SUMMARY

Eighth International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames

3 – 5 August 2006
Heidelberg, Germany

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INTRODUCTION

The series of workshops on Measurement and Computation of Turbulent Nonpremixed Flames (TNF) is intended to facilitate 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 nonpremixed and partially premixed flames, as revealed by comparisons of measured and modeled results for selected flames. Several participating research groups have strong interest in applying this same framework for detailed measurement – model comparisons to the areas of premixed- and stratified combustion. There is also growing interest in the use of detailed simulations to complement experimental benchmarks for model testing and validation. Our goal in these combined efforts is to accelerate the development of advanced combustion models that are soundly based in fundamental science, rigorously tested against experiments, and capable of predicting the behavior of a wide range of turbulent combustion situations.

TNF8 was attended by 80 researchers from 14 countries. Thirty-nine posters were contributed, with abstracts included in the proceedings, and several additional posters were displayed to augment the invited presentations. Discussion sessions addressed the topics listed below:

- Comparison of measured and modeled results on bluff-body and swirl-stabilized flames
- Recent modeling progress on other TNF target flames
- Progress on measurement of scalar dissipation and small-scale turbulence structure
- New experiments and high-speed diagnostics
- Strategies to reduce simulation costs for chemistry and mixing
- LES quality assessment
- Issues for comparing LES and Experiments
- What can be learned from DNS
- Progress and challenges for validation of premixed combustion models
- Perspectives from industry
- Priorities and planning for future work and TNF9 (Montreal, 2008)

For each main topic a session leader (member of the organizing committee or invited speaker) provided an overview, which included the work of others as well as their own, and outlined key issues for discussion and further work. This format has proven effective in maintaining the focus and continuity of the workshop series, while allowing for inclusion of relevant work by people outside the core of active participants in this collaborative process.

This summary briefly outlines highlights of presentations and discussions on these topics. 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 TNF8 Proceedings and also the summaries from previous TNF Workshops because each workshop builds upon what has been done before.

The complete TNF8 Proceedings are available for download in pdf format from the Internet at www.ca.sandia.gov/TNF. The pdf file includes materials from the proceedings notebook that was distributed to workshop participants in Heidelberg, as well as additional materials (such as PowerPoint slides) contributed after the workshop.

Several papers relevant to TNF8 topics and target flames were presented at the 31st Combustion Symposium. Most of these papers may be found in the sections on turbulent combustion within the *Proceedings of the Combustion Institute*, Vol. 31. References to several recently published papers are also given in the Proceedings. An effort will be made to continually update the bibliography page on the TNF web site, so that these relevant papers may be easily identified.

This collaborative research process was initiated more than ten years ago, with preparations for the 1st workshop in Naples, 1996. Accordingly, perspectives on the evolution, current status, and future directions of the TNF Workshop series are included at the end of this summary.

ACKNOWLEDGMENTS

Local arrangements for the TNF8 Workshop were coordinated by Andreas Dreizler, Simone Eisenhuth, and Bernd Radermacher. Sponsorship by General Electric, the German SFB-568 research program, Fluent, Rolls-Royce, ANSYS, Dantec, La Vision, Sirah Lasers, Continuum Lasers, and Coherent is gratefully acknowledged. These contributions allowed for reduction of the registration fees for university faculty and students. Support for Rob Barlow in coordinating TNF Workshop activities is provided by the U. S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences. Sandia National Laboratories is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94-AL85000.

AN IMPORTANT NOTE OF CAUTION

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 may be inappropriate to quote or reference specific results from these proceedings without first checking with the individual authors for permission and for their latest information on results and references.

HIGHLIGHTS OF PRESENTATIONS AND DISCUSSIONS

Comparisons on the Sydney Bluff-Body Flames and Swirl Flames

A comparison of model calculations and experimental measurements for several of the Sydney Bluff-Body and Swirl cases was coordinated by Andreas Kempf. The full Proceedings include summaries of the computational methods, comments by the contributing modelers, and graphical comparisons of results. These graphs include profiles of mean and fluctuation velocity, mixture fraction, and temperature. Comparisons generated discussion in three parts: the originally scheduled session on the first morning of the workshop; a separate committee discussion during the first afternoon, the highlights of which were presented to the full audience on the second day; and further discussion of these points by the full group.

Perspectives on the overall process were collected after the workshop and summarized by A. Kempf for inclusion in the Proceedings. A few points are paraphrased here.

- At TNF8 the flow and mixing fields for the bluff body HM (hydrogen/methane) flames were predicted with good accuracy. This progress triggered discussion on whether these flames should be dropped from future workshop comparisons. However, there are strong support from the modeling community to continue using the HM series of bluff body flames as a vehicle for developing turbulence-chemistry interaction models, for improving sub-models, and to examine effects of detailed chemistry in the context of extinction and re-ignition.
- The flow and mixing fields for the swirl flames are not predicted well enough, at this stage, to justify their use for combustion sub-model development, but further progress may be expected at TNF9.
- There was a comment from one of the participants from the gas turbine industry that the Sydney swirl flames had more complete stability maps than gas turbine combustors and that a configuration more closely aligned with gas turbine combustors might actually be easier to model.
- With LES evolving into a more common tool used by TNF contributors, it is becoming more obvious that LES validation places additional demands upon experiments. A major concern is that detailed information on inflow conditions is needed, including for example, the complete stress tensor and information on length and time scales of turbulence. Information on velocities upstream of the exit plane would allow more reproducible results using calculations that start upstream.
- The broader topic of developing appropriate approaches for verification and experimental validation of LES was also discussed, and these issues are addressed further in the sections that follow.
- There was some concern expressed regarding possible effects of different fuels (CNG for velocity experiments in Sydney vs. CH_4 for scalar experiments at Sandia) on flow fields in cases with local extinction, but no specific course of action was agreed upon.
- It was suggested that future comparisons attempt to include previously reported model results. This suggestion points to a broader problem that much of the information from model calculations, even the most successful examples, is not preserved and available in a convenient digital format. A consideration for the future is whether the TNF Workshop community should be making a greater effort to preserve this information in order to facilitate future comparisons, document progress over time, and avoid reinventing previous results.

The Post-Workshop Information, included in the Proceedings at the end of the section on Sydney flame comparisons, also summarizes opinions expressed regarding future directions and priorities for this sort of collaborative comparison of measured and modeled results, and the reader is encouraged to refer to the complete text.

Recent modeling progress on other TNF target flames

In order to maintain a reasonably narrow focus at the workshop itself, only the Sydney Bluff-Body and Swirl flames were considered for a broad collaborative comparison of model calculations and experiments. However, work continues on other TNF target flames. Accordingly, a session was included to provide an overview of recent work on several flames, including the DLR simple jet flames of $CH_4/H_2/N_2$, the Sandia and Delft piloted flames, the Darmstadt opposed jet flames, and the Berkeley and Sydney lifted jet flames in vitiated coflow. This session was coordinated by Dirk Roekaerts, who invited Robert Gordon and Andreas Kronenburg to present material on lifted and auto-igniting flames. The overview slides include references to more than 20 publications from 2005 and 2006 on modeling of these "other" flames using various methods. Many of these deal with the DLR and Delft jet flames, which have not received much attention in the past, and this is a welcome development that serves to improve understanding of combustion phenomena in the progression of available target flames, as well as improve understanding of the effectiveness of various models in addressing these phenomena.

Over time, the Sandia piloted flames have been most modeled and are perhaps best understood. At this stage it is important to acknowledge the extensive parametric studies conducted by the Cornell group to investigate the coupled effects of chemical mechanisms, mixing models, and the choice of the time scale ratio, C_ϕ, on predictions of localized extinction using RANS/PDF methods. References to this work are included in the TNF8 Proceedings, and additional parametric calculations were presented in a 31^{st} Combustion Symposium paper (Cao and Pope, 2007). Other notable developments are the application of CMC (Kronenburg and Kostas, 2005) and LES/FDF (Raman and Pitch, 2007) to predict effects of local extinction in flame E.

Experimental work has continued at Sydney University on the vitiated coflow burner configuration that was developed at UC Berkeley, and there has been corresponding computational work on these lifted flames in high-temperature coflow. Key issues addressed are the sensitivity of lift-off height to coflow temperature and to chemical mechanism and the presence of auto-ignition markers upstream of the flame stabilization location. These flames are expected to receive even more attention in the future, due to the importance of developing predictive models for the transition between partially premixed propagation and auto-ignition in a variety of combustion regimes. The presentation materials include information on these experiments, as well as related experiments on auto-ignition (Markides and Mastorakos, 2005), and modeling based on RANS/PDF and LES/CMC methods.

Progress on measurement of scalar dissipation and small-scale turbulence structure

The challenges associated with quantifying the effects of noise and spatial resolution on scalar dissipation measurements were a major discussion topic at TNF7 (Chicago, 2004). While some information on error sources has been included with previously published results on scalar dissipation, it became clear that the accuracy of such measurements could not be evaluated without knowing something about the scalar dissipation spectrum in flames and without knowing the local Batchelor scale.

Significant progress has been made toward understanding the scalar structure of turbulent flames at the smallest scales of turbulent fluctuations. An overview of developments in this area was presented by Noel Clemens and Rob Barlow. Key points were: 1) The measured energy and dissipation spectra of temperature fluctuations in jet flames are well represented by the model spectrum of Pope (Turbulent Flows, 2000) for fluctuations in turbulent kinetic energy. 2) High-resolution imaging of Rayleigh scattering may be used to determine the local equivalent of the Batchelor scale in the jet flames considered and possibly in more complex flames. 3) The dissipation cutoff scale for mixture fraction fluctuations is always equal to or slightly larger than that for temperature fluctuations. 4) Effects of noise are easily identified through spectral analysis. 5) These developments bring us closer to quantifying the accuracy of scalar dissipation measurements in flames. Additional information on this topic was presented at the 31st Combustion Symposium (Wang and Barlow, 2007; Kaiser and Frank, 2007).

New experiments and high-speed diagnostics

High speed diagnostics have seen rapid developments in recent years, due to advances in high-power diode-pumped solid-state lasers and improvements in CMOS detector technology. Andreas Dreizler presented an overview of recent applications of high-speed two-dimensional imaging diagnostics in turbulent flows and flames. The aim of this session was to provide examples and begin a discussion on the type of new information that might be extracted from high-speed diagnostics, with a focus on validation of numerical modeling.

Most of the studies outlined are based on sequences of chemiluminescence images obtained at rates of 7–10 kHz. Such "movies" are qualitative in nature, although there is potential to extract information that is spatially and temporally quantitative. However, they can be very informative with regard to transient phenomena, such as ignition, extinction, or flash back, because the transient events may be captured and slowed down to allow physical interpretation by the observer.

Combined imaging of chemiluninescence and Mie scatter offers the potential to obtain conditional velocity statistics around transient or intermittent events, such as local extinction in a turbulent opposed-flow flame. For example, the combination of OH chemiluminescence and velocimetry by PIV/PTV, could be used to obtain velocity statistics conditioned on extinction. High-speed PIV allows for mapping three-dimensional volumes. This can be achieved either by rapid scanning of laser-light sheets or by employing Taylor´s hypothesis. In each case the repetition rate is much faster than typical time-scales of the turbulent flow. Finally combined techniques, such as PIV and PLIF imaging of combustion-produced radicals at high repetition rates, are currently evolving. In these approaches quantitative scalar fields can be recorded in addition to the quantitative flow field information. This type of information is expected to validate models for flame transients, such as misfire vs. successful ignition or local vs. global flame extinction.

Strategies to reduce simulation costs for chemistry and mixing

In past TNF workshops there have been several sessions fully devoted to mixing models and alternative methods for efficient representation of chemical kinetics, particularly in the context of RANS/PDF methods. J-Y Chen presented an overview of recent developments in these areas.

With regard to mixing models, comparisons of several mixing models from DNS studies (Mitarai et al., 2005; Wandel and Klemenko, 2005, 2006) and from LES/PDF studies (Bizetti et al) were summarized. One observation was that LES results are less sensitive to the mixing model than RANS calculations. The expectation is that the localness requirement on the mixing model becomes relaxed as LES resolution increases.

With regard to chemistry, there were contributions covering work at TU Darmstadt on various applications of ILDM, from Cornell on recent developments and implementations of ISAT, from Fluent on *A priori* tabulation and ISAT implementation, from the University of Zaragoza on artificial neural networks (ANN) for representing chemistry and on cost comparisons of ILDM and ANN, and from UC Berkeley on experiences with reduced chemistry, ISAT, and ANN.

LES quality assessment

LES is a promising technique to accurately predict turbulent flows. However, many fundamental problems are unsolved, and no single LES procedure has emerged as a standard. Within the context of the TNF Workshop, validation of combustion LES against experimental results, particularly in flames with strong effects of turbulence-chemistry interaction, cannot be carried forward effectively until issues of code verification and LES quality assessment are addressed. An overview of methods used to quantify the accuracy of LES calculations was presented by Markus Klein, with attention to four points of view:

- The academic approach where one tries to minimize (a priori) numerical and modeling errors using: high-order, non-dissipative, conservative schemes; elaborated models; and high quality grids.
- The engineering approach where one tries to estimate (a posteriori) the modeling and numerical errors arising from a nonperfect numerical scheme, sgs model, and a rather low quality grid.
- The optimal strategy, where one tries to understand the interaction of modeling and numerical errors and to derive optimal LES strategies, using a large data base of decaying isotropic turbulence.
- Adaptive mesh refinement, where the computational grid is optimized in order to minimize a measure of the energy contained within the subgrid.

Although the methods proposed for quantification of LES accuracy are still in their early development, the examples presented show encouraging results. It is proposed to apply and refine the presented measures using the HM1 case as a collaborative exercise before TNF9 (Montreal 2008). We can also expect to gain insights from other workshops on combustion LES and LES quality assessment that are planned for 2007.

Issues for comparing LES and Experiments

So far, within the TNF Workshop series, we have compared LES and experiments in the same way that we compare RANS and experiments, on the basis of time averaged statistics (mean and rms) of velocity and selected scalars. Such comparisons can be informative but only scratch the surface of potential ways in which LES and experiments may be synergistically used to promote the development of predictive capabilities. The combustion community as a whole is only beginning to deal with the complex issues associated with more detailed comparisons of LES and experiments, and it is hope that our existing collaborative framework can serve to accelerate this important process.

Andreas Kronenburg, Venkat Raman, and Chenning Tong coordinated a session to highlight some of the complex issues associated with the coupling or comparison of LES and experiments. Their conclusions slide begins with the statement that the session generated more questions than answers, which is to be expected at this stage. It is broadly believed that we can do better that the current practice of comparing time averaged profiles. For example, high speed movies can help to identify coherent structures and large-scale dynamics, while measured and computed time series may be used to quantitatively compare dominant frequencies. However, there is significant work to be done to identify appropriate ways to validate LES through quantitative comparisons with experiments or to extract information from experiments that may be used in the development of combustion LES models.

One of the central challenges is that experiments and LES yield different filtered realizations of velocity and scalar fields, and careful consideration must be given to the influence of these different filters on the comparative results. Experimental results may be influenced by spatial averaging and noise, and the resolution of LES and experiments will not generally match. There are few if any experiments that can yield the equivalent of DNS results in flames (fully-resolved, three dimensional, and time evolving). However, fully resolved line and planar imaging experiments offer some potential to be used in developing and validating subgrid models for reacting scalar fields.

A few other discussion points were:

- It is possible to use LES solutions to evaluate the effects of experimental errors (e.g., noise, beam steering).
- Availability of complete, accurate, and repeatable boundary conditions is essential.
- Assumptions behind experimental procedure might affect comparisons and should be considered carefully.
- There is potential to simplify experiments and reduce overall uncertainties by comparing raw quantities, such as Rayleigh scattering signals or fluorescence signals.
- Comparisons should be conducted using flame series that include variation of a key parameter that offers a sensitive test of model capabilities.

What can be learned from DNS

DNS capabilities have expanded significantly in recent years. This session was included to promote discussion of what role DNS might play in the TNF process of model validation. Evatt Hawkes presented an overview of recent DNS of nonpremixed combustion. Examples from numerous contributors covered four general areas of activity:

- DNS with simplified models (e.g., pure mixing, one-step chemistry, homogeneous, 2D)
- Trends toward more advanced problems (3D, detailed chemistry, shear flows)
- Trends to include more physics (e.g., radiation, soot, spray)
- Attempts to simulate laboratory scale flames

Discussion of example DNS studies touched on the objectives and limitations, as well as specific results. There was a general consensus the DNS is an increasingly useful tool in the process of model development and validation. Furthermore, participants thought that the primary role should be to use DNS as "numerical experiments" to investigate specific phenomena with simple configurations under strictly controlled conditions. Several groups are using DNS with some success to understand fundamentals, then develop and test models. This needs to be done with due consideration of the parametric space to which DNS is limited. With terascale computing, a few 3D cases with detailed chemistry are being addressed, but this is not yet routine, and there are significant challenges associated with handing, mining, and sharing the very large data sets.

Progress and Challenges for Validation of Premixed Combustion Models

Johannes Janicka presented an overview on the status of validation efforts involving premixed and partially premixed (or stratified) combustion. This included input from S. Cant, J. Chen, S. A. Dreizler, A. Masri, and L. Vervisch. The presentation (in the Proceedings) addressed challenges, current models, validation cases, and DNS as a modeling tool. One challenge that was addressed in some detail was that of LES resolution relative to physical parameters of the burner and flame, and this was discussed in terms of an LES regime diagram for premixed flames. Four modeling approaches are outlined in the context of LES applications: subgrid Bray-Moss-Libby model, artificially thickened flames, G-equation, and the linear eddy model (LEM). Partially premixed (and stratified) flames were highlighted as having growing practical importance, and modeling approaches for partially premixed flames were outlined, again in the context of LES. A key issue here is that a major motivation for use of partially premixed or stratified flames in practical systems is their potential to yield reduced emissions. However, these emissions (NO_x, CO, UHC) can depend upon post-flame kinetics, which are not addressed by kinematic models. General data needs and specific experimental cases on premixed and stratified flames that are either in the literature already or are in the process of being measured were discussed. However, there was not a clear consensus pointing toward a single flame target or series at the time of the workshop, because complete data from new configurations are not yet fully available.

Perspectives from industry

TNF8 included several participants from the gas turbine industry or from CFD software companies who are closely involved with industry needs. These participants were invited to provide industry perspectives on the TNF Workshop process. They gathered as a small group (listed in the proceedings) on Friday afternoon, and a summary was presented by Jorge Ferreira during the regular session on Saturday morning. The broad message was that the TNF process provides access to good experimental data sets, good insights on the status of current models, and useful information about advanced experimental methods. The TNF focus on "basics" was encouraged. However, it was also suggested that any new flames should have relevance to "real life." The summary slides cover several important points of concern to industry regarding issues of accuracy, speed, and reliability of models. The slides also list areas of interest with respect to future target flame configurations.

Priorities and planning for future work and TNF9 (Montreal, 2008)

TNF9 is planned tentatively for July 31 – August 2. It will most likely be held in one of the hotels booked for the 32nd Combustion Symposium, with a schedule similar to TNF8. There are a few areas that are clear priorities for collaborative work in preparation for the next workshop:

- Conducting LES quality assessment, based on a selected TNF flame or flames. Andreas Kempf and Joe Oefelein have volunteered to coordinate this effort.

- Extending LES validation work to include effects of strong turbulence-chemistry interaction, such as local extinction. This will eliminate some combustion sgs models and is likely to require significant computational resources. However, because the primary focus of the TNF Workshop series has been on fundamental issues of turbulence-chemistry interaction and because we already know a great deal about the modeling of these effects in the RANS context, it is important to begin to systematically extent LES validation into problems with strong effects of turbulence-chemistry interaction.

- Developing a better understanding of how to appropriately compare LES and experiments and how such comparisons might extend beyond what has been done in comparing RANS and experiments. This will require close collaboration between experimental and computational researchers.

- Acquiring and making available new data sets for premixed and stratified combustion that are appropriate validation targets for models and address combustion phenomena relevant to practical systems. Several experiments have been conducted recently on such flames or are in progress. However, before any broad comparison of results can be carried out, there must be a consensus among several modeling groups that a particular flame or flame series is an appropriate target.

- Exploring ways to make better use of internet tools to facilitate collaboration and exchange information, including larger data sets, more types of data, results of model calculations and detailed simulations. There is currently a significant level of interest, within some funding agencies, related to developments in cyber infrastructure to support advancement in combustion science.

This list suggests emphasis on LES, due in part to the fact that the state combustion LES validation is not nearly as far along as for RANS, at least with regard to finite-rate chemistry effects in the TNF target flames. It should also be emphasized that RANS and hybrid schemes are expected to be widely used by industry for many years, and RANS methods will continue to play an important role within the TNF Workshop process.

Thoughts on the status and future of the TNF Workshop series (R. Barlow)

The TNF Workshop series has been running since 1996, and over that time the character of the workshops and the associated research collaborations has evolved. Early in the process, many of the modeling groups were working on the same flames, such that the main focus of each workshop during the first several years was on broad collaborative comparisons of results from a small number of cases. The first five workshops were conducted as annual events, collaboration and information exchange on the few target flames was active and ongoing, and several experiments were conducted in direct response to consensus requests from modelers. Progress toward understanding the capabilities of various RANS methods for combustion modeling was rapid, as was the process of understanding the relative performance of specific submodels.

During most of the first 10 years of activity, the emphasis of the TNF Workshops was clearly on fundamental issues of turbulence-chemistry interaction and the corresponding submodels. Attention was given to other aspects of the modeling problem (e.g., turbulence modeling, chemical mechanisms, and radiation effects) to the extent that these effects and submodels needed to be sufficiently understood and controlled to allow for unambiguous comparisons of the modeled effects of turbulence-chemistry interaction. Overall, the contributions of the TNF Workshop series and its regular participants toward better understanding and improved modeling of turbulence-chemistry interaction in nonpremixed and partially premixed flames has been substantial. This success may be attributed to the philosophy of collaboration and progressive research that underpins the TNF Workshop process. This philosophy is outlined in a 31st Combustion Symposium invited paper (Barlow, 2007).

With the passage of time and the addition of new target cases, the collaborative work has become more diffuse. Modeling and experimental efforts have branched out again, so that the overall process has become less tightly focused. Furthermore, with the growth in emphasis on LES within the overall community as an emerging and promising approach for combustion modeling, there has been a corresponding growth in emphasis on LES in the past few workshops. However, to some extent, this has diverted our focus away from issues of turbulence-chemistry interaction.

In order for the TNF Workshop process to be as effective in the future as it has been in the past, we should maintain a strong emphasis on fundamental issues of turbulence-chemistry interaction, as we refocus our efforts to address the next level of challenges, both experimentally and computationally. These challenges include:

- Expanding the array of validation-quality experiments to include a broader range of combustion regimes: nonpremixed, partially-premixed, stratified, and premixed flames in geometries that are appropriate for advanced models, have unambiguous boundary condition, and address phenomena of practical interest.
- Increasing the completeness of comparisons by: ensuring that velocity and scalar fields are obtained at well matched conditions (or simultaneously), going beyond comparisons of mean and rms point statistics, making a broader array of experimental data types easily accessible on the web, using web-based tools to reduce the effort required to submit and compare results, and including more parametric studies of the sensitivity of results to parameter changes.
- Paying more attention to issues of verification and quality assessment by developing some forms of standardization and by establishing benchmark cases that are based on the combination of detailed experiments and highly resolved (expensive) simulations.
- Doing a more complete job of archiving results of calculations and comparisons, so that it will be easy to call up results of previous calculations, particularly the better ones, so that the community can avoid reinventing wheels as we attempt to achieve predictive computational tools as rapidly as possible.

It is anticipated that specifically directed funding will be necessary to accomplish some of these goals because the level of complexity of the validation process has grown beyond that which can be handled effectively using the manually intensive tools that served the TNF process through the past decade. For example, the development of web based tools that specifically address the needs of the TNF Workshop is unlikely to happen without specific funding and ongoing support. Therefore, it will be important to educate funding agencies and contract monitors as to these additional needs, which are typically viewed as unglamorous, and find ways to increase the sophistication and thoroughness of the combustion model validation process without significantly increasing the work load required of those who volunteer their time to support this effort.