SUMMARY AND CONCLUSIONS

Fifth International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames

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INTRODUCTION:

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

TNF5 was hosted by the Thermal and Fluid Sciences Section, Delft University of Technical and was attended by 68 researchers from 11 countries. Thirty posters were contributed and abstracts are included in the proceedings. Calculated and measured results were compared for three target flames:

- Piloted CH4/air jet flame series, with emphasis on extinction/re-ignition and NO formation
- Bluff-body stabilized flows and flames
- The TECFLAM burner for confined swirling natural gas flames

In addition, there were presentation and discussions on specific modeling issues, including:

- Accuracy of chemical mechanisms in calculations of laminar, opposed-flow, partially-premixed CH_4/air flames
- Adequacy of the optically thin radiation model
- Sensitivity of piloted flame results to the choice of mixing model
- Sensitivity of results to changes (uncertainties) in inflow conditions
- Statistical accuracy of pdf calculation

As in previous TNF workshops there was an open and productive atmosphere with numerous discussions in small groups, during breaks and poster sessions, as well as larger discussions, during the technical session. It is this situation, together with the exchange of information during the year among collaborating groups at various locations, which forms the basis for progress on the selected target flames. TNF participants are encouraged to continue and expand these collaborations and discussions, as we pursue a better understanding of turbulent combustion.

This summary briefly outlines accomplishments on the three target flames and other focus topics. It also summarizes discussions at TNF5 regarding research priorities and planning for the next workshop (TNF6). The TNF5 Proceedings are available in pdf format on the web at www.ca.sandia.gov/tdf/Workshop. The pdf file includes all materials from the proceedings notebook that was distributed to workshop participants in Delft (preface, agenda, list of attendees, selected comparisons of measured and modeled results for the three target flames, information on other focus topics, and poster abstracts). Several vugraph presentations have also been included. The pdf file has 236 pages taking roughly 22 Mb, and it includes bookmarks and thumbnails for navigation.

ACCOMPLISHMENTS:

Accomplishments on various topics are outlined in the order of the TNF5 agenda.

Piloted Flames:

- **General Progress** – Significant progress has been made in recent years in the modeling of the piloted CH_4/air jet flames. It can be concluded that it is now possible to obtain very good agreement between model and experiment. In particular, the pdf calculations contributed by Tang, Xu, and Pope (Cornell) and by Lindstedt, Louloudi, and Vaos (Imperial College) each do well in accounting for local extinction, as well as getting reasonably good agreement on Favre averaged profiles, conditional means, and fluctuations. These calculations, which are described in more detail in papers contributed to the 28^{th} Combustion Symposium, are representative of the state of the art in modeling turbulent jet flames with local extinction. We have also achieved a better understanding of several aspects of the models and the sensitivity of results to the choice of chemical mechanism, radiation model, mixing model and mixing constants, constants in turbulence models, and boundary conditions.

- **Chemical Mechanisms** – Comparisons of measured and modeled results in steady, opposed-flow, partially premixed laminar flames served to clarify the similarities and differences among various detailed chemical mechanisms for methane combustion. It may be concluded that the detailed mechanisms used in the various calculations of the target flames (the Lindstedt mechanism and versions of GRI Mech) yield similar results for the major species profiles in laminar flames and that predictions agree with experiments. There are large differences among mechanisms, with regard to the prediction of NO. The proceedings include laminar flame results using mechanisms from Lindstedt, Li & Williams, Warnatz, and GRI-Mech (2.11, 3.0, and reduced versions of these). More work is needed to fully compare the available data with calculations using all the major mechanisms. However, the comparisons contained in the TNF5 proceedings show that GRI 3.0 significantly over predicts NO levels in lean and near-stoichiometric regions of the laminar flames, while GRI 2.11 under predicts NO levels in fuel-rich conditions. Calculations from Lindstedt and from Li & Williams appear to do a better job than GRI-Mech in predicting the measured shape of the NO profile.

- **Radiation** – Accurate modeling of radiation is important in the context of NO formation. Measured radiant fractions are now available for many of the jet flames in the TNF data library, and these are reported by Frank et al. (28^{th} Combustion Symposium). There is some evidence to suggest that the optically thin model recommended for TNF calculations over predicts the radiant fraction in all of the TNF jet flames except for the H_2 flames. The strength of absorption of the 4.3-micron band of CO_2 is the main issue. Further work is needed in this area to quantify the absorption effect and, if necessary, to develop an improved radiation model that is not computationally expensive.

- **Mixing Models and Constants** – The measured degree of local extinction in the piloted flame series is expected to be difficult to reproduce in calculations. Therefore, it is important to emphasize that calculations from the groups at Cornell and Imperial College each show good results on extinction. The Cornell group used the EMST mixing model, while the Imperial College group used the modified Curl's model. Both groups made adjustment to the mixing model constant in order to achieve agreement with measurements. This suggests than both mixing models are capable of capturing the main features of the local extinction process. However, it also demonstrates the sensitivity of extinction results to the choice of the mixing model and constants. Parametric calculations of flame F by J-Y Chen also show that different mixing models yield significantly different results, when constants are not tuned. The Cornell group has also demonstrated that the degree of extinction in very sensitive to inflow conditions. Specifically, they observed that ± 10K changes in the pilot temperature produced significant differences in burning index for flame F.

- **Unfinished Business** – Comparisons of results for piloted flame D, which were presented first in TNF3 (Boulder, 1998), showed that the steady flamelet model and the CMC model yielded significantly higher levels of CO and H_2 in fuel-rich conditions, as compared to pdf models and the measurements. The reasons for these differences are still not fully understood. Laminar flame comparisons have shown agreement between measured and calculated results for partially premixed flames at relevant strain rates. Thus, the problem appears to be with something other than the chemistry.

Bluff Body Flames:

- **Flow Field** – In contrast to the situation for piloted flames, predictions of the flow field for the bluff-body flames are not yet in satisfactory agreement with measurements. Computations of the velocity and turbulence fields are adequate in the upstream regions of the jet covering the recirculation zone and the necking zone. However, further downstream and starting at about two bluff-body diameters, calculations show increasing deviation from the measurements. This is true regardless of the numerical approach used and of the modifications made to the model constants. For the results at this workshop the contributions using modified eddy viscosity models did get better results than those using second moment closure approaches without modifications.

- **Chemistry** – The chemistry models used were simple and were based on one of the following assumptions: flamelet, fast chemistry, full or constrained equilibrium. Computations were presented for temperature and the mass fractions of OH and NO in the recirculation zones. It was clearly concluded that detailed chemical kinetics are needed to adequately compute the mass fraction of minor species such as OH and NO even in regions where local extinction is not prevalent such as in the recirculation zone.

- **New Wall Temperature Data** – Measurements of the temperature of the ceramic face of the bluff-body yielded 650 C for flame HM1 and 750 C for flame HM2. These new boundary conditions should be implemented in future calculations.

- **New CO Data** – Data on CO collected using LIF was presented in a poster by Dally et al. showing a vast improvement on the existing Raman CO measurements. These data, which were acquired during the original experiment but only processed recently, will be added to the current bank on bluff-body stabilized flames.

In the closing discussion it was agreed that focus should now shift to compute the compositional structure in the recirculation zone of bluff-body stabilized flames. Measurements show that, the mean radial location of the reaction zone shifts from the inner edge (close to the fuel jet) of the large vortex to the outer edge (close to the air side) depending on the fuel jet velocity and the fuel mixture. This is an important issue and a good test case for the computations. A list of candidate flames, having the mean reaction zone occurring at different locations in the recirculation region, will be made available as target flames for TNF6.

TECFLAM Burner:

For the TECFLAM burner the main accomplishment was the presentation of a complete, consistent data set. First modeling results are encouraging, but the problem of getting good agreement with experiment is even more open than in the case of the bluff body flames due to the complexity of the flow. The question is which strategy now has to be followed. Is it possible to identify the minimal ingredients both in turbulence modeling and in turbulence-chemistry interaction model to get at least the flow field to agree well. Incorporation of radiation in the model here needs more than an emission only assumption, which adds to the complexity.

RESEARCH PRIORITIES:

- **Piloted Flames** – There is no longer a strong incentive to keep the piloted jet flames as primary target flames for future TNF workshops because they have been extensively studied over the past years, and some good results are being published. Nevertheless, some arguments in favour of keeping them were given. Since the correct prediction of the velocity field is easily possible, the discussion can focus on detailed issues related to chemistry and turbulence-chemistry interaction. Piloted flames will remain useful as a test for NO and radiation modeling. Further comparison of micromixing models to better document the true reasons for success are to be made (e.g. compare EMST model and modified Curl model). It was also suggested that updated measurements in piloted flames of pure methane (or CH_4/N_2) and new data in ethylene flames would be of interest.

- **More Complicated Flames** – The main challenge for the TNF workshop participants is to extend the success obtained for partially premixed methane/air piloted jet flames to more complicated flames. Good datasets should be selected and made available on the web. Flame types that are in the picture are bluff-body flames, swirl flames, and opposed jet flames. With each of these geometries the accurate documentation of inflow and boundary conditions will be very important. Due to the difficulty in modeling just the flow field in these cases, it may be appropriate to consider bluff-body and swirl flames with little or no local extinction. Modelers should always first try to produce correct flow fields and mean mixture fraction profiles for the new flames. This needs understanding of the turbulence and a certain minimal level of chemistry model. The second step, is to get the profiles of main combustion species (including hydrogen and CO) right. The third and final step focuses on the prediction of minor species as NO. The succesful completion of the third step will need a completion of the discussion on radiation modeling started at TNF5

- **LES** – Large eddy simulation should also be done, because of its intrinsic value and because of the light it may shed on some of the modeling issues in PDF, CMC or flamelet models. Setting up LES may require a preliminary study on inlet boundary conditions.

- **Chemical Mechanisms** – The GRI mechanisms and various reduces versions are widely available. However, other mechanisms have shown better agreement with measurements of

NO in partially premixed CH_4/air flames. Therefore, it would be beneficial if detailed and reduced versions of mechanisms from Lindstedt, Li & Williams, and perhaps Miller could be made available on the web in broadly compatible format with corresponding thermodynamic data.

- **Laminar Flame Comparisons** – More work is needed to complete and fully document the cross comparison of various measurements and calculations of NO and other scalars in laminar flames. It was suggested that additional data at lower strain rates and lower fuel-side equivalence ratios would be useful. Detailed laminar flame data from ethylene flames was also requested.

- **Scalar Dissipation** – Available models of scalar dissipation in jet flames are not in agreement with each other. It appears that further work is needed in the area of experimental validation of scalar dissipation models.

- **Other Fuels** – In general, changing the fuel leads to mean reaction zones at different locations relative to shear layers and recirculation zones (because of other stoichiometry) and therefore changes in regime of turbulence-chemistry interaction. Therefore, it can be interesting to plan experiments with other fuels, in either piloted or a bluff-body geometry providing new challenges. In the case of piloted flames, it can be interesting to turn to the more difficult case of pure methane. Also ethylene was suggested as an interesting fuel because it is a key component in many combustion processes. Two candidate fuels for bluff body flames are CH_4 (for which some results are already available) and H_2/CO. The turbulent diffusion flame lab in Sandia is available for experiments, but there is a need for someone to do the measurements: e.g. visiting students from groups worldwide

ORGANIZATION OF TNF6:

The Sixth TNF Workshop will be held in Japan in 2002 just before the 29th Combustion Symposium. Details regarding target problems, location, and dates will be announced.

Arguments were put forward to enlarge the scope of the TNF workshop to include also spray flames and even premixed flames. The preliminary conclusion on this was that such excursions are possible provided a sufficient number of both experimentalists and modelers are actively involved. It is the strength of the group of contributors to TNF workshops that there is a strong interaction between modellers and experimentalists and this should be maintained.

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