Next generation of guiding questions for basic turbulent combustion research

A two-day workshop was held at the University of Michigan, Ann Arbor, MI, on June 9&10, 2014 to identify and articulate research needs and opportunities for progress on the scientific and engineering foundations of turbulent combustion processes.

The first half-day of the meeting featured five overview presentations that were open and attended by a public audience.

James Driscoll: Experiments on gas turbine and supersonic combustion instabilities
Laurent Gicquel: Simulations of ignition and acoustic instabilities in gas turbines
Matthias Ihme: A unifying combustion model
Joe Oefelein: New discoveries from LES of fuel sprays
Andreas Dreizler: Diagnostics in unsteady combustion systems: IC engines

The attendees (see listing at the end of the report) then met in three sub groups to discuss the following questions.

- What are key bottlenecks that limit breakthrough developments?
- How can the impact of sub-scale modeling of combustion and fluid process be quantitatively assessed?
- What scientific and infrastructural efforts are needed to create the experimental data foundation for building and validating turbulent combustion models (in general) and key model assumptions (in particular)?

The sub groups reported out to the joint audience and then focused on preparing written documentation that formed the basis for this report. All participants contributed to this report and reviewed and edited its contents in preparing the final version as submitted here.

Summary:
A two-day workshop was held to identify and compile research questions and needs to advance basic turbulent combustion research towards capabilities that allow predictive simulations at the design level for practical devices. Recognizing the state-of-the-art simulation capabilities and inherent limitations with computational resources the focus is on Large Eddy Simulations as a pathway to this goal. This report documents not only scientific and technical questions related to shortcomings in our current understanding of turbulent combustion, but also addresses procedural challenges. Key bottlenecks and research needs are addressed and described but the report also emphasizes that the conduct of research has to adapt to the complex nature of turbulent combustion by fostering collaborations and long-term funding horizons.

Background

The goal of fundamental research efforts in turbulent combustion is to identify and understand controlling basic principles – the physics and chemistry of turbulent combustion and use that knowledge to develop, test, and validate physics-based simulation tools that eventually will have predictive capability for design purposes. For practical reasons, largely given by limited computational capabilities, the description of some aspects of physics and chemistry and their interaction must often be simplified with models. Ideally, these models have input parameters that are (more or less) directly measureable in experiments to support rigorous and highly accurate validation work.

Substantial progress has been made in the past decades to understand basic principles of turbulent combustion through enormous advances in experimental and computational capabilities and resources as evidenced in the scientific literature and in policy reports such as one of the DoE Basic Research Needs reports [1]. However, to date, our understanding is still limited due to the complex nature of turbulent combustion, including a huge range of spatial and temporal scales that govern critical steps such as mixing for fuel and oxidizer, ignition, reaction to products, and pollutant formation, and so forth.

Simulation capabilities have been advanced to levels of astounding complexity and level of microscopic and macroscopic detail[2]. Yet, only for fairly benign flame conditions, typically simplified from practically relevant geometries, can such simulations be carried out as full Direct Numerical Simulations (DNS). In other words, a direct numerical simulation without modeling processes below a particular spatial scale is still rarely feasible. This is in particularly true for high-Reynolds number combustion systems and systems with variable geometric boundary conditions, including reciprocating-piston internal combustion engines. Research and development for modern combustion systems points to the need to operate combustion at conditions that are, unfortunately, close to inherently unstable conditions, such as very lean operation. Therefore, the risk of combustion failures increases and substantial research efforts need to be geared towards experimental and computational studies of stochastic processes in combustion. Recognizing the resource limitations for the widespread use of DNS, Large-Eddy-Simulation (LES) approaches have been advanced and are beginning to enter design-stage use in the community. It is evident, though, that the need for and efforts in reducing the complexity and magnitude of the computational problem leads to the use of models. These models are typically systematically developed and validated for a limited set of conditions where the results of the simulations can show a high level of fidelity and agreement with experimental observations. The use of a simulation package for any other combustion problem might result in unstable or unphysical solutions, or predictions inconsistent with experimental observations.

How can efforts be developed and coordinated to result in the next level of predictive combustion simulation capabilities? Simulation approaches that utilize different, yet applicable, models for subscale processes should eventually result in comparable results within the uncertainty limits of the simulation and the experimental validation databases.

[1] A. McIlroy et al., http://www.sc.doe.gov/bes/reports/files/CTF_rpt.pdf

[2] J. H. Chen, Proceedings of the Combustion Institute, 33 (1), 99-123 (2011)

1 Key bottlenecks that limit breakthrough developments

The following sections provide a listing of topics that are deemed essential to achieve levels of insights into combustion processes that will allow it to build and use better design tools that require less, if any, calibration data from model experiments or prototype setups. These bottlenecks include aspect related to experimental, theoretical, modeling, and simulation limitations present in today's portfolio of combustion research tools. Also included is an emphasis on how research work is being and could be conducted.

1.1 Insufficient foundation (first principles or experimental-observations based) for LES models

For most LES models, key model assumptions'/building blocks' representativeness of and consistency to the underlying physics has not been clearly established and quantitatively evaluated. Impacts of unresolvable/subgrid scales on resolvable scales have not been clearly understood and sufficiently quantified. Addressing these problems forms the foundational steps for any LES model development and should be a key component of any research investment strategy into the development of turbulent combustion models. This should be done collaboratively in the areas of combustion, turbulence, and applied mathematics based on first principles consideration and experimental observations rather than on ad-hoc, convenient assumptions.

1.2 Direct numerical simulation and experiments addressing key challenges

Turbulent flows involving heterogeneous chemically reacting and/or multiphase mixtures (as is the case for all advanced high-performance combustion systems) have a variety of complicating factors including highly nonlinear chemical kinetics, small-scale velocity and scalar-mixing, turbulence-chemistry interactions, compressibility effects (volumetric changes induced by changes in pressure), and variable inertia effects (volumetric changes induced by variable composition or heat addition). Coupling between processes occurs over a wide range of time and length scales, many being smaller than can be resolved in a numerically or experimentally feasible manner. Further complications arise when liquid phases are present due to the introduction of dynamically evolving interface boundaries and the complex exchange processes that occur as a consequence. At the device level, high performance, dynamic stability, low pollutant emissions, and low soot formation must be achieved simultaneously in complex geometries that generate complex flow and acoustic patterns. Flow and combustion processes are highly turbulent; i.e., integral-scale Reynolds numbers of O(100,000) or greater, and the turbulence dynamics are inherently dominated by geometry or various operating transients. In modern systems, operating pressures now approach or exceed the thermodynamic critical pressure of the fuel (or oxidizer in the case of liquid rocket engines). Operation at elevated pressures significantly increases the system Reynolds number(s), which inherently broadens the range of spatial and temporal scales that interactions occur over.

No one experimental or simulation technique is capable of providing a complete description of the multi-scale processes described above. The highest quality experiments only provide partial information due to limitations associated with various measurement techniques. Likewise, solving the fully coupled equations of fluid motion, transport, and chemical reaction using DNS can only be applied over a limited range of turbulence scales in highly canonical domains of only a few centimeters in size due to prohibitive computational demands. While petascale computing has enabled the application of DNS for treatment of three-dimensional reacting flows with detailed chemistry, the largest DNS runs to date are off by more than an order of magnitude in Reynolds number compared to practical devices. The limited dynamic range and indirect relation to actual device level operating conditions introduces limitations for using DNS directly for model development that underlie practical combustors.

Despite these clear limitations and shortcomings, DNS remains a fundamental and highly complementary numerical tool of particular importance for canonical configurations designed from the ground up with experimentalists and theorists that identify key uncertainties and gaps in our knowledge. Complementary to experimental data, the DNS data are also required to develop and validate predictive mixing and combustion models for engineering Reynolds-Averaged Navier Stokes (RANS) and LES. Some of key scientific challenges in turbulent combustion that could be addressed this way include with complementary canonical experiments are:

a. High-Reynolds number turbulent premixed flame propagation in moderate-to-high temperature preheated reactant mixtures (750-1300K) with or without vitiates at ambient and high pressures
b. Geometrical effects (e.g. spherically expanding flames, counterflow flames, turbulent jet flames, swirl-stabilized flames)
c. Lewis number effects (thermo-diffusive effects in both lean and rich limits)
d. Hydrodynamic effects coupled with aerodynamic stretch especially with increasing pressure
e. Stratification of reactants causing front or back support of enthalpy and composition
f. Stratification of products causing front or back support of enthalpy, radicals, or dilution with products
g. Effects of turbulent flame propagation into negative-temperature-coefficient conditions that is chemistry dependent, and issues associated with competing ignition delays and residence time (from localized turbulent mixing rates)
h. Understanding the spectral consistency and scaling of turbulent premixed flames and turbulence at different Damköhler numbers, Karlovitz numbers, density ratios, fluctuating Mach numbers, and Reynolds numbers compared with incompressible flows and passive scalars

1.3 Lack of an accessible database of DNS, LES and experimental results for premixed turbulent combustion similar to the TNF database for nonpremixed flames

The creation of such a resource requires decisions (perhaps made by a committee) about what data are acceptable, what geometries are included, and how to define the parameters. Issues also include that DNS databases are so large that not all computed quantities can be stored. There seems to be a consensus that important canonical geometries for premixed turbulent flames include Bunsen (rim-stabilized) flames, low-swirl flames, spherical (fan-stirred chamber) flames, and flames in compressible flow in a wind tunnel. More collaboration is required to agree on the details of the geometries and the quantities to store in the database. In the long term, the database should be expanded from premixed turbulent flames to include partially-premixed flames, flames in compressible high-speed flows, and combustion instabilities.

1.4 Enhanced collaboration among theory, experiment, and numerical simulation/modeling

Even though there are a number of good examples of strongly integrated long-term research collaborations, it is noted that there is still a tendency for researchers to work in isolation. To accelerate progress, it is essential to establish and maintain meaningful long-term collaborations among researchers who approach turbulent combustion using theoretical, experimental, and computational methods. This goes beyond simply communicating more, to fundamentally changing the way in which the combustion research community identifies research priorities and shares resources and results.

There has been significant progress in establishing an effective framework for connecting DNS with theory, and DNS with modeling. For these purposes, a priori and a posteriori analyses are being used effectively, and should continue to be used going forward. The main bottlenecks pertain to archiving, documenting and manipulating large data sets.

On the other hand, the connection between experiment and numerical simulation/modeling remains primitive. For example, modern optical diagnostics that are used to measure up to four-dimensional (including time) velocity and/or scalar fields require extensive processing (including modeling) to derive physical quantities of interest from measured radiative intensities. Typically, a few low-order statistical quantities from an experiment are compared with the corresponding quantities from a simulation. Within the next five-to-ten years, it should be feasible to compute the radiation signals corresponding to various luminosity-based and laser-based optical diagnostics in high-fidelity DNS and LES. This has the potential to reduce uncertainties in comparing experimental and simulation results, to better interpret experimental measurements, and to quantify the effects of spatial and temporal filtering in both experiments and simulations. To be successful, the development of such "numerical diagnostics" will require close collaboration among theory (to provide models for how lasers interact with molecular gas species and with soot particle, and detector response), experiment (to quantify spatial and temporal resolution), and modelers (to come up with tractable algorithms for computing spectrally resolved intensity at a detector).

Rigorous uncertainty quantification (UQ) will be essential at all stages of experiment and simulation. Uncertainties in measurements, models and numerical methods, and operating conditions/boundary conditions must be propagated through the simulations to establish uncertainties and sensitivities. This will allow informed decisions to be made regarding which DNS study or experiment should be performed next, or which aspect of the modeling most urgently needs to be improved, to reduce the uncertainty in our ability to predict a key metric such as pollutant emissions. Currently such decisions are made subjectively through consensus among experts. Further development and application of UQ would allow such decisions to be made based on an objective and rigorous basis, and this would accelerate the rate of progress dramatically by focusing on the aspects of the problem that are really the most important ones.

1.5 Limitations in diagnostics

High-speed, planar measurements are becoming increasingly common in the community, particularly for velocity and certain scalars. However, rate measurements, particularly of heat release remain highly undeveloped. Line-of-sight measurements of CO_2*, OH*, and CH* are commonly used indicators, as well as simultaneous measurements of CO and OH, or OH and CH_2O. Nonetheless, direct planar measurements of key formation rates or heat-release rates do not really exist, yet are arguably some of the most critical combustion parameters.

Two-dimensional measurements of flamelets do not enable characterization of flamelet orientation, significantly confusing interpretation of iso-surface displacement speeds, and thicknesses. As such, volumetric measurements of scalars and velocity are needed, including development of seedless velocimetry approaches. Seedless approaches are necessary, as window coating for contained vessels at high pressures is extremely problematic, as well as rendering Raman diagnostics impossible.

1.6 Practical means for including chemical-kinetic effects in modeling of turbulent combustion

For example, it is not known how important the low-temperature (NTC) chemistry may be in turbulent combustion. This is especially true when the mix of multicomponent fuels of practical interest is taken into account. Most descriptions of that kind of chemistry involve hundreds of chemical species with thousands of chemical steps, which is incompatible with the capabilities of modeling procedures. Descriptions of the chemistry that are both reasonably accurate and amenable to application in the modeling are needed to overcome this bottleneck. Such descriptions would be important in interpreting experimental results as well as in facilitating modeling efforts. Finally, kinetics in mixing situations with hot product gases, leading to flameless combustion, and the impact of radiation that is important in many industrial combustion systems are not well-understood and implemented in models.

1.7 Processes controlling turbulent burning rates

One of the most profound impacts of turbulence on combustion is the augmentation of burning rates with increasing turbulence intensity. One type of physical description of this process, promoted, for example, by Damköhler, emphasizes "global" arguments relating to flame area - i.e., in constant-burning-velocity flames, the turbulent burning velocity increase is considered to be directly proportional to the increase in flame-surface area. An alternative approach, discussed by Zeldovich and others, to understand turbulent augmentation of burning rates is based upon "leading points", which may be considered to be intrinsically local properties of the turbulent flame. A key implication of the latter approach is that, if flames are controlled by leading points, then the augmentation of burning area is an effect, not a fundamental cause, of augmentation of burning rates. A similar idea is that in sufficiently intense turbulence it is mainly flamelet collisions that consume reactants most rapidly, and periodic rapid consumption events control the spread rate, while the remaining flamelet combustion simply determines the turbulent flame thickness. Work by Sabelnikov and Lipatnikov, using language of "pulled" and "pushed" fronts, suggests that more than one description is valid, but in different physical regimes. There are a number of other ideas, such as control in propagation of flamelets along vortices.

Are all these various descriptions equivalent descriptions of the same phenomenon, or is one more fundamentally physically correct under a given set of operating conditions? In the case of the latter, what does a "regime diagram" look like that differentiates between "pulled" and "pushed" fronts, for example? What kind of analysis of computations or experimental data would be needed to isolate processes controlling turbulent burning rates? Any one such description can form the basis of modeling concepts that will predict turbulent burning velocities.

In a related framework, issues naturally arise on what processes control turbulent burning rates as preheat temperatures increase (or, more fundamentally perhaps, as overall temperature sensitivities of heat-release rates decreases)? As systems move into regimes where fast autoignition occurs (e.g., aircraft engines with preheat temperatures > 1000K) burning rates may become ignition-dominated. What is the role of turbulent mixing on burning rates in this limit?

1.8 Turbulent flame – wall interactions

Wall interactions relevant to intrinsic flashback safety, wall heat transfer, and shock-turbulence-flame-wall interactions at high Mach number at ambient and high pressure are inadequately understood. It is also necessary to understand the coupling between hydrodynamic instability and turbulent boundary layer structure in their interaction with the flame, and the influence of fuel stratification on flame propagation near walls and in the bulk flow.

Most canonical turbulent-combustion databases are envisioned as homogeneous system without wall effects. In many applications, however, ranging from unexpected flashback in combustors of gas turbines when small amounts of hydrogen are added to natural gas, to upstream jumping of the flame-holding positions in scramjet configurations, turbulent flame propagation along walls is the dominant mechanism. An important bottleneck is our lack of understanding of the physics of this kind of turbulent flame propagation. Common experimental and computational studies of these processes therefore are important, with development of the needed theoretical understanding that can facilitate rational approaches to the design and development of procedures to mitigate associated practical challenges.

1.9 Shock-wave interactions with chemically reacting mixing layers

How are shock waves and detonations affected by turbulence, and how do they modify the turbulence? The lack of knowledge in this area is a bottleneck to efficient development of scramjet propulsion, for example.

1.10 No reliable LES model for spray combustion

There is a need for LES models of sprays because DNS of sprays requires excessive computational time while the use of empirical formulas to characterize a spray at the input boundary is not sufficiently scientific. A LES approaches should be validated by comparison to DNS or drop-size measurements, to be sure that the proper spray characteristics can be simulated without requiring excessive computational time.

Concerning the evident need for addressing the bottleneck of developing reasonable turbulent descriptions of multiphase turbulent flows, it may be observed that, even in the laminar combustion of a mono-disperse spray stream in a mixing layer with a hot air stream, decidedly non-monotonic mixture-fraction profiles develop, complicating modeling challenges appreciably.

1.11 Gap between many of the premixed flames studied (at 1 atmosphere for simple geometries) and real devices

The physics and chemistry of combustion at elevated pressure can substantially change compared to those at atmospheric pressure. Reduce spatial scales impose severe restrictions to experimental studies as do collisional effects on optical measurements. Simulations often do not account for effects that relate to real-gas behavior and also are impacted by the decrease in spatial scales that have to be resolved. Research must be expanded to better handle high-pressure conditions for measurements and LES/DNS simulations. Even for atmospheric-pressure conditions, the transition to real, or near-realistic, combustion devices creates increased complexity for measurements (run time, windows, etc.) and for simulations (boundary conditions, meshing problems, etc.)

2 Quantitative assessment of the impact of sub-scale modeling

The need for sub-models is recognized as essential and inevitable in simulations, be it for practical, time-sensitivity, financial, or other reasons. Unfortunately, it is not necessarily known how well models capture the physics and chemistry at spatial and temporal scales below the simulation's resolution. It may also not be known how well the coupling between resolved and modeled scales works. Therefore, it is essential that experiments or DNS should be designed to specifically and directly probe assumptions/models in LES to which the final solution is highly sensitive.

It also has to be addressed how well a simulation or isolated sub-model captures what can be measured. Key metrics and tools for comparison of simulations and experiments are needed. This leads to questions about what actually should be compared beyond just mean and fluctuating values of relevant or accessible parameters.

2.1 Development of better quality metrics for LES

Current combustion models for turbulent reacting flow require closures for turbulent stresses, turbulent scalar fluxes, and chemical sources terms, as well as other terms arising from the closure of higher-order nonlinear terms and turbulence-chemistry coupling. Currently, those closure models are inherited for different - and often unrelated - problem configurations (examples are isothermal, incompressible, or irrotational flows, or idealized flame-problems). As such, their applicability in simulations of relevant combustion environments is commonly not comprehensively assessed. Furthermore, the underlying assumptions to individual submodels are often not consistent with each other. Therefore, any calibration or adjustments of model coefficients are most-likely case-specific and their mutual interactions are not fully appreciated. Therefore, guidelines for understanding the submodel interaction and the development of consistent closure submodels are needed.

Development of predictive LES is complicated by the interdependence of different subgrid-scale models, competition between modeling and numerical errors, model variability, and numerical implementation. Errors and ambiguities are multiplying, and control of accuracy has become a critical aspect in the development of predictive LES for design. Results can be misleading and intractably erroneous due to accuracy-limiting factors such as poor numerics, poor grid quality, lack of appropriate spatial or temporal resolution, ill-posed boundary conditions, and inaccurate models.

The need for improved quality metrics for LES has been recognized now for many years. A major deficiency with the quality indicators used to date is that none of them account for the various sources of error rigorously. Only the bulk error from multiple competing sources has been considered instead of the distinct sources of error. Discretization and modeling associated with LES introduces three distinct forms of error: 1) discretization errors associated with the numerical techniques (i.e., temporal integration, spatial differencing, and related stabilization schemes), which can induce damping and dispersion of the broadband flow processes; 2) the total model residual error, which is caused by discretization of the sub-models themselves; and 3) the error associated with the model approximation itself due to both the basic model assumptions and the related range of subgrid- or subfilter-scales it is specified to work over.

2.2 Understanding competition between sub-models and numerics

It is recognized that the sub-grid model contributions can be influenced by the nature of the numerical scheme. For instance, numerical schemes may provide a dissipation sink to under-resolved and un-resolved scales that serves as an inherent sub-grid model (as exemplified by implicit-LES approaches). It is also recognized that such an implicit-sub-grid model cannot capture real physical phenomena such as energy backscatter. Nevertheless, the presence of numerics complicates the formulation of sub-grid schemes. In fact, it becomes necessary that the sub-grid model automatically account for such inherent dissipation effects such that the sum effect of the sub-grid model and the numerics provides an accurate representation of the physics. A related notion that deserves further scrutiny is the distinction between explicit and implicit filters and their relationship to numerical dissipation effects.

2.3 Validation experiments

Experiments have traditionally focused either on a) revealing physical configurations of turbulence, combustion, and turbulence/combustion interaction and/or b) providing statistics for the purpose of verifying global results of simulations. A new class of experiments that is accessible using modern laser-based measurement techniques is those that directly assess the underlying assumptions of LES and specific subgrid closure models. This includes topics that are fairly general across LES methods, such as scale-similarity, and those that are specific to a particular implementation, such as reaction-rate closure models. Although the mathematical formalism of LES facilitates use of powerful identities associated with filtering that eliminates the need for tuning constants, other assumptions such as the local turbulence equilibrium, local gradient mixing, and quasi steady state often underlie many closure models. Experiments specifically designed to address and check these assumptions will provide important information for model development. Where possible, a range of parameters should be investigated to help understand the regimes of validity for the assumptions.

Experiments should be designed that specifically and directly probe assumptions/models in LES to which the final solution is highly sensitive. Such experiments must be designed in close collaboration with the researchers developing and implementing LES in order to ensure that the resultant data addresses the targeted issue in an effective manner. Moreover, the assessment should be performed over a sufficient parameter space to identify the regimes of applicability and metrics quantifying these regimes. In designing the experiments, initial efforts should be made to identify assumptions/models to which the final the final solution is most sensitive.

2.4 Validation and discovery using DNS

DNS are an important tool that provides access to the flow dynamics, where the smallest flow-relevant scale in the continuum model is resolved. DNS provides a useful complement to experimental studies due to the inherent access to the detailed flow field information. The use of DNS is valuable both for verifying the ability of closure models for turbulent combustion to capture the key physical properties of the flow and for discovering new physical effects in the regimes, which have been previously unexplored or not explored with sufficient detail.

In this role, however, DNS faces a limitation in the range of the regimes accessible to the investigation. The need to resolve all key flow scales combined with the increasing separation between the targeted large scales of the flow and the Kolmogorov scale limit the Karlovitz and Reynolds numbers that can be accessed in a DNS. This requires development of new computational approaches that enable the exploration of high-Ka, high-Re regimes that cannot be probed with full DNS. Such approaches would provide solution fidelity that matches, or is close to, that of DNS. Do all scales in the flow indeed need to be resolved in all regimes in order to capture accurately the flow dynamics and to obtain the same information as provided by full DNS? For instance, does the Kolmogorov scale need to be resolved when it becomes much smaller than the characteristic flame width: i.e., do the system dynamics exhibit asymptotic behavior as Re approaches infinity? In what regimes does such asymptotic behavior exist?

Alternatively, depending on the regime, various physical components of the model may be understood to a different degree, and their relative importance for the overall system dynamics can vary. Thus, it may be possible to use combined approaches, in which some aspects of the system are modeled from first-principles, e.g., flame dynamics, while other are captured with a subgrid model, e.g., dissipation scales.

2.5 New physics evaluation

As activities in turbulent combustion have grown, it has become clear that there are aspects of combustion physics that are still poorly understood. For example, broken reaction zones, premixed flame structure at high turbulence levels, flame-wall interactions, flame-shock interaction, etc., can be important in some applications. Experiments designed to explore these processes are needed to provide the basis for the development of new modeling concepts that may be required to address these more complex physical processes.

An additional class of experiments designed to check basic modeling concepts is needed. There are several basic modeling assumptions that are specific to LES such as scale similarity and approximate factorization. Additional modeling assumptions such as local turbulence equilibrium, local gradient mixing, and quasi-steady-state often underlie many closure models. Experiments specifically designed to address and check these assumptions will provide important information for model development. Where possible, a range of parameters should be investigated to help understand the regimes of validity for the assumptions.

2.6 Data assimilation for model development

A comprehensive approach to model evaluation and model development also creates a need for innovative methods for data assimilation. This refers to the use of detailed experimental and/or DNS data to systematically aid in the design of sub-grid models. One can envision this taking many forms, including but not limited to, model derivation, model optimization, physics regime inquiry, uncertainty quantification, stochastic enrichment, and design of experiments. It is anticipated that many of these topics will lead to new areas of research inquiry that may well benefit from multi-disciplinary research in big data, machine learning and intelligence.

2.7 Stochastic model issues

Although most available turbulent reacting flow LES closure derives from a pseudo-statistical context, the large-scale features deterministically set the final system of transport equations. For safety as well as scientific reasons, we need to understand the fundamental limitations of probability-based turbulent combustion models (such as transported or presumed-PDF, LEM, etc.) and the limits of such models to predict low-probability or "rare" events (say, at the tails of the distribution) that may contribute to unexpected ignition, extinction or unstable events with possible catastrophic consequences on aviation propulsion systems. The capability to predict such events is crucially important and research results and approaches from other fields such as meteorology could be fruitfully leveraged.

3 Experimental data foundation for building and validating turbulent combustion models

Creating, sharing, and maintaining trusted experimental data for the combustion community to build upon is a task that requires improvements from various angles. Not only does this relate to instrumentation needs and the type of combustion systems studied but it also requires game-changing modifications in how research is coordinated and supported. The following section addresses some of the key aspects in this context.

3.1 Start with a model/canonical problem – "from simple to complex"

For solving key problems in turbulent combustion the following well-organized and strategic approach is recommended.

a. Start from an agreed-on technologically relevant device (gas turbine combustor, internal combustion engine, power plant, …) to identify the primary shortcomings. This step is crucial to answering the important questions or, in other words, to avoid answering questions that no one has asked.
b. Canonical geometries should then be extracted that aim for a much-reduced number of mutually coupled phenomena compared to the complete technological case. The concept of such a canonical device should provide full control of inflow and boundary conditions, reproducibility and compatibility to experimental, theoretical and numerical approaches.
c. Starting with the design phase of such a canonical flow/flame geometry a close interaction/communication between experts from experimental, theoretical, and numerical combustion science is mandatory (too often we have seen experiments showing interesting phenomena, but with flow devices that were unfeasible for computational investigations – often because of unknown or incompatible boundary conditions).
d. Experimental, (theoretical) and numerical tools should be adapted to the canonical geometry. As a result of such an adaptation, the limits of the present methodology should be identified as accurately as possible. Such an insight might trigger accompanying research projects, e.g., to resolve diagnostics shortcomings or required model extensions. However, it should be emphasized that in a close collaboration between experimental, theoretical, and numerical disciplines, for example, not all parameters have to be measured. Instead the capabilities, for example, of a validated numerical simulation can be exploited to extract physical insights that are hard or even impossible to be measured. Exploiting such a synergy might prevent taking costly and unproductive directions.
e. A parametric variation should be realized. Dependent on the case, this could comprise the nozzle exit Re-number, the turbulence intensity, integral length and time scales, the equivalence ratio, the pressure, heat losses, etc. The primary aim of such a parametric study should be to identify sensitivities that guide our physical/chemical understanding and that are mandatory for developing models. Implemented into a code, a model at least must correctly reproduce such trends or sensitivities to be useful at all.
f. At the highest level of defining canonical problems, more than a single flow/flame configuration should be deduced. Different aspects of the technological device might require specialized configurations and methodologies. Depend-

ent on the problem, this may directly imply not only close interactions between experimental, theoretical, and numerical disciplines, but inside these disciplines interactions between specialists from heat transfer, multiphase flows, diagnostics, etc., are triggered.

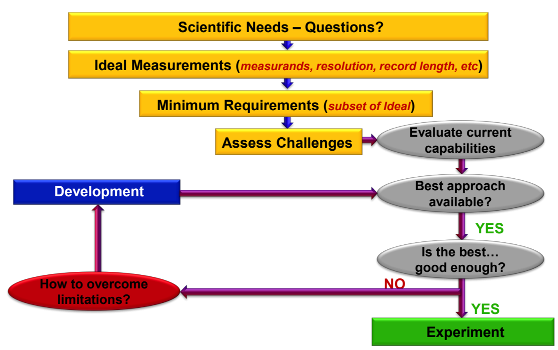
g. The next level of complexity should account for mutual interactions between different physical and/or chemical processes. Non-linear coupling is one of the great challenges in turbulent combustion research and should be addressed in depth. From an experimental point of view this requires (at least in part quantitative) multi-parameter diagnostics. Cinematographic measurements in all spatial dimensions are desirable, but in practice there is a trade-off between precision/dynamic range/resolution and capturing multiple dimensions. The diagnostics must follow the primary needs that are set by the problem. Similar to the previous level of studying canonical problems, parametric variations are of high importance.
h. At the final level all of the most relevant and mutually coupled phenomena should be studied in a device that already is close to the technical device (semi-technical scale). The intention hereby is that in a transfer to the real world problem the risk of missing a key issue should be minimized. Of course, infrastructural needs both for experimental and numerical approaches can be significant. As a consequence, suitable research locations should be selected and supported to build up such an infrastructure. This implies a long-term commitment, but one that can be shared between public and private institutions.
i. As a rule of thumb, the higher the level of system complexity, the fewer parameters can be measured. In other words, in this sequence from "simple to complex" diagnostic tools change, the range of resolved scales will shrink, and so on. A comprehensive validation as is possible for the canonical flows/flames most often is not feasible anymore. However, the measurable quantities should be taken for validation. This implies as well that the process of measuring itself might be implemented into the numerical simulation (for example, if chemiluminescence as a cheap and popular technique for high-pressure combustion devices is frequently used, chemiluminescence might be easily implemented to the chemical model; this allows a direct comparison between simulation and experiment that is not based any more on a local quantity). In addition to simplifying experiments, this also is a pathway to increased accuracy because then complicated and simplifying correction procedures (e.g. to account for fluorescence quenching) for optical signals are no longer needed.
j. As a result of this approach the primary outcome is a fundamental understanding of isolated and mutually coupled phenomena and validated models that at least are capable to predict most important trends once they were calibrated. However, future numerical combustion methods should be predictive for the most important properties of a combustion device! Such outcomes are not only restricted to the last level of the semi-technical device but will be produced as a constant flow of improved understanding and improved models at each level of this "from-simple-to-complex" approach.

3.2 Experimental best practices

First, it must be emphasized that turbulent combustion measurements are not trivial, are not without limitations, or are even impossible in certain configurations, especially more realistic, technical devices. Second, it is noted that model performance is typically evaluated using multiple data sets from multiple experimentalists and multiple experimental campaigns.

Measurements in turbulent combustion systems are challenging as the environment is characterized by the complex coupling between finite-rate chemical kinetics and turbulent fluid mechanics, which occurs over a broad range of length and time scales. Generally speaking, there are two overarching goals to experimental research: (i) to elucidate key physical and chemical processes underpinning the system of interest, and (ii) to provide benchmark data for assessing turbulent combustion models. Each of these goals dictates specific measurement requirements, which may differ. Targeted or desired measurement quantities can include velocity, temperature, species concentrations, and reaction rates (among others), all of which are changing in space and time. Commonly, "instantaneous" realizations are desired (or required) which places an increasingly higher level of difficulty on the measurement in terms of accuracy and repeatability.

To provide reliable data for model development or assessment, a common set of measurement guidelines across the turbulent combustion community should be adopted. It is appropriate to define the general logic for measurements in the context of any project's specific goals. A sample flow path of an ideal process is outlined in the adjacent figure, noting that this is neither always possible nor practical depending on certain project constraints.



First, the scientific needs or objectives of the experiment need to be defined. As a target example, one can consider that the scientific objective of a certain experiment is to provide a high-fidelity database that can be compared to turbulent combustion modeling results. After the scientific objectives have been identified, the "ideal" measurements (for the targeted objective) should be identified. In practice, even the most detailed experimental campaigns can provide only a limited number of measurable quantities as compared to the complete system of interest, thus it is important to identify the necessary "minimum measurement requirements" to satisfy the scientific objectives. After establishing the necessary requirements, important, but often neglected steps, include evaluating current capabilities, choosing the best approach available, and making an important decision on whether the "best approach available" is sufficient for satisfying the goals of the experiment. If satisfied, the experiment can be deemed valid and used in the context of the project's goals. If this criterion is not satisfied, this does not necessarily invalidate the role or goals of any given experiment, but it should prompt the experimentalist (or the community at large) to consider how the overcome the limitations, which may necessitate diagnostic development or refinement.

An additional point of consideration is the need for developing a common set of definitions and experimental procedures to characterize an experiment in terms of its accuracy, precision, and resolution, all of which contribute to an overall uncertainty in the measurement. While proper definitions of turbulent flame quantities (i.e., Reynolds number, Karlovitz number, etc.) are largely debated (but not agreed upon), the characterization of the "quality" of any given experiment is seldom discussed, and a consensus of "best practices" has not been reached. In the context of experimental vs. model comparison and, in particular, using multiple data sets from multiple research groups, it is imperative that the limitations of any individual experimental set is considered in the broader landscape of model assessment. A consistent set of definitions and measurement procedures should be established for determining spatial resolution, temporal resolution, signal-to-noise ratio (largely precision), and accuracy. This approach should not only be applied to any given "active" experiment, but the same definitions should be used to determine the minimum requirements at the design stage. A common criterion should be established for the *required resolution*. This is important as the targeted experimental resolution largely depends on the length and time scales of the process of interest, which are often difficult to estimate in reacting flows. However, establishing an accepted protocol can help to reduce an additional level of uncertainty in comparison between experimental and model results. Equal consideration needs to be given to calibration procedures, systematic errors, and the protocol to minimizing these.

3.3 Coordination of research efforts

Development and validation of robust, predictive models for combustions systems is a goal common to all the agencies funding combustion research programs. Combustion applications vary significantly, and a spectrum from fundamental to applied research is supported, but there is significant overlap with respect to combustion phenomena that must be captured by models. All applications involve complex, multi-scale, multi-physics problems that present significant modeling and simulation challenges. Validation of models for such problems is similarly complex and cannot be carried out effectively or efficiently by separate, individual research efforts on three-year funding cycles. While important progress has been made toward creation of experimental and DNS foundations for testing model performance on simple canonical flames (e.g., through the activities of the TNF and Premixed Turbulent Flames workshops), greater coordination of efforts will be required to extend the model development and validation process to more complex conditions that must be addressed on the way to achieving predictive capabilities for combustion applications.

As validation target cases become progressively more complex, the levels of effort required to design and construct appropriate hardware, fully define boundary conditions, create data sets of sufficient completeness and accuracy to differentiate among models, carry out the simulations over a range of parameters, and systematically evaluate and compare results all increase. Furthermore, particularly in the context of LES, it is paramount that the level of rigor applied in the process of evaluating models be increased beyond that applied to date. First, the basis for comparison of measured and modeled results needs to be expanded beyond point statistics (mean and rms) of velocity and scalars to include multidimensional, time-resolved data. The combustion community has only begun to address this challenge, and close coordination among experimental and computational researchers will be essential in developing appropriate techniques for data extraction and statistical comparison for experiments and simulations. Second, the community needs to more effectively address the challenges of developing quantitative metrics for the quality of simulations, as well as guidelines for best practice in documenting experimental and computational uncertainties and sensitivities. Such efforts are likely to evolve toward inclusion of uncertainty quantification (UQ) methods into both experiments and simulations, which will further increase the level of effort associated with a given validation target and reinforce the need for collaboration among multiple investigators with complementary capabilities and expertise. These needs have been identified in TNF Workshop summaries beginning in 2006. However, only modest progress has been made due to the lack of specific support.

Many experiments have intrinsic value in providing physical insights on combustion phenomena and in their educational role. However, experiments that are not specifically designed as model validation experiments are not likely to be useful for that purpose because models can only be effectively tested if boundary conditions are well defined and experimental data are sufficiently complete to allow unambiguous comparison of measured and modeled results. Furthermore, validation experiments are most effective if they isolate, as well as possible, specific combustion phenomena over a parameter space that shows particular sensitivity; experiments at single operating conditions have limited utility no matter how carefully executed. These considerations point to the need for engagement of modelers in the experimental design process. They also point to the need to applying multiple diagnostic techniques to the same target cases, and this implies involvement of multiple research groups having complementary experimental capabilities, application of careful quality control over experimental conditions, documentation of uncertainties and repeatability, and execution of extended research campaigns that may extend over multiple funding cycles.

Collaborative research has been essential in developing target cases model comparisons that have been addressed in the TNF Workshop series. The Engine Combustion Network (ECN) and the Large Eddy Simulation Working Group (LES-WG) are other examples for national and international collaborations. However, those collaborations have been developed on a strictly voluntary basis, relying on fortuitous availability of separate funding to the groups involved. This suggests that the research culture and funding constraints within the US discourage or inhibit collaborative research compared to the level in Europe.

Collaborative efforts are a key to the advancement of turbulent combustion research because they can build and utiliz synergies that enable more targeted and faster progress towards research outcomes and education of the next generation of scientists than can be achieved by isolated efforts. However, collaborative efforts are often limited in their reach by a lack of resources for travel, exchange of students, and the cost of collaborative tools. Funding agencies may want to more strongly encourage coordinated and linked research efforts as a means to multiply the effectiveness of research funding. Support should be provided to put volunteer-based collaboration networks in a position to be more effective and coordinated by enabling organizational frameworks that do not have to rely on someone's spare time.

It is not expected that any single agency can transform and accelerate the process of combustion model validation. Rather, all agencies, beginning with those emphasizing basic combustion research, should adopt a programmatic orientation that specifically encourages and supports collaborative research, including multiagency collaborations and coordination. Close coupling between experimental and computational efforts should also be specifically encouraged and supported. Potential benefits include more effective use of complementary resources, better design of validation experiments that can pace model development, more complete data on select target cases, better connections between basic and applied research, better understanding of applicability and performance of various models, and greater impact with available budgets.

3.4 Documentation, archival procedures, and cyber infrastructure

Science and Engineering are informed by and draw inspiration from the work done by others either contemporarily or in the past. The body of peer-reviewed literature is a trusted resource in this context and in many cases serves the required needs quite well. However, it is also clear that some research produces and/or needs access to large amounts of raw or processed data, such as input in the form of chemical kinetic reaction schemes, thermodynamics data, or large experimental or simulation results for comparisons or further analysis. Perpetual electronic access is critical in this context to make this information the most useful. Shared and open access to well-documented data is key to progress in combustion research.

Owing to the multidimensional and time-dependent nature of turbulent combustion processes, experimental and numerical investigations generate large amounts of data that often will provide a rich source of information for data mining by researchers with other expertise, interests, and resources. Databases for simulation input, for validation and exploration, for experimental methods and analysis tools, etc. need to be available to the research community for immediate, longterm, and archival use.

Key problems related to creating, sharing, and maintaining databases are rooted in a lack of guidance for authors on how to properly document and illustrate the posted information but more so on strategies and means to providing the longevity of access to the information. While a federal mandate exists that results from publically funded work should be made available publically, there is no financial support to actually enable this beyond the lifetime of the research grants that support the generation of the information. Continued financial support is necessary to maintain the physical preservation of the data and to keep it in accessible, i.e. currently readable, format.

Is a federal repository the right way to approach the creation and maintenance of the archive of the 'combustion knowledge'? Should it be located at a National Laboratory? Should a professional society, e.g. the Combustion Institute, be charged with such an effort? Should it be left with the original source of the information and support be provided to maintain the data locally?

3.5 Need for instrumentation/facility support

Combustion research has, historically, required a large investment in instrumentation. The payoff has been that combustion scientists and engineers can now quantify a range of critical combustion parameters, including the temperature and velocity fields (usually in two-dimensions, defined by a "laser sheet"), concentrations of combustion species (including pollutants and combustion intermediates and products), the two-dimensional representation of the flame surface, and under ideal conditions, approximations of the heat-release rate. Over the last twenty years, this instrumentation has typically included pulsed lasers (typically commercial Q-switched Nd:YAG and dye lasers but also mode-locked picosecond and femtosecond lasers and even custom laser sources), image intensified digital cameras, optical components (lenses, dielectric mirrors, etc.), and custom electronics (high-bandwidth oscilloscopes, power supplies, etc.). More recently, there has been a move toward time-resolved, kHz-rate imaging diagnostics that has exacerbated the "investment problem," as the required kHz-rate instrumentation is even costlier. Indeed, there are currently very few laboratories across the US (or even in Europe) that have sufficient equipment and financial resources to study fundamental combustion process in sufficient detail (temporal and spatial) to enable progress in both a theoretical understanding of combustion processes (e.g., turbulent flame speed) and computational model development (to enable true, predictive capability). It should be recognized that enhancing our theoretical understanding and simulation capability for combustion processes is a critical national need that requires infrastructural investments for experiments and computations.

This could be addressed by:

a. More investment from US government funding agencies (NSF, DOE, DoD, etc.). Currently, there are very few avenues for acquiring significant resources for instrumentation at the university level.
b. Encourage teaming arrangements between research groups (with/between both university and US government laboratories), to mitigate the burden of equipment requirements. This encouragement must come from US funding agencies (and perhaps from universities too), but "buy in" is also required from US government laboratories involved in combustion research, since their investment in equipment/instrumentation is generally greater than at universities.

Participant list (alphabetical order):

Arvind Atreya (University of Michigan)
Robert Barlow (Combustion Research Facility, Sandia National Laboratory)
Cam Carter (Wright Patterson Air Force Base), via video conference
Chiping Li (AFOSR)
Jackie Chen (Combustion Research Facility, Sandia National Laboratory)
Ruey-Hung Chen (NSF)
Andreas Dreizler (TU Darmstadt, Germany)
James Driscoll (University of Michigan)
Dan Haworth (Penn State University)
Matthias Ihme (Stanford University)
Tim Lieuwen (Georgia Institute of Technology)
Laurent Gicquel (CERFACS, Toulouse, France)
Joe Oefelein (Combustion Research Facility, Sandia National Laboratory)
Norbert Peters (RWTH Aachen, Germany), via written input
Alexei Poludnenko (NRL, Washington, DC)
Chris Rutland (University of Wisconsin, Madison)
Venke Sankaran (Air Force Research Laboratory)
Volker Sick (University of Michigan), organizer and local host
Adam Steinberg (University of Toronto, Canada)
Jeffrey Sutton (Ohio State University)
Foreman Williams (UC San Diego)