Third International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames

Boulder, Colorado
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Comments from the Program Co-Chairs

The following comments highlight some of the major discussion topics and outcomes from the Boulder workshop. They are not intended as a complete summary of the target flame comparisons, and they do not necessarily represent a consensus of opinions of the TNF3 participants and contributors.

The Target Flames

One of the primary objectives of the TNF Workshop is to establish and maintain a library of data sets on turbulent nonpremixed and partially premixed flames that is appropriate for testing various turbulent combustion models. In developing this library we have started from the simplest cases (hydrogen jet flames in coflow) and are gradually increasing the complexity of the flow field and the fuel. Our goal is to provide a sufficient number of reliable and reasonably complete data sets to test a wide range of turbulent combustion models and better understand the capabilities of models to capture important fundamental combustion processes. Flames may be added or deleted from the library based upon the availability of new data and the interests of the modelers participating in the workshop.

These collaborative comparisons provide experimentalists with useful feedback on the completeness and appropriateness of each data set, including documentation of boundary conditions and experimental uncertainty. In some cases the process points to gaps in the documentation or questions that call for additional measurements.

The four TNF3 target flames all include CH_4 as a primary component of the fuel, but they represent a range in flow field complexity. They were presented at the workshop in order of increasing complexity. Each of these flames is at a different stage with regard to the process of comparing measured and modeled results, and so we include here a few comments to outline the status of each flame and place it in the context of the overall workshop process.

Simple $CH_4/H_2/N_2$ Jet Flame (DLR Flame)

The DLR flame was a late addition to the list of target flames that appeared in the first announcement of the Boulder workshop. Scalar measurements were contributed by Wolfgang Meier and coworkers at DLR Stuttgart, while velocity measurements were provided by Egon Hassel and coworkers at TU Darmstadt. Three modelers contributed calculations.

An important attribute of this flame in the context of the data library is that it combines methane kinetics with the simple jet geometry. Thus it provides a logical bridge between the simple H_2 jet flames and the pilot- or bluff-body stabilized methane flames. In fact, the burner is the same as that used for the "H3" hydrogen flame in the library. The inclusion of H_2 in the fuel stream makes differential diffusion a significant issue near the base of the flame. This point was made clear by results from Heinz Pitsch (not included here) comparing flamelet calculations with Le=1 vs. Le≠1. The differential diffusion effect is believed to be responsible for some of the differences among measured and modeled results in Section 1. Consequently, this flame is not as simple a test case for methane chemistry as one might like. However, the relatively clean boundary conditions at the nozzle make it a useful target, particularly for the few models that include effects of differential diffusion. Also, imaging data on this flame provide information on turbulence structure that are useful in the interpretation of near-field effects.

The figures comparing measured and modeled results for the DLR flame have been revised since the workshop to combine the different calculations onto the same graph wherever possible. In addition to the three calculations represented in these figures, the poster abstract from H. Pitsch includes comparisons of calculations using three different chemical mechanisms.

Additional scalar measurements on this flame would be useful. The available scalar point data do not include simultaneous point measurements of OH or NO. Also, the Raman scattering measurements of CO are affected by fluorescence interferences and may not have sufficient accuracy to really test the details of the reduced chemical kinetic mechanisms and the turbulence-chemistry coupling models. Experiments to fill in these data are planned as a collaboration between DLR Stuttgart and Sandia.

Piloted CH_4/Air Flame (Flame D)

Flame D is one in a series of piloted flames measured recently at Sandia. Velocity measurements were obtained at TU Darmstadt using the piloted burner and a set of calibrated flow controllers loaned from Sandia. While the pilot adds some flow complexity, it does not appear to present a special problem to the turbulence models, and most calculations were conducted using the same model constants as for simple jet flames. The participating modelers generally agreed that one could not expect current RANS models to accurately predict the near field (x/d<5) of simple or piloted jet flames, and detailed comparisons in the near field were not carried out. In fact, several of the models required special treatment of the near field in order to produce a stable flame, and some comments on this are included in the model descriptions. Comparisons starting at x/d=7.5 show that some models did better than others in calculating the overall velocity and fixture fraction fields. However, these differences were not discussed in detail, and the general view was that all of the models were close enough on the mean axial velocity and mixture fraction profiles to allow comparison of the details of the species results.

The discussions of Flame D focused mainly on issues of chemistry. Plots of conditional means in Section 2 provide the most direct information regarding chemistry in this flame. There is close agreement between measurements and most of the models for fuel-lean conditions. However, the plots of measured and predicted conditional means show wide variations among calculations of species mass fraction in fuel rich conditions. The reasons for these differences are not fully understood at this time, and this is one obvious area for further investigation. All of the calculations, except the PDF/ILDM calculation from TU Darmstadt, were based on the GRI-1.2 or GRI-2.1 mechanisms. Therefore, it appears that differences in the turbulence-chemistry coupling models, rather than differences between the mechanisms, are responsible for the wide variations observed in the results on conditional means. It is quite possible that relatively minor changes in the parameters of the models could improve agreement with the measurements. However, this has yet to be demonstrated.

We note that the ILDM calculation is limited by the fact that the ILDM table used in this calculation was based on a manifold that was only defined for a limited interval in mixture fraction surrounding the stoichiometric condition. Outside of this region the calculated results for H_2 and CO are unrealistic, due to the assumptions used in constructing the table. The same observation is made in the poster by Hinz et al. and also in the discussion of the Delft flame calculations (Section 3), which were based on a similar ILDM implementation. An ILDM approach using different assumptions in constructing the table or an approach using more than two progress variables might well provide better agreement with the measurements, and there is room for further work here.

Piloted Natural Gas Flame (Delft III)

The boundary conditions for this piloted flame are more complicated than for Flame D, and measurement problems caused by interferences from soot precursors and soot are more severe. However, there is now a significant bank of data for this flame using different techniques in different labs. In particular, the poster by Versluis et al. reports recent CARS temperature measurements that are in good agreement with Rayleigh scattering measurements from Sandia. Such redundant measurements are very useful with regard to model validation and the establishment of reliable benchmark data sets. The Delft flames also uses a "practical" fuel, which may be an important consideration, at least politically, when making the connection between fundamental research and industrial applications.

The Delft III flame was used already as a target for the Second Workshop on Aerodynamics of Steady-State Combustion Chambers and Furnaces (A.S.C.F) held in Piza, Italy on November 28-29, 1996, and only one modeler outside of TU Delft contributed results to the TNF3 Workshop. Accordingly, Tim Peeters presented a status report on the Delft flame (Section 3) rather than a comparison of measured and modeled results.

One important aspect of the TU Delft calculations of their own flame is their comparison of three different mixing models. Some comments on this are also included in the poster abstract from Peeter Nooren. This type of study on the effects of changing one submodel at a time are very useful, both for understanding the sensitivity of results to such changes and for evaluating the accuracy, applicability, or efficiency of specific submodels. We encourage more work on this type of parametric investigation.

Bluff-Body Stabilized CH_4/H_2 Flame

The recirculating flow field of this case represents a significant challenge for turbulence models, and the emphasis of the TNF3 round of comparisons on the bluff-body cases was on the flow field calculations. Nonreacting and reacting cases were considered, and relatively simple models for the chemistry were used. Assaad Masri, the coordinator for this flame, has provided a good overview of these comparisons in Section 4.

One area of discussion in Boulder had to do with the apparent qualitative differences between predicted streamline patterns in the recirculation zone (lower center image on the proceedings cover page, for example) and the pattern derived from the measurements (not included in these proceedings). Some people expressed the opinion that such qualitative differences were an indication of an overall deficiency in the RANS models and that large eddy simulation (LES) should be pursued if one wished to improve the accuracy of flow-field calculations for this type of flame. We note that comparisons in a recent paper by Dally et a. (Combust. Theory Modelling

2:193-219) of the measured and computed flow patterns for one of the nonreacting bluff-body cases show reasonably good qualitative agreement.

Experimental Uncertainly

The determination and clear documentation of experimental uncertainty is a critical issue for the process of establishing benchmark data sets and testing models. Norm Laurendeau commented on this in Boulder, and we wish to emphasize some of those comments. First, none of the comparisons of measured and modeled results include error bars on the experimental data. These should be included in the future. Second, confidence levels should be provided as part of any estimates of uncertainty, and the method of establishing the uncertainties and confidence intervals should be documented.

While most of the experimentalist contributing data to the workshop library have included some estimates of uncertainty, it is clear that we can and should do a more complete job in this area. We will continue to try to emphasize the documentation of uncertainties. We will also consider the possibility of providing specific guidelines for the determination and reporting of experimental uncertainties in connection with data sets to be included as TNF target cases. Comments and contributions on this topic are welcome.

In a similar vein, modelers are encouraged to document such things as tests for grid independence, sensitivity to boundary conditions, sensitivity to changes in model constants, and any special procedures used to start a calculation or establish a stable solution.

Some Areas for Further Work on the TNF3 Target Flames

There are several areas where further work is needed in connection with the four target flames. We hope to address some of these over the coming year and at the TNF4 Workshop in Darmstadt, Germany during the summer of 1999. These include:

- additional measurements of minor species in the DLR flame
- investigation of the reasons for the large differences in predicted conditional means for fuel-rich conditions in Flame D
- comparison of results on NO formation (Some calculations of Flame D included NO, but this was not discussed in detail in Boulder.)
- additional measurements and analysis of flame radiation as it influences NO formation in these hydrocarbon flames
- extension of calculations to piloted flames E and F, which have significant localized extinction
- inclusion of more complete chemistry in the calculations of the bluff-body flames
- investigation of the LES models for calculating these target flames, particularly the bluff-body flame

Some Possibilities for Future Target Flames

While the above list may already imply more work than can be accomplished in time for the TNF4 Workshop, there was also discussion in Boulder about the next types of flames that should be addressed. Swirling flames are a prime target for those who have research connections with practical applications. Several groups are already working on swirling flames, as reflected by the posters. A few data sets are already in the literature, other experiments are in progress, and two or three groups are considering new experiments on "simple" swirling flames. We strongly recommend that the experimental and computational people interested in swirling flames collaborate on: i) the evaluation of existing data sets to determine whether they are appropriate for the sort of model testing that the workshop is doing, ii) the design of new or supplementary experiments to ensure that boundary conditions, flow parameters, measured quantities, and measurement accuracies are consistent with the requirements for model testing, and iii) the acquisition of complete and complementary data on selected flames in different laboratories. Several workshop participant also expressed interest in turbulent counterflow flames as being useful for testing certain aspects of combustion models. Discussions on both types of flames are continuing.

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