight, and their different properties hence stem from the chemical structures. The review presented at TNF11 considered DME and covered a number of different aspects, including a new DME flame series, some of the chemistry background, recent modeling efforts, and the influence of differential diffusion in the context of transport approximations. To date, corresponding work on ethanol flames has not been performed. It is in this context important to note that the TNF community serves to identify and encourage collaborative research, but cannot provide direct funding streams.

Perhaps the key reason for the success of the TNF community has been the ability to evaluate the importance of turbulence-chemistry interactions in a coherent framework that is inclusive and permits a focus on the primary topic while reducing other complexities. In this context, the Sandia A-F flame series has served as a key component, and it is particularly important that the corresponding data sets are now in the process of being extended to alternative fuels. Experimental work on a new piloted DME flame series (A-G) currently features collaboration between Sandia National Laboratory and Ohio State University, with further contributions expected from TU Darmstadt and UT Austin. The applied diagnostics at Sandia include PIV, LIF, and Rayleigh scattering at low repetition rates as well as velocity and scalar imaging at high repetition rates. Raman spectroscopy and line measurements of temperature and species are being pursued in collaboration with the other institutions mentioned. As with the piloted CH4/air flames, these DME flames show increasing probability of local extinction with increasing jet velocity (Re up to ~68,000). Preliminary experimental results are highlighted in the presentation. More extensive velocity and scalar measurements should be available before TNF12.

The chemistry of DME has been covered comparatively extensively by several groups with proposed mechanisms available. The latter include the work by Kaiser et al. (2000) and Zhao et al. (2008) as outlined by Fuest et al. (2012). There has also been a number of experimental low-pressure premixed flame studies, and a comparison of modeled species profile with measurements by Cool et al. (2007) was presented. There are indications that the key initial branching of DME leading to either methoxy (CH_3O) or formaldehyde (CH_2O) remains less well reproduced than desirable – particularly given the very different reactivities of methoxy and formaldehyde – and hence some updating of the chemical mechanisms may be required. The impact of differences in combustion chemistry is further highlighted by the LES-CMC computations performed at ITV Stuttgart by Kronenburg and co-workers, with very significant differences obtained in formaldehyde concentrations depending on the chemical mechanism used. The work thus further emphasizes the need to revisit key initial branching ratios. The need for accurate reduced mechanisms of DME remains a priority and should arguably form a focus point ahead of TNF12.

The impact of transport approximations (differential diffusion) upon the ability to predict DME flame structures was investigated in a collaboration between TU Bergakademie Freiberg, Engler-Bunte-Institute KIT, and TU Darmstadt. The work shows that differential diffusion effects are non-negligible and that problems in predicting the outer regions of the flames measured by Fuest et al. are present.

Oxy-fuel combustion and fuel composition effects in MILD combustion: The objective of this session was to review state of the art and identify research questions of particular relevance for the participants in the TNF-workshop.

In oxy-fuel combustion the oxidiser stream is oxygen or enriched air. Oxy-fuel combustion is used in partial oxidation (gasification) and in high temperature furnaces (e.g. glass furnaces), and it is part of a potentially efficient solution for carbon capture and sequestration (CCS). Oxy-fuel combustion is often used with CO_2 recycled into the oxidiser stream in order to lower NO_x emissions. In order to decide on recommended modeling approaches in applications of oxy-fuel combustion, it is of interest to investigate the role of turbulence-chemistry interaction and also the role of turbulence-radiation interaction in a range of configurations, from simple to semi-industrial.

In MILD or ‘flameless’ combustion, one or more of the fuel and oxidizer streams is diluted with products of combustion, which are at lower than adiabatic temperature. The combined effects of lowering of oxygen concentration and lower enthalpy have impact on the combustion process. Because high values of temperature are less frequent, NO_x formation by the thermal mechanism is lower. In flameless combustion, auto-ignition is observed to play an important role. To be able to exploit the benefits of MILD combustion in a wider range of applications, fundamental understanding is needed on how fuel composition influences the boundaries of operation in the MILD regime. The jet-in-hot-coflow (JHC) burner (with coflow of vitiated air) allows study of the MILD combustion phenomena in a turbulent jet flame configuration.

Results from several experimental and numerical studies on oxy-fuel and MILD combustion were highlighted, with emphasis on localized extinction, differential diffusion effects, radiation modeling, flame lift-off behavior, fuel effects with different hydrogen/hydrocarbon mixtures, and chemistry reduction. The reported experimental results provide interesting new opportunities for modeling studies. For example, the datasets on oxy-fuel jet flames can be used to study whether models capable to predict local extinction in turbulent jet flames burning in air are performing equally well in the case of oxy-fuel and whether they are able to capture the additional effects due to differential diffusion and influence of presence of CO_2 level in the oxidizer on CO-level in the flame. Datasets on jet flames of natural gas diluted with H_2 or CO_2 burning in vitiated coflow can be used to study whether models are able to predict the trends in lift-off height and the observed appearance and growth of ignition kernels. Datasets on MILD combustion in a lab-scale furnace can be used to study which level of modeling is needed to predict the boundaries of the regime with low emissions

Interpretation and Utilization of Temporally Resolved Data

Coordinators: Adam Steinberg, Wolfgang Meier, and Luc Vervisch

The two focus topics for this session were: 1) experimental considerations for creating ‘well-posed’ time-resolved experiments and 2) requirements for comparing time-resolved experiments and simulation.

The main experimental considerations highlighted were out-of-plane effects, limited detectible quantities, and data analysis. Experimental methods that accounted for out-of-plane effects were identified, which typically employ cross-plane or parallel plane imaging. The combined use of planar imaging with line-of-site integrated techniques also was discussed. Limitations imposed by detectable species arise due to the relatively low pulse energy of continuous duty-cycle high repetition- rate laser systems. Consequentially, OH PLIF, tracer PLIF, and 1D Rayleigh scattering are the most commonly reported high-repetition-rate spectroscopic techniques. Experiments must therefore be designed such that these measurements reveal the phenomena of interest. Moreover, effort should be made to visualize simulations in the same manner as experiments. The potential of custom-built pulse-burst laser systems, capable of achieving much higher pulse-energies for short-duration bursts (ca. 10-100 pulses), also was discussed. Several different analysis techniques for time-resolved data were then presented, and experiments that employ these techniques reviewed. Efforts should be made to standardize certain common techniques, such as proper orthogonal decomposition, and/or have a few common data sets on which different versions of the techniques can be tested.

The following issues were discussed during and after the workshop:

1. Attention must be given to the different meanings between ‘time-resolved’ in the context of experiments and simulations. What is the effect of the LES time step, pulse duration, and inter-measurement time on the interpretations?
2. For model development and validation, specific target phenomena should be sought in which time-resolved experiments can yield important new insight. What are the most important dynamic phenomena to model properly? An advantage of time-resolved image sequences is that the statistics can be conditioned and that it is possible to catch events which happen quite rarely.
3. Effort must be made to analyze time-resolved experiments and simulations using the same tools (filtering, POD, DMD, etc.). Standardized data sets should be used to test different versions of analysis algorithms. This will allow more quantitative comparisons of experiments and simulations.
4. It was proposed to distinguish between ignition dynamics and flame dynamics:
    a. Ignition relates to a single instant in time and space, which must be isolated in both experiments and simulations; time series may be collected before and after ignition to better understand ignition conditions and implication on the subsequent flame development.
    b. Flame dynamics studies rather go with time sequences (not always time resolved), with a necessary check of the statistical predictions to validate the simulation.
5. In simulations, the time analyses may be performed in either Lagrangian or Eulerian frameworks. Eulerian implies storing many fields and Lagrangian motivates the development of specific methods to track meaningful trajectories (not always matching the flow path-lines). Specialized budget equations may also be derived to isolate time evolution of a given quantity. It may be desirable to rewind time, which is not always that easy in practice.

LES/DNS Quality and Best Practice

Coordinators: Joe Oefelein, Luc Vervisch, and Steve Pope

LES and DNS have become topics of central interest in the TNF workshop due to 1) the potential benefits LES has over classical Reynolds-Averaged Navier-Stokes approaches, and 2) the potential DNS has for providing insights toward model development. There are still many open questions, however, related to implementation of these methods and the sensitivity of various inputs on the results and model accuracy. Efforts over the past several workshops have been focused on establishing robust performance metrics to assess the “quality” of a given simulation in a manner that minimizes potential sources of error. The goal for TNF11 was to continue to build off of these past efforts by first providing a broad summary of what has been learned to date followed by development of a new more formal set of criteria that provides improved quality metrics to assess model accuracy.

The need for improved quality metrics has been recognized now for many years. In TNF8, for example, attempts to model the bluff-body flames (e.g., HM1) produced many ambiguities. Two issues arose from initial comparisons: 1) uncertainty with respect to boundary conditions, and 2) uncertainty with respect to code and simulation parameters (i.e., numerics, grid-resolution, time-step, integration time, etc.). The combined uncertainties made it difficult to draw any conclusions regarding model accuracy. Codes with a variety of different numerical schemes and capabilities (e.g., with and without explicit artificial dissipation added for stability) were used. Geometric details of the burner (which are surprisingly complex) were not resolved in most cases. Limited computational resources imposed significant constraints on the levels spatial/temporal resolution applied, all of which is a typical dilemma. These types of uncertainties are even more severe for applications.

For TNF9, algebraic error indicators were applied to the HM1 flame to explore their utility in the context of the observations above. It was shown that these indicators could produce anomalous results. Dissipative schemes (or application in laminar flows) produced misleading performance trends. Use of bulk averages instead of instantaneous quantities was problematic. Measures of turbulent kinetic energy were shown to be divergent and/or anomalous (e.g. for dissipative schemes velocity fluctuations are damped and low values of turbulent viscosity suggests good “resolution” as a consequence). Detailed analysis of results led to the conclusion that these types of indicators do not account for various sources of error correctly.

A second focal point in TNF9 and TNF10 was application of the error-landscape concept to LES (Geurts et al.). This method inherently accounts for the competing effects of numerical and modeling errors simultaneously. The primary advantage of this technique is that it identifies combinations of grid, filter, and model parameters that introduce incorrect flow and combustion physics. Thus, it allows one to simultaneously minimize the competing effects of modeling errors and numerical errors. The disadvantage, however, is that the error cannot be reduced to any arbitrary level and the method is expensive to implement (but still cheaper than refining the grid to eliminate non-optimal minimization of errors). Likewise, grid dependence studies were presented as part of TNF10 with emphasis placed on parametric uncertainties and recursive filter refinement.

Based on these findings, improved performance metrics, based on a new local resolution, criteria were proposed and presented. The new criteria are based on quantifying the sub-filter scales that a given turbulent combustion model is capable of representing as a function of critical parameters. The analysis and discussion led to the following progressive set of recommendations to guide ongoing research:

- Grid resolution and coupling between grid and filter spacing must be quantified
    - Simple global refinements are not sufficient
    - Pros/cons of implicit versus explicit filtering need to be better quantified
    - Local resolution criteria needs to be established as function of sub-filter scales
    - Local grid distributions need to be reported and checked in critical regions of flow
- Metrics for model applicability and implementation need to be reported
    - Grid spacing … numerical parameter
    - Filter width … model parameter
    - Competition between numerical and model errors
- More documentation of key simulation parameters is needed
    - Algorithmic characteristics of codes (spatial, temporal, stabilization method)
    - Local grid resolution, key length/time scales, related parameters
    - Boundary conditions and sub-model implementation
- Work toward UQ to determine sensitivity of uncertain parameters
    - Boundary conditions, model parameters, baseline model assumptions
    - Large space of uncertain parameters, general guidelines

The goal for TNF12 will be to apply these new criteria to key target flames to demonstrate the method and define a more precise set of requirements based on the recommendations above.

Turbulent Opposed Jet Flames

Coordinators: Dirk Geyer and Alesandro Gomez

The presentation started with an overview of the characteristics of existing turbulent opposed jet configurations, focusing on the last decade, and the experimental data available for these configurations. Currently, two main designs are available. The first is the turbulent opposed jet version from Darmstadt (DA), having a nozzle diameter of D=30 mm as well as nozzle separation of H=30 mm (H/D=1), which was especially designed to allow for laser beam access along the centerline, aiming for the measurement of scalar gradients over the reaction zone. This version was further developed by the group of Peter Lindstedt at Imperial College (IC) with an emphasis on the enhancement of the turbulent velocity fluctuations. The level of the turbulent fluctuations was enhanced by a factor of two by employing fractal grids instead of simple perforated plates. Moreover, the distribution of energy containing length scales was also substantially increased. The second design (D=12.7 mm, H/D=1.5), is from Sandro Gomez’s group at Yale. Here, the turbulence generation is based on a different scheme, forcing the flow through a high-blockage plate with a daisy-shaped orifice far upstream of the burner outlet. Using this scheme, turbulent Reynolds number up to approx 1200 could be realized. The discussion showed that the turbulent flow established near the stagnation plane exhibits different features, depending on the use of fractal grids (IC) or high blockage plates (Yale).

The most prominent difference is that large scale instabilities in the region of the reaction zone are much more pronounced in the Yale burner. Such instabilities necessitate the use of suitably formulated conditional statics.

Detailed information on the inflow conditions is crucial for all turbulent opposed jet configurations since the flow field depends strongly on the way the turbulence is generated. Such data are available for all opposed jet configurations (DA, IC, Yale). In particular, the DA group also ran high-speed PIV downstream of the turbulence generating plates. Different LES simulations performed for all configurations directly after the turbulence generating device by Andreas Kempf's group at IC were able to capture all prominent characteristics of the flow field very well. The compact domain of turbulent opposed jet geometries allows for a high resolution of the simulations inside the nozzle.

During recent years, the number of fuels and flame conditions was increased. While the earlier work focused methane as fuel, higher hydrocarbons like C_2H_4 or C_3H_8, and liquid fuels like JP-10 have been investigated at IC. The flame conditions are ranging from non-premixed to very lean premixed, with the latter established in the fresh reactant versus burnt product configuration. Experiments with conditions of local extinction were briefly discussed under conditions of direct relevance to gas turbine operations.

A number of simulations (Monte-Carlo PDF, 2nd moment U-RANS, LES-Flamelet) have been performed in the past years on the three burner configurations and were compared to experimental data. Flow fields as well as scalar data obtained by experiments are available for all configurations, where in particular the type of scalar data varies from line concentration/temperature data up to 2D imaging at low and high speed. The compact computational domain in conjunction with aerodynamic stabilization of the flame provides potential advantages computationally, in particular for LES. Simulations with different methods (LEM, W. Calhoon or LES-PDF, S. Pope) are under way. The concluding discussion showed that there is an ongoing interest in the turbulent opposed jet flames in parts of the TNF community, especially since the recent increase of the turbulent Reynolds number allows for investigations more relevant to technical applications.

Priorities and Planning for TNF12

The TNF12 Workshop will be held in the San Francisco area prior to the 35th Combustion Symposium (San Francisco, August 3-8, 2014). It is likely that there will be some coordination on schedule and venue between the TNF Workshop and the International Sooting Flame (ISF) Workshop.

It is anticipated that more extensive model comparisons will be carried out for the Darmstadt and Cambridge stratified burners and for the Sydney Piloted Premixed Jet Burner. Interested modeler should contact Andreas Kempf or Matt Dunn, respectively. There is also ongoing interest in opposed jet flames and in lifted flames in hot coflow and crossflow. We anticipate significant new experimental progress on the series piloted DME jet flames, so model comparison should be possible. It is possible that other target flames will be added, and such announcements will be made as early as possible. Those interested in modeling these or other flames that are relevant to the TNF process are encouraged to contact the authors of work on those specific flames and appropriate members of the Organizing Committee.

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, uncertainty quantification, and the roles of DNS and highly resolved LES in model validation are likely to be on the agenda. Development of better methods for quantitative comparison of experiments and LES, particularly in the context of high speed imaging, will also be a priority for the next workshop.

In recognition of his hard work on preparations for TNF11, Benoit Fiorina has been invited to join the TNF Organizing Committee.