SUMMARY

Twelfth International Workshop on Measurement and Computation of Turbulent Flames (TNF12)

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INTRODUCTION

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

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

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

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

TNF12 was attended by 93 researchers from 13 countries. The main sessions topics were:

- Turbulent stratified flames and model comparisons
- Sydney Piloted Premixed Jet Burner (PPJB) update
- Experiments and simulations in turbulent opposed jet flames
- Piloted DME jet flames
- Utilization of temporally-resolved experimental and simulation data
- Enclosed flames and unsteady combustion
- Flame-Wall Interaction
- LES quality assessment and uncertainty quantification
- Modelling of DNS cases

The complete TNF12 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 44 contributed posters.

The sections that follow briefly outline 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 TNF12 Proceedings and also the Proceedings of previous TNF Workshops, because each workshop builds upon what has been done before.

PLANNING AND PRIORITIES

The 2016 TNF Workshop will most likely be held in Seoul, Korea prior to the 36th Combustion Symposium. It is likely that there will again be some coordination on schedule and venue between the TNF Workshop and the International Sooting Flames (ISF) Workshop.

Each of the topics from TNF12 will be included in the next workshop, assuming there is sufficient progress and interest. Early coordination to select target cases, define ground rules for model comparisons, and establish priorities for collaborative experimental and computational work is strongly encouraged. Regular communication among members of the organizing committee and key contributors is also strongly encouraged. Suggestions for new topics should be communicated to the organizers.

ACKNOWLEDGMENTS

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HIGHLIGHTS OF PRESENTATIONS AND DISCUSSIONS

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

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.

Turbulent Stratified Flames and Model Comparisons

Coordinators: Andreas Kempf and Benoit Fiorina

Recent simulations of turbulent stratified flames were compared against experimental data. Burner configurations from TU-Darmstadt and Cambridge University provided the target cases, both burning methane. Eight 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), the CORIA laboratory (Rouen), the Hanyang University (Seoul), Imperial College London (IC), and Duisburg-Essen University (UDE).

With one exception (RANS-PDF from Hanyang), 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 but coupled with a level set approach, LUND described the combustion chemistry through a 4-step mechanism combined with Implicit LES, UDE used an artificially thickened flamelet generated manifolds technique on many low cost cells, CORIA applied the filtered laminar flame PDF model, Imperial used the stochastic fields technique, and Hanyang applied a three environment PDF technique with IEM mixing based on a k-epsilon RANS model. All modeling strategies were designed to produce the correct laminar flame speed.

The Darmstadt stratified burner consists of three 5-mm-staged concentric tubes placed in a 0.1 m/s co-flow. Burnt gases exit from the central tube (pilot) to stabilize the flame. Numerical studies focused on the TSF-A operating conditions, which promotes moderate fuel stratification within the flame. Both adiabatic and isothermal assumptions were 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 750K.

In addition to different modeling approaches, simulations differ by the CFD codes, the combustion chemistry, the numerical methods and the computational grids. Although based on different assumptions, all these computational strategies are designed to capture the filtered flame propagation speed both when subgrid-scale flame wrinkling occurs and when the flame wrinkling is fully resolved at the LES filter scale. In addition, as these models account for non-adiabatic effects on the combustion chemistry, they are able to capture quenching phenomena induced by heat losses.

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 was observed between the numerical predictions and the measurements. All adiabatic computations predict a flame anchoring at the burner lips, while the non-adiabatic simulations show a flame lift-off 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. Quantitative comparisons exhibit strong similarities in the mean flame brush position. It is also observed that the absence of turbulence combustion modeling at the subgrid scale has an influence on the mean flame front position. Instantaneous flame comparisons exhibit differences in the size of the resolved flame wrinkling patterns. The first reason is that each computational strategy (with different grids, numerics, and LES combustion models) implicitly filters the flame at a specific scale. As wrinkling patterns bellow this cut-off scale are not resolved on the LES grid, differences are observed in the flame front visualizations. The second reason for the differences in the size of the flame wrinkling pattern is linked to the influence of the LES combustion model on the flame dynamics.

The Cambridge/Sandia burner also consists of three concentric tubes in a laminar co-flow, 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, UDE, CORIA, Hanyang, and Imperial. Two cases were considered: 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). Further contributions were made for a highly stratified case (SwB9) with 1.125 and 0.375 equivalence ratio from Hanyang and UDE.

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 were presented at various downstream locations. A good overall agreement between experiment and simulation was observed, with considerable progress since TNF11.

One key to accurate predictions of this flame is the inclusion of the effect of heat loss to the bluff body, which does affect flame standoff. The temperature of this bluff body is known from new measurements that were performed jointly by experimentalists from Cambridge and Darmstadt.

An interesting issue specific to the Cambridge flame is that of differential diffusion, which is visible in the region downstream of the bluff body, manifesting itself through an apparently increased mixture fraction – beyond the mixture fraction of the richest stream at the inlet. This behavior has been captured by the contribution from CORIA, which transported an additional mixture fraction with a source term that represents the effect of differential diffusion. The effect of this differential diffusion has been shown by an interesting study from EM2C: they found that for the conditions of SwB1, differential diffusion and heat loss effects can compensate each other, such that considering both heat loss and differential diffusion effects will lead to the same temperature as an adiabatic simulation for unity Lewis number. This compensation of errors will, however, not occur for SwB5, since differential diffusion does hardly alter the flame temperature in these conditions.

On the side of experiments, the mentioned temperature measurements for the bluff body surface have become available. There are also new statistics for the single shot data, including species concentration plots conditional on temperature and scatter plots of equivalence ratio vs. progress variable. These statistics should be considered in the comparisons at the next TNF.

Overall, good progress has been made for both the Darmstadt and Cambridge flames through the inclusion of the effects of heat-loss and differential diffusion and the availability of new surface temperature boundary conditions provided by the experimentalists. Given the good agreement in the first two velocity and scalar moments, it is not clear how strong the effect of stratification is beyond altering the laminar flame speed, which can be well resolved by the present simulations. For the strongly stratified SwB9 case, however, the agreement between experiment and simulation is not yet satisfying, requiring further research.

Sydney Piloted Premixed Jet Burner (PPJB) Update

Coordinators: Matthew Dunn and Assaad Masri

The purpose of this session was to review recent progress on the piloted premixed jet burner (PPJB) and to consider how the PPJB might feature in future TNF workshops. Previous comparisons (TNF10 and TNF11) focused exclusively on the PM1 series of four flames in which jet velocity was increased, hence increasing the importance of finite-rate chemistry effects. Both RANS and LES based calculations at TNF10 and TNF11 showed encouraging results for the lower velocity PM1-50 and PM1-100 flames. However, no numerical modelling methodology was able to capture the degree and impact of the finite-rate chemistry effects in the higher jet velocity PM1-150 and PM1-200 flames. This led to many questions: Are the chemical mechanisms sufficiently accurate under the conditions encountered in the PPJB? Is LES mandatory to sufficiently capture the flowfield dynamics and statistics? What is the minimum necessary dimensionality of the chemical manifold necessary to sufficiently capture the extinction and re-ignition of the higher velocity flames?

Rowinski and Pope (CTM 2013) investigated the sensitivity of LES/PDF results in work that was published after TNF11. They observed significant sensitivity of finite-rate chemistry effects to the pilot velocity. This motivated experiments on the sensitivity of the PPJB flames to variations in pilot velocity, coflow temperature, and central jet fuel type, with results presented for the first time at TNF12. It was found that by decreasing the pilot velocity the PM1-100 flame could display a similar degree of extinction to the standard flame PM1-150. Conversely, the degree of extinction could be reduced in the PM1-150 by increasing the pilot velocity. For high velocity flames it was found that the coflow temperature had a significant impact on the degree of extinction. Flames of ethylene and DME were observed to be far more robust than methane flames.

Previous modelling results had shown a significant sensitivity to the inlet conditions, especially to the pilot inlet conditions. In response, preliminary OH LIF measurements of both temperature and OH concentrations at the exit plane of the burner were presented that will allow more accurate specification of the pilot boundary conditions in models that can accept non-equilibrium inlet conditions. Initial results for the PPJB from Jeff Sutton's group at Ohio State University were introduced, including proof of principle high-speed Rayleigh scattering and PIV measurements.

In summary, recent experimental results exploring the sensitivities in the PPJB offer an opportunity to better understand modelling difficulties associated with the higher velocity PM1-150 and PM1-200 flames. Whilst there is a renewed experimental interest in the PPJB, a strong commitment from the modelling community will be required to further explore computational sensitivities. Such an exploration will be required to understand why many models fail to adequately predict extinction in the PPJB flames, and it should be based on the experimentally identified sensitivities in the PPJB.

Experiments and Simulations in Turbulent Opposed Jet Flames

Coordinators: Bruno Coriton and Steve Pope

The session on turbulent opposed jet flames highlighted the latest measurements and simulations in the *reactant-to-product* configuration in which a turbulent stream of premixed reactants is opposed to a second stream of combustion products in thermo-chemical equilibrium. The *reactant-to-product* configuration allows for a unique variety of premixed combustion regimes in a compact geometry. Turbulent premixed flames can be stabilized under intense turbulence and strain thanks to the "back-support" of the counterflowing combustion products.

To date, two burners designed at Yale University and Imperial College are available in this configuration. Both burners employ turbulence-generating plates (TGP) housed inside the nozzle. The stream of hot combustion products is generated by premixed flames enclosed inside the bottom nozzles. Fluid properties (Re_t, K_{bulk}) as well as the stoichiometry of the reactants and the temperature and equivalence ratio of the combustion products can be varied independently.

New experimental results from these two burners and DNS results for a single lean premixed H_2/air flame were summarized. At Imperial College, simultaneous PIV and OH-LIF measurements have been performed in lean premixed flames for different fuels (CH_4, JP-10, DME). At Sandia, PIV and LIF (CO, CH_2O, OH) measurements were performed in the Yale counterflow burner. Data are available for $CH_4/N_2/O_2$ premixed flames over a wide range of Reynolds numbers (470-1050), bulk strain rates (1400/s-2240/s), product temperatures (1500K-2000K), and equivalence ratios (lean-to-rich). Under these conditions, the flames exhibited varying amounts of localized extinctions.

Simulations of turbulent opposed jet flames performed by four research groups (Brandenburg, CRAFT Tech, Duissburg-Essen, and Cornell) were presented. Although a broad range of flow conditions were simulated, no target flame was identified and therefore no direct comparison between the simulations could be made. In counterflow jets, implementing the inflow velocity boundary conditions is a challenge. Two strategies were identified and compared: 1) the boundary conditions are prescribed directly at the nozzle exit planes (Brandenburg, Cornell) or 2) the solution domain also includes the flow inside the nozzles, either up to the TGP (Duisburg-Essen) or further upstream of the TGP (CRAFT Tech). Conclusions from the four modeling group contributions are summarized below:

- Brandenburg performed an ODT simulation of the Sandia H_2/air premixed flame for which DNS data are available. Although ODT is a reduced order model, it was able to achieve good agreement with the DNS data (temperature, major species, etc). ODT appeared to yield satisfactory species profiles, but to under-predict heat release and ignition. The Yale/Sandia $CH_4/N_2/O_2$ experiments were also attempted with ODT; however, there was difficulty in capturing ignition.
- CRAFT Tech's LES simulations of the Yale *reactant-to-product* burner included the full burner geometry. The fluid dynamical aspects of the counterflow were studied in a non-reactive case (N_2/products). The GMLI was found to oscillate slowly between the nozzles and at larger amplitude than in the experiments, which affected the unconditional statistics. Preliminary

simulation of the $CH_4/N_2/O_2$ premixed flame was also conducted with a simple algebraic Pocheau model. In the future, the extinction/ignition events observed experimentally will be modelled with an LEM-CF model.

- The group at Duisburg-Essen performed LES/FDF simulations of the Darmstadt and Imperial College CH_4/air twin-premixed flames. Good agreement between simulations and Darmstadt's experiments were achieved. Future work will include different fuels (C_2H_4, C_3H_8).
- Cornell's group performed simulations of both non-premixed and premixed flames in the Yale burners. The domain included the flow between the nozzles. Inflow boundary conditions were prescribed based on Pettit's LES data of nozzle inflow. Good agreement for velocity statistics and progress variables were obtained. LES/PDF methods tend to predict less extinction than in the experiments.

Overall, calculating the flow field was a challenge, even when the domain included the turbulence-generating plate. The simpler treatments used by Brandenburg and Cornell appeared satisfactory and yielded good agreement with the experimental data. Specifying inflow conditions at the nozzle exits may decrease or eliminate large-scale flow instabilities.

More calculations are expected in the future now that groups have satisfactory flow calculations and many different experimental conditions to investigate. To study turbulence-chemistry interactions, conditional statistics should be used in order to reduce the sensitivity to imperfections in the flow calculation and to large-scale flow instabilities. Comparison of conditional statistics that reveal more about the turbulence chemistry interaction would be desirable.

Piloted DME Jet Flames

Coordinators: Jonathan Frank and Andreas Kronenburg

This session focused on turbulent piloted partially premixed dimethyl either (DME)/air jet flames. The DME/air target flame series has varying probability of localized extinction and is analogous to the piloted CH4/air jet flame series that has been well studied in the context of the TNF Workshop. In the DME/air flame series (D-G), jet velocities are varied to provide jet exit Reynolds numbers from approximately 29,000 to 73,000. DME is a relatively simple oxygenated fuel, and the inclusion of DME target flames is part of an effort to address the combustion of alternative fuels within the TNF Workshop. This series of turbulent jet flames was introduced at TNF11, and the results presented at TNF12 represent early stages of comparisons between numerical simulations and experimental measurements. Experiments were performed at Sandia and included PIV, OH-LIF, and CH_2O-LIF imaging measurements, as well as joint Raman/Rayleigh/CO-LIF line measurements. The numerical simulations consisted of four different approaches, including RANS-MEPDF (Hanyang), LES-PDF (Beijing/Cornell), LES-CMC (Stuttgart), LES-FPV (Freiberg).

An important issue in DME combustion is that the rich-side chemistry presents challenges for both experiments and modelling. Fuel decomposition produces significant concentrations of hydrocarbon intermediates that complicate the interpretation of diagnostic techniques, such as Raman and Rayleigh scattering. The turbulent transport of hydrocarbon intermediates can result in a broad spatial distribution of these species, as evidenced by CH_2O-LIF imaging measurements from Sandia. Diagnostics complications include the overlap of Raman spectra from different hydrocarbons and differences between the Rayleigh scattering cross-sections of hydrocarbon intermediates and DME. Strategies to account for these issues in Raman/Rayleigh scattering measurements are being developed in a collaborative effort between Sandia, Ohio State, and TU Darmstadt. The current approach uses a modified mixture fraction construct and an assumed scalar structure that depends on strain rate, transport, and the chemical mechanism. Comparisons with computations require care in using the same mixture fraction construct.

Chemical kinetics challenges include relatively large mechanisms, convergence issues due to stiffness, and strong dependencies of some intermediates on the mechanism (e.g. CH_2O, CH_3OCH_2). As noted at TNF11, there remains a need to develop more accurate kinetic mechanisms with a reduced number of species. Four different DME mechanisms were considered using laminar flame calculations. The Zhao mechanism predicted significantly larger CH_2O mole fractions than the Kaiser, Burke, or Aramco mechanisms. Similar discrepancies in CH_2O were observed in LES calculations of the turbulent Flame D using the Zhao and Kaiser mechanism.

Four different approaches to turbulent flame simulations were applied to Flame D, and limited initial comparisons showed largely good agreement with experiments. The somewhat larger deviations in species predictions for RANS-MEPDF and LES-PDF computations are not necessarily associated with issues of these specific modeling approaches. The discrepancies in the predicted radial profiles using RANS-MEPDF could be attributed to inflow boundary conditions that had not been matched with measurements, shortcomings in the RANS-based turbulence model, and the use of the IEM mixing model. The LES-PDF results presented by Beijing/Cornell originated from LES on rather coarse meshes leading to relatively large local discrepancies in the measured and computed mixture fraction fields. Improvements can be expected for TNF13. LES-CMC and LES-FPV agree well with measurements. However, the current CMC implementation fails to capture the fuel decomposition that is observed at and beyond z/D=40. For the LES-CMC and LES-FPV calculations, preliminary comparisons with experiments included OH and CH_2O distributions. For these comparisons, the LES calculations were used to simulate OH and CH_2O LIF signals, and the downstream evolution was compared. The OH field was captured well, but the radial spreading rate of the CH_2O field was particularly sensitive to the LES grid resolution. The simulation of CH_2O-LIF signals requires additional care.

The significance of differential diffusion in these jet flames remains an open question. At TNF11 some results indicated that differential diffusion effects need to be considered when modeling these flames. The presentation at TNF12 included contradictory results concerning the role of differential diffusion. LES-PDF show large effects of differential diffusion on all species and temperature throughout the entire domain. In contrast, LES-FPV computations do not suggest a large influence of differential diffusion on most species (major and OH) with the exception of CH_2O. Here, non-premixed flamelets and unity Le yielded the best agreement with measurements.

Goals for TNF13 should include more detailed comparisons of experiments and simulations as additional data become available, the extension of simulations to flames with higher probability of localized extinction (Flames E-G), advances in chemical mechanisms, and an improved understanding of the impact of differential diffusion in this flame series.

Utilization of Temporally-Resolved Experimental and Simulation Data

Coordinators: Adam Steinberg and Benjamin Böhm

This session built off of the TNF 11 session, *Interpretation and utilization of temporally resolved data*, and addressed methods by which temporally resolved experiments can be rigorously and quantitatively compared with simulations. This included limitations of measurements, potential cross-platform analysis techniques, and uncertainty considerations.

A summary was presented of high-repetition-rate laser diagnostics. General considerations regarding high-speed experiments and simulations were outlined, and differences in interpretation of the sampling frequency, spatial resolution, field-of-view, and output quantities were discussed. It was proposed that an experimental equivalent of the CFL number be reported, wherein it is required that the frequency of the measurements be sufficient to capture the time-scales associated with the targeted phenomena. For the case of turbulent combustion, this generally is the time scale associated with the smallest resolved turbulence length scale, which generally are larger than the Kolmogorov scale.

Several examples of cooperative use of time-resolved experimental and simulation data were presented, including: autoignition of hydrogen jets in crossflows (DLR, Argonne), autoignition and stabilization of hydrogen jets in co-flows (DLR, Ohio State), lagrangian tracking through 4D data sets (U. Toronto, Sandia), local extinction of opposed jet flames (TUD, Duisburg-Essen), proper orthogonal decomposition of IC engine data (U. Michigan), and data assimilation (NS State).

Even though time-resolved measurements are becoming more and more popular, their cooperative use with time-resolved data from simulations is still rarely found in literature. Many comparisons performed so far, although using time-resolved measurements, focus on the first statistical moments of the quantity of interest disregarding the information on the available time history. The examples highlighted different levels of comparison between simulations and experiments useful for validation purpose.

The major take-away item was that the only way to rigorously compare experiments and simulations is with some form of statistics. In contrast to conventional data, these statistics may explicitly involve temporal derivatives or may be conditioned on a particular delay relative to a detectible phenomenon. A continuing need exists in finding appropriate metrics to handle the huge data sets and to extract the relevant information from both the experiments and simulations in a meaningful statistical manner which depends on the phenomenon of interest.

Enclosed Flames and Unsteady Combustion

Coordinators: Benoît Fiorina and Matthias Ihme

The first part of this session provided an overview of experimental and computational work on several enclosed burner configurations, including both nonpremixed and premixed reactant supply, as well as modular burners designed for operation across multiple combustion modes. Examples included the TECFLAM nonpremixed swirl burner, the MOLECULES burner, two MILD combustion configurations from IST Lisbon, the DLR dual-swirl model gas turbine combustor, the PRECCINSTA burner, a new partially-premixed methane/air swirl burner (similar to the DLR dual-swirl burner) developed for studies of acoustically active flames under the collaborative project SFB606, a new single-sector staged-combustion facility at TU Darmstadt, a multi-mode multi-fuel swirl burner at Cambridge, a Cambridge-UCL bluff-body swirl burner for unsteady combustion studies, and dual-swirl micro-turbine burner from Sunchon National University and Sydney University.

The second part of the session focused on experimental and LES studies of the EM2C confined premixed swirl combustor, which was designed to study the effects of fresh-gas composition, heat transfer, and flow dynamics on flame shape and stabilization. The burner includes a cylindrical injection tube with a 14-mm exit diameter. The flow is put in rotation by a radial swirling vane located upstream of the injection tube. A central rod installed on the burner axis helps anchoring the flame at the injection unit outlet 2 mm above the dump plane. The mixture enters the burner through a plenum and subsequently passes through a grid/honeycomb/grid-arrangement before entering a water-cooled convergent nozzle to reach a nearly uniform top-hat velocity profile at the entrance of the swirler. A loudspeaker is placed at the bottom of the injection system to operate pulsed flame regimes. Steady and unsteady (350 Hz forcing) cases have been studied. Experimental data include velocity measurements by PIV, longitudinal and transverse OH-PLIF imaging of flame shape, surface temperature measurements by laser induced phosphorescence, and gas temperature measurements in the outer recirculation zone using thermocouples.

Lund University (LUND), the University of Texas at Austin (TX), and EM2C laboratory at Ecole Centrale Paris have performed LES using Low Mach Number solvers. EM2C and TX applied the model F-TACLES based on filtered premixed flamelet tabulation, whereas LUND employs a skeletal mechanism combined with an Implicit LES approach. Velocity measurements a few mm above the exit of the injection tube have been used to define the simulations BC's. Detailed temperature measurements at the walls have been used to characterize the thermal BC's. Cold and reactive flow LES of the steady case were performed. For each group, LES assuming a fully adiabatic combustion chamber predicts an M-shape flame and completely mispredicts the thermochemical conditions within the domain. LES which accounts for non-adiabaticity predicts a V-shape flame and shows good agreement with experiments. Preliminary experimental and numerical results on the unsteady configurations were presented and need to be further consolidated.

Flame-Wall Interaction (FWI)

Coordinators: Francesca di Mare, Johannes Janicka, and Andreas Dreizler

The flame-wall dynamics play a central role in the development of new combustion technologies for propulsion and power generation under the increasingly stringent regulations on emissions. In modern gas turbine combustors operating in the lean premixed regime a large amount of the air flow is diverted from liner cooling, thus giving rise to a sparse, unstable film. The presence of a strong swirling flow in the main body of the combustor induces hydrodynamic disturbances which disrupt the labile cooling layer and allow the flame to approach the liner wall. In the presence of fuel-rich gases the cooling air also affects the reaction patterns by providing oxidant for high-temperature combustion, thus increasing the formation of NOx in the forward part of the combustion chamber. Further oxidation of the exhaust gas can be promoted by the presence of cooling air in proximity of the metallic surfaces of the high-pressure turbine stage, with consequent shortening of the component's life. In internal combustion engines the downsizing of the combustion chamber results in a large fraction of the charge burning de facto in proximity of the walls.

The interaction of the flame with cold walls is a complex phenomenon involving hydrodynamic, chemical and thermal effects. FWI can be described in terms of head-on quenching (HOQ) or sidewall quenching (SWQ). In the first case the flame propagated perpendicularly to the wall and is arrested at a distance comparable to the flame brush thickness. In the second case the flame propagates parallel to the wall and is quenched at a distance larger than that observed in HOQ. As the flame extinguishes the heat flux toward the wall reaches its maximum, estimated to be equal to one third of the flame power, although in SWQ smaller heat fluxes have been observed. As the flame modifies and is in turn affected by the turbulent field in proximity of the wall, the combustion regime undergoes a transition from flamelet in the core flow to thickened flame near the wall, opening new questions regarding the appropriate modelling of the turbulence/chemistry interaction.

The time and length scales involved in FWI present significant challenges for both experimental and numerical investigations. Only recently, simultaneous quantitative measurements of temperature and CO concentration in the context of FWI have been carried out in a laboratory scale configuration at moderate Reynolds numbers. DNS studies have been carried out to gain more detailed information on the fundamental mechanisms of FWI in turbulent flows. However, as these numerical experiments were carried out in highly idealized conditions, the results fail to address the issue of modelling the complex turbulence/chemistry interaction in technologically relevant devices where complex fuels are used.

In the near wall region closure is necessary for both hydrodynamic phenomena and chemistry. Whilst Large Eddy Simulation (LES) can be effectively used to address the former, it is likely that a reduced chemistry approach, such as the FGM technique, might break down when applied to FWI. In particular, whilst temperature and CO-concentration can be well captured using reduced chemistry, the composition of the burnt or partially burnt mixture in the post-quenching period can only be predicted using skeletal mechanisms. On the basis of the information gained in idealized cases through DNS, it appears that the classic modelling paradigms (premixed/nonpremixed, PDF-FGF) cannot be applied without possibly major extensions. Important modelling questions remain to be answered; among these:

- How can the information obtained from laminar quenching be exploited to understand the dynamics of FWI in turbulent combustion?
- Is the formulation of a well-founded turbulence/chemistry interaction model at all possible in the near wall region?
- How existing modelling approaches should be extended to encompass FWI? Moreover, should only extension be considered (e.g. heat losses in FGM), or rather a conceptual re-thinking of existing models is required?
- Which approach can offer the best perspectives in terms of UHC and CO modelling?

This new TNF session on FWI was aimed at presenting the open issues related to this research topic and sketch possible future research strategies. As the latter require close interaction between modelling and simulations on one side and experimental studies on the other, the TNF forum is decidedly an ideally conducive environment to carry forward systematic research on FWI. To support a fruitful modelling and simulation activity by all interested researches, the FWI-burner configuration investigated by Mann et al. (CNF 161:2371-2386, 2014) is proposed as benchmark.

LES Quality Assessment and Uncertainty Quantification

Coordinators: Guilhem Lacaze and Joe Oefelein

The need to understand the range of errors that can affect a given LES calculation and establish better metrics related to LES implementation is well recognized. To address this need, past TNF sessions have been aimed at investigating different approaches to measure the "quality" of LES calculations. Initial focus included the potential merits of various algebraic error indicators using the Sydney HM1 flame as a test platform (e.g., Pope criterion, Celik, etc.). The Error-Landscape concept (e.g., Geurts, Kempf et al.)

and Recursive-Filter-Refinement techniques (e.g., Klein, Raman) were also investigated. In TNF11, a summary of efforts to date was presented, followed by attempts to develop better local resolution criteria based on relevant subfilter scales (e.g., Vervisch et al.). The idea was to better understand and quantify the range of subfilter scales over which a given system of sub-models can work effectively. While some progress has been made, the challenges of establishing robust criteria and methodologies are still significant. The question of LES quality is still open due to the inherent complex interconnections between the various sources of error (models, numerics, boundary conditions, etc.).

Given the current status, the objective of the session on this topic in TNF12 was to further extend ideas by presenting the feasibility and potential benefits of probabilistic Uncertainty Quantification (UQ) methods to assess the quality of LES models and predictions. The session contained three interrelated elements. First, a brief summary was presented to highlight the needs and status in the context of TNF flames. Second, a focused "tutorial-like" presentation of Bayesian inference methods was given to establish the basic concepts, tools, and their potential utility in TNF examples. A key element that makes UQ affordable for LES is the construction of a surrogate model that reproduces the dependence of quantities of interest on relevant model parameters. This model is built using a number of sampled LES computations using sparse quadrature methods. Using this model, Bayesian methods are then used for model calibration, comparison, and validation. The third element was a set of example studies that demonstrated the current state-of-the art in this area. Following the tutorial by Najm, Lacaze showed how in practice a non-intrusive UQ technique can be coupled to a LES solver using the HM1 Sydney burner as an example. Mueller then demonstrated how UQ can be used to estimate error bars on LES results due to uncertainties in chemical models. Di Mare presented the latest developments in terms of quality indices for LES in complex geometries. Finally, Sankaran showed comparisons between different LES solvers applied to the same reacting case, which demonstrated that numerical and model errors must be considered simultaneously and decoupled to do any meaningful analysis.

Subsequent discussion revolved around the following points:

- Comments on the quality of present TNF calculations:
  - Different models are tested in different codes. Models should be tested across different codes. The objective is to quantify better what combination of numerical methods, models, and implementation approaches are required for robust application of LES.
  - It was suggested that the TNF cases were somewhat "forgiving" and were not "breaking" models enough. For cases where models agree well with measurements, parametric studies would bring useful insights with respect to grid dependence, parameter dependence, etc.
- How can we decouple numerical and model errors?
  - Numerical errors depend on the type of numerics and decrease as spatial and temporal resolutions are refined. Grid sensitivity studies should be systematically performed to distinguish grid requirements for the different combinations of codes and models.
  - Explicit filtering can be used in theory, but is still expensive in practice. Models require a sufficiently resolved scale-separation, but achieving this with explicit filtering could imply prohibitively large grids that quite possibly approach DNS resolutions. This requires further investigation.
- What is the path for relevant code comparisons?
  - Different codes employ different numerical approaches, which can have very different broadband damping and dispersion characteristics. Hence, fixing the spatial and temporal resolution across codes using the same models does not necessarily provide a

good basis for comparison. Instead, resolutions need to be consistent with the order of accuracy of respective codes.
    - Codes and models should first be demonstrated to perform well on non-reacting flows. A systematic grid sensitivity analysis should be performed to find the grid spacing required to capture cold-flow statistics and related scalar-mixing processes. This will help separate problems with mixing from problems with the combustion closure.
    - Once scalar mixing characteristics are quantified, analogous reacting cases should be considered. The cold flow results should then be included with the reacting flow results.
- What is the path for relevant model comparison?
    - First, perform grid sensitivity analyses against cold flow measurements to find the resolution at which numerics no longer impact simulation results.
    - Model results should be code independent and should be implemented in different solvers to perform meaningful comparisons.
- What cases should we focus on to address LES quality issues at the next TNF?
    - Bluff-body burner HM1 from Sydney.
    - Turbulent counter-flow burner.

Modelling of DNS Cases

Coordinator: Evatt Hawkes

The objective of the session was to do with direct numerical simulation (DNS) databases what has been done with experimental databases in this workshop since its inception, i.e. to understand and improve the performance of practically useful models of turbulent combustion.

Used in this way, as a "numerical experiment", there are several advantages to DNS: the sub-model inputs, such as chemical kinetic rates, are completely specified; there are minimal uncertainties associated with boundary and initial conditions; there are no measurement errors; elements of the modelling (for example scalar dissipation rate) can be determined or at least guided by the DNS; much more data are available for comparison (complete time-varying 3D fields of scalars and velocity); and the DNS can be examined in detail to understand why models work or not. Taken together, these advantages represent a significant opportunity in that many possible reasons for differences between model and "experiment" can be eliminated, and in that the remaining reasons can be better understood.

On the other hand, we also have to be mindful of the limitations of DNS. DNS is limited by computational expense to certain parameter regimes. Principally it is restricted to problems which do not exhibit a large disparity of length and time-scales. For example it is restricted to low Reynolds numbers (currently jet Reynolds numbers ~10,000). It is limited by computational expense in terms of the amount of statistics that can be collected much more than are typical physical experiments, so that statistical error is much more significant. It is affected by numerical errors. DNS is after all just another model. It is possible that due to model inputs or physical assumptions being inaccurate, it does not represent reality accurately enough. It could also be simply wrong due to coding errors, etc., though most DNS codes are quite well verified.

It was decided early on that the focus of the session should be on *a posteriori* tests, i.e. tests of the models where the model is run and the resulting statistics are assessed against the DNS statistics. This is in contrast to the *a priori* testing of models, where elements of the modelling a directly examined using the DNS data, without actually running the model as a whole. While there is a huge body of work on *a priori* testing, reports of *a posteriori* tests are much fewer. The focus on *a posteriori* tests was considered appropriate for TNF first because there has been so many *a priori* tests that it would have been impossible to review them within a TNF session, but more importantly because things that work extremely well in *a priori* tests often fail in practice, while things that work well in practice often fail in *a priori* tests.

Two sets of DNS modelling non-premixed, temporally evolving, plane-jet flames featuring extinction and reignition were considered. These databases were selected because a number of modelling investigations of the data already existed, and because an initial focus on non-premixed jet-flames mirrored the initial focus of the TNF workshop. The first DNS database considered syngas fuel and a series of cases having different Reynolds numbers, keeping the Damköhler number fixed. One case was also considered where all species had unity Lewis number, in order to understand any possible influences of differential diffusion. The second DNS database considered ethylene fuel with a series of cases having different Damköhler numbers, keeping Reynolds number fixed. In the syngas cases, higher Reynolds number resulted in more extinction, while in the ethylene cases lower Damköhler number resulted in more extinction. Comparison of the results between the two different fuels was also of interest, since in the case of syngas the reaction zone was much broader than for ethylene, and the PDF of radicals conditional on mixture fraction was mono-modal in the case of syngas and bi-modal in the case of ethylene.

Four groups contributed modelled results for comparisons. UNSW contributed RANS/transported PDF results using four different mixing models for all the DNS cases. Cornell/Peking contributed LES/TPDF results for the highest Re syngas case. Utah contributed ODT modelling of the syngas series. Brigham Young contributed ODT modelling of the ethylene series. Georgia Tech also previously modeled the syngas cases using LEM coupled with LES. As per previous comparisons with experimental jet flames, the most challenging situation for the models arose in cases that exhibited large amounts of extinction.

Regarding mixing models, RANS context, UNSW results show that, when uncertainties of turbulence modelling, chemistry, etc., are eliminated, all mixing models are capable of good predictions in strongly burning conditions. In conditions approaching extinction, models that feature locality of mixing (EMST, SPMM) generally provide good predictions of mean quantities, but greatly under-estimate conditional fluctuations. In contrast models that do not feature locality of mixing (IEM, MC) fail for predicting the means but do better for conditional fluctuations. SPMM is a newer model for which the optimal parameter settings are not yet known. It was shown to provide results similar to EMST or IEM with different parameter choices. Regarding LES, Cornell and GA-Tech show good results with LES, particularly for syngas case H, which is on the edge of global extinction. Reignition is stronger than in UNSW's RANS, suggesting that spatial structure in LES may be helpful for capturing reignition. Regarding ODT, some great results were demonstrated after parameter tuning to get the jet spreading right. Results were noticeably better in syngas cases, which are thought to be reigniting by flame-folding (represented in ODT), compared with ethylene, which are thought to be reigniting by edge-flame propagation (not represented in ODT).

There was a lively discussion after the session. Model parameter tuning was one issue raised several times. Some of the models had certainly benefited from parameter adjustment, some had not, and for others it was unclear whether there had been tuning or not. One view was that excessive parameter adjustment suggests that something deeper is deficient with the model. The other was that parameter adjustment is needed in order to understand sensitivities, and that the objective is to build up enough experience about how to set the parameters in different contexts and preferably embed this into the model in ways that end users can easily take advantage of.

Future sessions will benefit from a more coordinated effort. In the TNF12 session, the modelling had been done by various groups over several years. With the exception of the UNSW set of results with an array of mixing models, too much had been varied between the models to make clear conclusions on any one modelling element. In addition with most groups reporting just one set of modelling results, understanding any parameter sensitivities was impossible.

To better coordinate this in future sessions it is suggested that the workshop could propose some specific DNS cases as targets, similar to what is done for the experimental targets. As per the experiments, the targets would have to be of interest to enough modelling groups to create a critical mass of effort such that useful conclusions can be drawn. DNS targets should probably be designed from the beginning with this particular use in mind, similar to the experimental databases, so as to maximize their usefulness to the modelling community. The databases should meet some quality standards, which need to be defined. They need a thorough characterization targeted at what modelers need to know. Finally, the databases need to be made readily accessible. For this to be useful for TNF13 we probably need to start the process now. A discussion therefore on whether this is a useful direction for TNF13 to pursue is needed. Several possible future target cases with references are given in the session summary in the full proceedings.