Proceedings of the First Model Validation for Propulsion (MVP 1) Workshop

2017 AIAA Science and Technology (SciTech) Forum and Exposition
January 9 - 13, 2017
Grapevine, Texas

Adam Comer, Matthias Ihme, Chiping Li, Suresh Menon, Joseph Oefelein,
Brent Rankin, Vaidyanathan Sankaran, Venkateswaran Sankaran

Abstract

The purpose of this report is to document the Proceedings of the First Model Validation for Propulsion (MVP) Workshop which was held at the 2017 AIAA SciTech Forum from January 9 - 13 in Grapevine, Texas. The Model Validation for Propulsion Workshop is an open forum bringing together researchers and modelers to help improve our understanding and capabilities of modeling turbulent reacting flows in relevant aerospace propulsion systems. The MVP 1 Workshop was attended by approximately 100 researchers from more than 5 countries. The main session topics included (1) validation metrics and interactions with experiments, (2) best practices in reacting large eddy simulations, and (3) the Volvo bluff-body premixed flame validation case. These proceedings summarize the objectives, final program, discussion topics, and conclusions for the MVP 1 Workshop. These proceedings and further information are available on the MVP Workshop website: https://community.apan.org/wg/afrlcg/mvpws

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INTRODUCTION

Objectives of MVP Workshop Series

The Model Validation for Propulsion Workshop is an open forum bringing together researchers and modelers to help improve our understanding and capabilities of modeling turbulent reacting flows in relevant aerospace propulsion systems. The objectives of the MVP Workshop series include the following:

- Define and evaluate procedures/metrics for grid convergence for reacting LES and quantify numerical error.
- Evaluate performance of physics models for combustion, turbulence and turbulent combustion closures.
- Identify the requisite data for validation of reacting LES.
- Identify fundamental gaps in current knowledge of reacting LES models to inform basic research programs.
- Use data and comparisons to guide the development of improved models.

Organizing Committee for the MVP Workshop Series

The organizing committee for the MVP Workshop series consists of the following members:

- Adam Comer, Air Force Institute of Technology
- Matthias Ihme, Stanford University
- Chiping Li, Air Force Office of Scientific Research
- Suresh Menon, Georgia Institute of Technology
- Joseph Oefelein, Sandia National Laboratories
- Brent Rankin, Air Force Research Laboratory
- Vaidyanathan Sankaran, United Technologies Research Center
- Venkateswaran Sankaran, Air Force Research Laboratory

Objectives of MVP 1 Workshop

The objectives of the MVP 1 Workshop include the following:

- Introduce the objectives of the MVP Workshop
- Discuss validation metrics and interactions with experiments
- Compare methods and results from simulations of the Volvo bluff-body premixed flame validation case
- Discuss best practices in reacting large eddy simulations
- Establish framework for future MVP Workshops

Planning for MVP 2 Workshop

The Second Model Validation for Propulsion Workshop will be held at the 2018 AIAA SciTech Forum from January 8 - 12 in Orlando, Florida. Early coordination is strongly encouraged for selecting validation cases, defining guidelines for model comparisons, and establishing priorities for collaborative work. Regular communication between members of the organizing committee and key contributors is also strongly encouraged. Suggestions for new discussion topics or validation cases should be communicated to the MVP Workshop organizing committee.

Important Note Regarding Use of Workshop Proceedings Material

Results in the MVP Workshop proceedings are contributed in the spirit of open collaboration. Some results represent completed work, and other results represent work in progress. Readers should keep this in mind when reviewing these materials. It is inappropriate to quote or reference specific results from these proceedings without first checking with the individual author(s) for permission and for the most recent information and references.

FINAL PROGRAM FOR MVP 1 WORKSHOP

Opening Session

Wednesday, January 11, 2017, 09:30AM-12:30PM

- Objectives of the MVP Workshop Series (Adam Comer)
- Validation Metrics and Interactions with Experiments Invited Panel Discussion
  - Moderated by Brent Rankin, Air Force Research Laboratory
  - Rob Barlow, Sandia National Laboratories
  - Christer Fureby, The Swedish Defense Research Agency
  - Laurent Gicquel, CERFACS
  - Tim Lieuwen, Georgia Institute of Technology
  - Adam Steinberg, University of Toronto

Technical Papers Session I

Thursday, January 12, 2017, 9:30AM-12:30PM

- Chaired by Adam Comer and Venke Sankaran
- **N. Chakroun**, S. Shanbhogue, G. Kewlani, S. Taamallah, D. Michaels, A. Ghoniem, "On the Role of Chemical Kinetics Modeling in the LES of Premixed Bluff Body and Backward-Facing Step Combustors," AIAA-2017-1572.
- H. Wu, P. Ma, Y. Lv, **M. Ihme**, "MVP-Workshop Contribution: Modeling of Volvo bluff body flame experiment," AIAA-2017-1573.
- **S. Drennan**, G. Kumar, S. Liu, "Developing Grid-Convergent LES Simulations of Augmentor Combustion with Automatic Meshing and Adaptive Mesh Refinement," AIAA-2017-1574.
- **C. Fureby**, "A Comparative Study of Large Eddy Simulation (LES) Combustion Models applied to the Volvo Validation Rig," AIAA-2017-1575.
- D. Maestro, A. Ghani, **L. Gicquel**, T. Poinsot, "LES reliability of the Volvo bluff-body stabilized flame dynamics," AIAA-2017-1576.

Technical Papers Session II

Thursday, January 12, 2017, 2:00PM-5:00PM

- Chaired by Adam Comer and Venke Sankaran
- **V. Sankaran**, T. Gallagher, "Grid Convergence in LES of Bluff Body Stabilized Flames," AIAA-2017-1791.
- **A. Potturi**, J. Edwards, "Advanced LES Models for Turbulent Combustion," AIAA-2017-1792.
- **J. West**, C. Groth, "Application of Detached Eddy Simulation to a Bluff Body Flame Stabilizer in Duct Flow," AIAA-2017-1793.
- **C. Wey**, "Model Validation for Propulsion – On the TFNS Subgrid Models for a Bluff Body Stabilized Flame," AIAA-2017-1794.

Closing Session

Friday, January 13, 2017, 9:30AM-12:30PM

- Best Practices in Reacting Large Eddy Simulations Invited Panel Discussion
    - Moderated by Matthias Ihme, Stanford University
    - Rob Baurle, NASA Langley Research Center
    - Graham Candler, University of Minnesota
    - Peyman Givi, University of Pittsburgh
    - Frank Ham, Cascade Technologies, Inc.
    - Z. J. Wang, University of Kansas
- MVP 1 Workshop Findings and Feedback (Venke Sankaran)

<u>SUMMARY OF MVP 1 WORKSHOP</u>

<u>Validation Metrics and Interactions with Experiments</u>

An invited panel session was organized to discuss validation metrics and interactions with experiments. The most significant topics from the discussion are summarized in this section.

- **Hierarchy of Configurations** – An enduring hierarchy of configurations with varying complexity need to be explored during the model validation process. The current focus of the MVP Workshop is on single-element configurations with increased relevancy relative to canonical problems yet sufficiently simplified geometries. The availability of comprehensive data sets of single-element configurations operating at relevant conditions with well-defined boundary conditions appears to represent a gap within the combustion community. The selection of future cases should consider the diverse interests and funding priorities of government, industry, and academia.

- **Unit Physics Problems –** Unit physics problems are more appropriate for the evaluation and validation of turbulence and turbulence-chemistry closure models. The model validation process requires detailed data at the flame location, and these localized effects are more readily assessed in unit physics problems that are simpler than single-element target cases such as the Volvo bluff-body premixed flame case. The extent to which unit physics problems should be incorporated within the MVP Workshop or other existing workshops in the future remains open for further discussion. The MVP Workshop needs to retain a sufficiently narrow focus to make a lasting impact while simultaneously having some overlap with existing workshop series.

- **Boundary Conditions –** The importance of having well-defined boundary conditions that can be matched between experiments and computations was emphasized. Specific attention should be focused on experimentally characterizing thermal and acoustic boundary conditions as these are often neglected but have been demonstrated to be important. Data on fluctuations at inflow and outflow boundaries are desired. Implementing boundary conditions using a consistent computational approach is a critical step for code-to-code comparisons. The repeatability of boundary conditions and the corresponding measurements should be demonstrated.

- **Operating Conditions –** The acquisition of experimental data sets for a range of operating conditions (e.g., temperatures, velocities, and equivalence ratios) is useful for evaluating the capability of computations to capture trends accurately. For example, computations of bluff-body premixed flames should be able to accurately predict trends for varying temperature/density ratios across the flame. Off-design operating conditions such as ignition, lean blowout, and thermo-acoustic instabilities are of interest for future validation cases. There is reasonable consensus that exploration of off-design conditions should be explored only after stationary combustion has been investigated thoroughly.

- **Sensitivity Analyses –** The importance of performing experimental and computational sensitivity analyses was discussed. Experiments should be designed to be as insensitive as possible to boundary conditions (e.g., background acoustics). It would be beneficial to utilize a combination of experiments and computations for assessing the sensitivity of the configuration to boundary and operating conditions before acquiring validation data. Computational sensitivity analysis would be useful for guiding the experiments and identifying the potentially largest sources of error.

- **Comparison of Measurements and Computations** – The importance of comparing global flow and flame features (e.g., flame position and shape) between measurements and computations before comparing detailed statistics was emphasized. The comparisons of global features can be made more quantitative through modal and frequency analysis for unsteady flows. Additionally, the experimental techniques (e.g., broadband imaging and chemiluminescence imaging) to detect and measure these aspects of the flow are more readily available at relevant conditions. However, comparisons cannot stop at the global flow and flame features level as this could encourage model adjustments and is not as rigorous as point measurements.

- **Challenges Associated with Comparing Measurements and Computations –** Several challenges associated with comparing measurements and computations were discussed. The differences in sampling times between measurements and computations could present challenges because experiments have relatively long acquisition times whereas computations occur over short physical times. The difference in spatial resolution and filtering operations between measurements and computations could also present challenges.

- **Statistical Comparisons –** Beyond the mean and RMS, statistical comparisons may push the limits of codes to collect sufficient data. Different sources of unsteadiness require different statistical processing techniques. Broadband turbulence and coherent structures both contribute to unsteadiness, but they are very different in their frequency characteristics and represent different underlying physics. A given statistic without detailed frequency information can be achieved in many ways, meaning many different flow or flame calculations could yield the same statistics but predict significantly different underlying processes.

- **Model Evaluation and Validation Process –** The differences between model evaluation/assessment, verification, and validation were discussed. The use of blind studies in which experimental results are not revealed until after the computations are complete has not yielded great results in the past. The use of partially blind studies in which some but not all experimental results (e.g., axial velocity profiles along centerline) are revealed may be a useful approach.

- **Validation Cases** – Due to the complexity of the model evaluation and validation process, focusing the community on one case (or a limited set of cases) and performing code-to-code comparisons will help distinguish the MVP Workshop and represents a promising path forward. Validation cases should be inspired by experiments but not overly constrained by them, at least initially. The consensus was that the bluff-body premixed flame is a logical choice for the first validation case for this workshop.

- **Interactions between Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES) –** Large eddy simulation is a tool for large practical problems for which we cannot perform DNS. The evaluation of closure models at resolutions significantly higher than the Kolmogorov scale (e.g., 100X) must be required of workshop participants. Spatial resolution is often treated as a variable that can be modified to make the simulation affordable, but perhaps resolution should be treated more like a requirement in the context of a validated model. The use of high-fidelity simulations for performing a very fine-grid LES of the target case may provide a baseline for course-grid LES and other codes. However, this approach should be pursued with caution because requiring high-fidelity fine-grid LES may exclude participants due to the large computational cost.

Best Practices in Reacting Large Eddy Simulations

An invited panel session was organized to discuss best practices in reacting large eddy simulations. The most significant topics from the discussion are summarized in this section.

- **Hierarchy of Configurations** – Some reservations were expressed about the complexity of the Volvo bluff-body premixed flame validation case caused by the geometrical configuration, large domain size, and low velocities (i.e., large flow through times). The current focus of the MVP Workshop is on single-element configurations with increased relevancy relative to canonical problems; however, one expected outcome of the MVP Workshop series is the identification of unit physics problems and canonical arrangements that would be useful for validating new combustion sub-models. Further discussion is anticipated to decide whether unit physics problems are formally incorporated within future MVP Workshop. It is important to recognize that over-simplified configurations present alternative challenges regarding the translation of findings to more complex applied configurations.

- **New Model Development Efforts** – There was substantial discussion regarding the current status of turbulent combustion model development. It was suggested that turbulent combustion model development has become stagnant with a significant reliance on old models often derived from non-reacting flows or Reynolds-averaged Navier-Stokes approaches. Significant investment in the fundamental development of new turbulent combustion models is needed. The underlying physical processes are fundamentally stochastic, and this realization must be incorporated into modeling and simulation.

- **Model Evaluation and Validation Process –** The validation process depends on the level at which it is being conducted. For example, evaluating and validating integrated models at the simulation level is an exercise in uncertainty management in an attempt to achieve the best estimate. Evaluating and validating individual models or sub-models involves different processes and requirements. It is critical to eliminate or mitigate numerical errors when performing model validation. Explicit filtering can reduce numerical error and isolate model effects by keeping the filter width the same while reducing the grid size. However, going to DNS level resolution eliminates the role of the model and hinders validation efforts as the model is not tested.

- **Benefits of Implicit Filtering** – The relative advantages and disadvantages of implicit and explicit filtering were discussed in detail. Implicit filtering is often favored over explicit filtering because (a) explicit filtering and differentiation do not commute and (b) explicit filtering is computationally expensive. Explicit filtering often requires the user to sacrifice resolution due to the higher computational cost.

- **Benefits of Explicit Filtering** – It is challenging to separate physical model errors from numerical errors using current implicit filtering approaches. This issue suggests the need for explicit filtering, in which filter width can be fixed while the mesh is refined. If filter width varies with grid size, a different differential equation is simulated for different meshes, which corrupts the model comparison and causes the results to be dependent on the numerical methods applied. There was reasonable consensus that explicit filtering is required to reduce error and enable definitive statements about model accuracy. However, implicit filtering also must be investigated because it is more cost effective for practical industry applications.

- **High-Order Methods for Controlling Dissipation and Dispersion Errors** – Higher order schemes or methods can be used to reduce the numerical error to be less than the sub-grid scale physics that influence turbulence-chemistry interactions. One must experiment by using different higher order schemes on the same mesh and tuning them to minimize the aliased error. Fourth order schemes have been developed that have some dispersive errors that are minimized by the user. For high order filters, the general approach is to consider the fundamental energy stability and then focus on ways to address the dissipation. Kinetic energy consistent methods are favored by some groups, and dissipation must be adjusted to balance stability and accuracy. More information than order of accuracy is needed to describe numerical performance of a given scheme. For instance, upwind schemes will be more dissipative and more prone to errors when compared to central schemes of the same order.

- **High-Order Methods Advantages and Disadvantages** – High order methods are typically more computationally efficient given the same accuracy requirement. In other words, for a given grid, higher order, low dissipation methods should provide more information. For the same number of degrees of freedom, higher order methods can resolve a higher frequency range. High order methods are highly scalable and should be able to handle complex geometry, as well as mixed elements. These methods also offer significant flexibility in refinement by enabling independent mesh and polynomial refinement. Initially, there was skepticism in the non-reacting community, but the merits of higher order methods now have been largely recognized. The largest impediment to widespread adoption of higher order methods is mesh generation. Coarser meshes (approximately one million elements) are needed with particular topologies (curved) for industrial calculations. Unfortunately, one needs smoothness for polynomial-base methods to work, but real applications have discontinuities that present challenges.

- **Non-Reacting LES** – For non-reacting LES, it was found that the SGS model does nothing more than add dissipation (at least for finite volume), so implicit LES is favored since the numerical schemes are sufficiently dissipative for stability. For finite volume methods with only one degree of freedom, the truncation error is so large that even with an exact SGS model, the potential benefit is overwhelmed by numerical error. However, the non-reacting conclusions probably do not translate to reacting flows, since there are significant sub-grid physical processes that affect the flow and turbulence cascade.

- **Mesh Generation** – Selection of a priori mesh resolution requirements still requires significant experience and judgment. Upstream and downstream elements are surprisingly coupled, and the critical regions of the flow are often difficult to identify. This matter is further complicated by transitions in complex grids that generate noise, which can be alleviated with careful numerical methods. Higher order methods offer grid flexibility that may be useful in resolution specification. However, there is still a need to evaluate the results after the simulation and analyze the spectra. It may not be possible to perform only one simulation in the foreseeable future because multiple simulations are needed to assess resolution requirements.

- **Adaptive Mesh Refinement (AMR)** – AMR can reduce simulation time by a factor of ten for certain problems (e.g., oblique shocks in a scramjet). It is critical that the refinement switch occurs outside the region of critical physics to minimize numerical error. As far as key metrics for detection, the divided difference technique using density has produced good results. However, AMR does not readily integrate into explicit filtering approaches.

- **Boundary Conditions** – LES is an exercise in balancing and controlling errors to achieve a result that is accurate enough to provide actionable information. Boundary conditions are critical to accurate simulations and are the most common source of error. Accurate modeling of heat transfer boundary conditions is important for capturing global flame features, but it is often neglected or performed using incorrect wall modeling.

- **Sensitivity Analyses** – The costs of sensitivity analyses and grid convergence studies present a major challenge, requiring significant support for allocating sufficient resources. Monitoring the statistics and energy cascade are the conventional approaches, but focusing resolution change in critical regions and the use of the adjoint method may provide cost savings for future investigations.

- **Grid Convergence -** It is important to consider both the grid and filter width as variables when performing grid sensitivity studies. Grid convergence is critical because without it, model comparisons are inconclusive. In general, more standardization will be needed to gain significant insights from grid convergence studies. One mechanism for encouraging sensitivity analysis is to incorporate it as a requirement for journal submission. For instance, AIAA journals currently require grid convergence to be demonstrated.

- **Statistical Convergence** – The evaluation of statistical convergence needs to be more rigorous and comprehensive than simply specifying the number of flow through times. For instance, the timescales associated with recirculation zones could be very long and much more demanding than an initial estimate based on flow through times. In addition, the issue of incorporating sub-grid values into the calculation of statistics should be addressed. For example, Favre averaging has a third order correlation with density because of the filtered density. This averaging affects the baroclinic torque, but it is rarely considered in comparisons.

- **Quantum Computing** – A practically useful quantum computer would exponentially improve the performance of certain algorithms, such as Monte Carlo mixing. However, the speed-up would occur only for certain aspects of reacting flow simulations where there is independence between successive calculations. Therefore, the time-marching process of current CFD algorithms may present a major obstacle. New algorithms would have to be developed to make full use of quantum computing. An example of the difficulties associated with changing architectures can be seen in the slow adoption of GPUs for CFD calculations.

Volvo Bluff-Body Premixed Flame Validation Case

Two technical paper sessions were organized in which 9 presentations were made on the modeling and simulation of the Volvo bluff-body premixed flame validation case. The most significant observations and conclusions from the presentations are summarized in this section.

- **Grid Convergence –** Most of the technical papers did not demonstrate grid convergence for the reacting conditions with one exception. One paper demonstrated grid convergence at mesh sizes of 30 to 100 million cells (0.5 to 0.7 mm) with a customized version of OpenFOAM. A grid resolution of 1 mm (approximately 11 million cells) was not sufficient for grid convergence.

- **Grid Convergence for Non-Reacting and Reacting Conditions** – It was more challenging to achieve grid convergence for the reacting conditions in comparison to the non-reacting conditions as expected.

- **Statistical Convergence** – It was more challenging to achieve statistical convergence for certain statistics (e.g., RMS, centerline profiles of axial velocity, and anisotropy) than it was for other statistics (e.g., transverse profiles of average velocity).

- **Turbulent Combustion Models** – Turbulent combustion models could be instrumental in achieving grid convergence, as laminar closure results tended to exhibit more variations between meshes. Other elements of the model, especially chemistry, can influence grid convergence. As expected, the results suggest more detailed chemistry than a global mechanisms is necessary.

- **Experimental Considerations** – The thermal (e.g., water cooling effects) and acoustic (e.g., reflective vs. non-reflective) boundary conditions must be considered to improve quantitative agreement between the measurements and computations.

Workshop Feedback

Many suggestions for improving future MVP Workshops and next steps related to the validation case were made throughout the invited panel sessions and technical paper sessions. The suggestions are summarized in this section.

- **Validation Cases**
    - Bluff-body premixed flames represent a relevant and challenging validation case. There is reasonable consensus that it is a logical choice for future MVP Workshops in the near-term.
    - Off-design operating conditions such as lean blowout are of interest for future validation cases. There is reasonable consensus that exploration of off-design conditions should be explored only after stationary combustion has been investigated thoroughly.

- Evaluating the capability of simulations to predict trends over multiple stationary combustion conditions would be a useful next step prior to exploring off-design conditions.

- **Grid Convergence**
  - Achieving grid convergence is imperative to making valid assessments of model performance.
  - Finer meshes and/or higher order methods are needed to achieve convergence. A more efficient grid topology (non-uniform) should be considered with some static refinement for critical regions (e.g., recirculation zone).
  - Explicit filtering may provide more rigor to the grid convergence studies, but it is also expensive and not readily available in many codes.
  - The computational cost of the Volvo bluff-body premixed flame is high. Approaches for decreasing the computational cost (e.g., higher inlet velocity or shorter domain to reduce flow through times) should be considered.
  - Future workshops should feature a more concerted effort to address uncertainty.

- **Direct Numerical Simulations and Unit Physics Configurations**
  - Developing a framework for sub-model evaluation may be achieved more efficiently on smaller unit physics problems. The workshop should lead to unit physics problem recommendations, even if those problems are not incorporated into the workshop.
  - To satisfy the need for a simpler test, the use of two cases was proposed: one based on a canonical experiment (physical model focus) and one based a unit physics problem (numerical methods focus). For the unit physics problem, explicit filtering could be more readily applied and enable separation of model and numerical errors. However, the ability to perform DNS at relevant conditions has been called into question.

- **Future Simulation Inputs and Outputs**
  - The workshop should coordinate which variables (e.g., temperature and vorticity distributions) to plot in order to identify global flame features for code comparisons.
  - The difference between actual (0.62) and reported (0.65) equivalence ratios for the Volvo bluff-body flame needs to be resolved for the next workshop.
  - The inlet turbulence specification should be reconsidered.
  - The number of flow through times for collecting statistics should be specified, and a process for assessing convergence should be identified. Higher order moments and/or spatial/temporal autocorrelations may be required for a more detailed convergence assessment.

- **Actions Related to MVP 1 Workshop**
  - Consider creating a database or repository of the computational results to compare how the codes performed on the Volvo bluff-body premixed flame
  - Consider performing a meta-analysis to gather lessons from the Volvo bluff-body premixed flame validation case. It is currently unclear whether grid convergence and standardization issues are too significant to invest significant time in detailed meta-analysis of the MVP 1 Workshop validation case results.

- Explore potential opportunities to interact with non-reacting LES community and associated workshops.
- Evaluate the advantages and disadvantages associated with scheduling future MVP workshops concurrent with the conference or prior to the conference.

CONCLUSIONS FOR MVP 1 WORKSHOP

The most significant outcomes and conclusions from the First Model Validation for Propulsion Workshop are summarized here.

- An enduring hierarchy of configurations with varying complexity need to be explored during the model validation process. The configurations should include unit physics problems for assessing the influence of numerical methods, canonical problems for assessing individual physical models, and single-element arrangements for assessing the capability of simulations to predict turbulent reacting flows in more relevant geometries and under more relevant conditions. The MVP Workshop series initially is focused on single-element arrangements with the objective of guiding the selection of unit physics problems which may be incorporated into the workshop in the future.

- The MVP workshop will focus on one validation case (or a very limited number of cases) and perform code-to-code comparisons in the near-term because of the complexity of the model evaluation and validation process. The consensus was that the bluff-body premixed flame is a logical choice for the first validation case for this workshop.

- Grid convergence was not demonstrated by most of the technical papers which reported results on the Volvo bluff-body premixed flame. One paper demonstrated grid convergence at mesh sizes of 30 to 100 million cells.

- The demonstration of grid convergence is a critical step in the model validation process because model comparisons are inconclusive without it. It is challenging to separate physical model errors from numerical errors using current implicit filtering approaches. This issue suggests the need for explicit filtering, in which filter width can be fixed while the mesh is refined. There was reasonable consensus that explicit filtering is required to reduce error and enable definitive statements about model accuracy. However, implicit filtering also must also be investigated because it is more cost effective for practical industry applications.

APPENDIX: Opening Session Presentation Slides

Model Validation for Propulsion (MVP) Workshop Opening Session

11 January 2017

Organizing Committee:

Adam Comer	Air Force Institute of Technology
Matthias Ihme	Stanford University
Chiping Li	Air Force Office of Scientific Research
Suresh Menon	Georgia Institute of Technology
Joseph Oefelein	Sandia National Laboratories
Brent Rankin	Air Force Research Laboratory
Vaidyanathan Sankaran	United Technologies Research Center
Venkateswaran Sankaran	Air Force Research Laboratory

AIAA Shaping the Future of Aerospace

Goals

- Define and evaluate procedures/metrics for grid convergence for reacting LES and quantify numerical error.
- Evaluate performance of physics models for combustion, turbulence and turbulent combustion closures.
- **Identify the requisite data for validation of reacting LES.**
- Identify fundamental gaps in current knowledge of reacting LES models to inform basic research programs.
- **Use data and comparisons to guide the development of improved models.**

AIAA Shaping the Future of Aerospace

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Schedule

Opening Session: Wednesday, 9:30AM-12:30PM
(*Room: San Antonio 5)*

- Goals of the MVP Workshop Series
- Validation Metrics & Interactions w/ Experiments: Invited Panel

Technical Paper Session 1: Thursday, 9:30AM-12:30PM
(Room: San Antonio 6)

Technical Paper Session 2: Thursday, 2:00PM-5:00PM
(Room: San Antonio 6)

Closing Session: Friday, 9:30AM-12:30PM
(Room: Palomino 2)

- Best Practices in Reacting LES: Invited Panel
- Inaugural Session Feedback and Findings / Future MVP Workshop Cases

AIAA Shaping the Future of Aerospace

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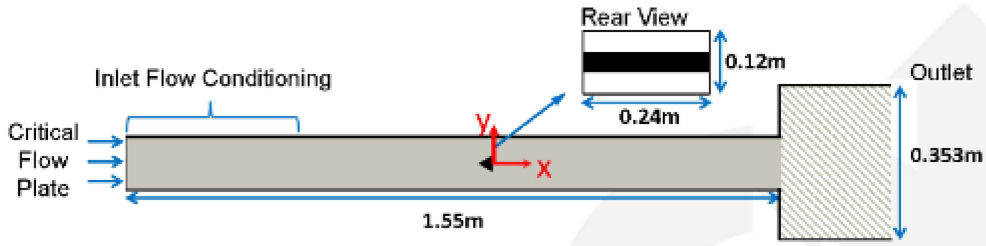
Volvo Configuration and Conditions



Operating Conditions	
Reynolds Number	47,000
Mach Number	0.05
Bulk Velocity	17.3 m/s
Inlet Temperature	288 K
Equivalence Ratio	0.65

Sjunnesson et al., 1991

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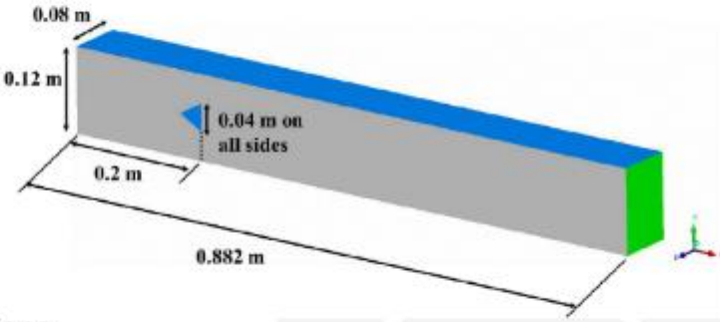
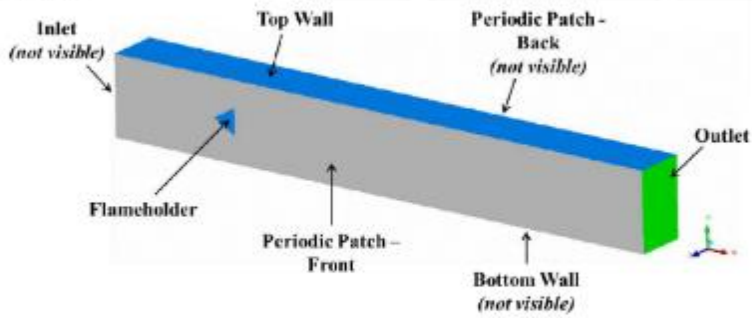
Case Setup

Dimensions



Boundary Conditions



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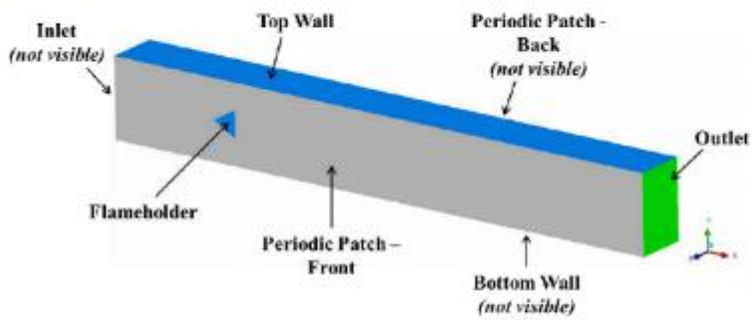
Case Setup



Patch	Boundary Condition
Inlet	Uniform $\dot{m}$=0.2083 kg/s, T_t=288.2 K, No turbulence, Φ=0.65
Top, Bottom, & Flameholder Walls	No-slip, adiabatic
Front and Back	Periodic
Outlet	Fixed static pressure of 100 kPa

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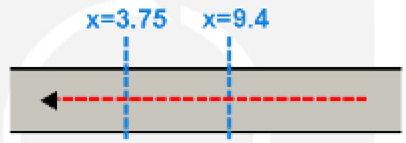
Grid and Data Comparison Guidance

- Recommended resolutions: 4 mm, 2 mm, and 1 mm
- Values of interest: U_x, U_y, T, CO, & CO_2
- Main Goal - Show convergence via the following statistics:
  - Mean – Axial & Transverse Profiles
  - RMS – Transverse Profiles
  - Turbulence Intensity – Axial Profile
  - One-Point Temporal Statistics
    - Temporal Autocorrelation



$$\rho(\vec{x},\Delta\tau) = \frac{\langle \varphi'(\vec{x},t)\varphi'(\vec{x},t+\Delta\tau)\rangle}{\langle \varphi'(\vec{x},t)^2\rangle}$$

    - Integral Timescale

$$\tau_I(\vec{x}) = \int_0^\infty \rho(\vec{x},\Delta\tau)\, d\Delta\tau$$

7

Panel Sessions

Validation Metrics & Interactions with Experiments (Today)

Rob Barlow	Sandia National Laboratories
Christer Fureby	The Swedish Defense Research Agency
Laurent Gicquel	CERFACS
Tim Lieuwen	Georgia Institute of Technology
Adam Steinberg	University of Toronto

Best Practices in Reacting LES (Friday)

Rob Baurle	NASA Langley Research Center
Graham Candler	University of Minnesota
Peyman Givi	University of Pittsburgh
Frank Ham	Cascade Technologies, Inc.
Z. J. Wang	University of Kansas

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Questions or Comments?

Opening Session: Wednesday, 9:30AM-12:30PM
(*Room: San Antonio 5)*

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- Best Practices in Reacting LES: Invited Panel
- Inaugural Session Feedback and Findings / Future MVP Workshop Cases

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Validation Metrics and Interactions with Experiments: Invited Panel Session

- Introduction to Model Validation for Propulsion Workshop (~30 min)
- **Introductory Remarks by Panel Members (~30 min)**
- **Validation Metrics (~30 min)**
  - Criteria for "validated" model
  - Moving beyond the mean and RMS
  - Non-stationary conditions (e.g. ignition, extinction, and thermo-acoustics)
- **Experimental Data Requirements for Model Evaluation and Validation (~30 min)**
  - Desired experimental data for validation
  - Boundary condition requirements
  - Spatial and temporal resolution requirements
  - Uncertainty quantification
- **Interactions between Experiments and Computations (~30 min)**
  - Interaction between experiments, theory, LES, and DNS
  - Selection of validation cases

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APPENDIX: Closing Session Presentation Slides

Model Validation for Propulsion (MVP) Workshop
Closing Session

13 January 2017

Organizing Committee:

Adam Comer	Air Force Institute of Technology
Matthias Ihme	Stanford University
Chiping Li	Air Force Office of Scientific Research
Suresh Menon	Georgia Institute of Technology
Joseph Oefelein	Sandia National Laboratories
Brent Rankin	Air Force Research Laboratory
Vaidyanathan Sankaran	United Technologies Research Center
Venkateswaran Sankaran	Air Force Research Laboratory

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Model Validation for Propulsion (MVP) Workshop

Best Practices in Reacting LES (invited panel session)

Rob Baurle	NASA Langley Research Center
Graham Candler	University of Minnesota
Peyman Givi	University of Pittsburgh
Frank Ham	Cascade Technologies, Inc.
Z. J. Wang	University of Kansas

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Best Practices in Reacting LES

- **Introductory Remarks by Panel Members (~30 min)**
- **Numerical methods (~60 min)**
  - LES filtering methods: *Implicit vs. explicit filtering; role of filter kernel functions; aliasing errors from numerical schemes*
  - Numerical discretization: *High-order vs. standard 2nd-order methods; separation of discretization error and physical errors*
  - Solution stabilization: *filtering, artificial dissipation; shock capturing; embedded conservation*
  - Mesh-refinement: *cost, merit, and potential issues of AMR; unstructured vs. block/structured discretization*
  - Use of UQ-techniques *for evaluating numerics and physics of models*
- **Best practice guidelines (~30 mins)**
  - Setting up a new simulation: *Recommendation on mesh-size; mesh-distribution; resolution requirement; use of resolution criteria (Pope's criteria, index of resolution quality, …)*
  - Mesh-convergence: *Assessment of grid convergence, How to define grid convergence for LES?*
  - Knowledge transfer *to full-scale combustor geometries; practical applications*
  - Physical models: *Combustion models; SGS-models, …*

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General Summary of Grid Convergence

Paper	Non-Reacting	Reacting
AFIT/AFRL	No	No
MIT	Not available	Not available
Stanford FV	Yes	No
Stanford DG	Not available	Not available
Convergent Science	No*	No
SDRA	Not available	Yes**
CERFACS	Not available	Not available
UTRC/Ga. Tech	Not available	No
Metacomp/NC State	Not available	No
UTIAS	Yes	No
NASA Glenn	Not available	Not available

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* To be updated and reviewed; averaging error
** Between 30 and 100 million cells

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General Findings

- Grid convergence is harder to achieve in reacting flows compared to non-reacting flows
  - For certain statistics, it is more difficult to achieve convergence
- Grid resolution of 1 mm is not sufficient for grid convergence but Fureby demonstrated convergence at 30-100 M cells
- Turbulent combustion models could be instrumental in achieving grid convergence
- Importance of reflective vs. non-reflective BCs
- Suggestion that explicitly-filtered LES may provide a basis for grid convergence

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General Findings

- For replicating the experimental data, the following must be considered:
  - Thermal boundary conditions
  - Acoustic boundary conditions
  - Acoustic wave propagation effects
  - Chemistry more complex than global is needed

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Recommendations

- Coordinate which global structures to compare
  - Temperature and vorticity contours suggested by Vaidya Sankaran
- Need finer meshes or higher order methods
- Specify flow through times for collecting statistics
- Need to identify sensitivity to model parameters
- Delay off-design calculations until stable combustion has been sufficiently investigated
  - However, predicting parametric trends would be a useful step

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Audience Feedback and Questions

http://mvpws.stanford.edu/

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APPENDIX: Validation Case Guidelines

MVP Workshop – SciTech 2017 Case

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Last Update: 22 September 2016, 1218EST, Summary of Edits

Abstract Deadline and Details: Please submit your abstract via the SciTech 2017 website. Please select "Propellants and Combustion" as the topic and "Turbulent Combustion" as the subtopic when submitting the abstract. These steps will help ensure that your paper is placed in the correct session. To request an extension or for other inquiries, please e-mailaiaa.mvpws@gmail.com.

Initial Validation Case Overview:

The first validation case in the MVP Workshop series is the premixed bluff body flame experiment conducted by Volvo. Participation in the workshop is open, and participants can contribute by performing reacting flow simulations of the selected test case. Non-reacting simulations are highly encouraged but optional. The geometry, conditions, recommended model settings and practices, and experimental data can be found below. The guidelines are provided in order to ensure consistency among the simulations presented and to facilitate code and model comparison. They are not necessarily the best model and simulation choices, and the organizing committee does not intend to imply that there is a consensus regarding these choices. In addition, sample meshes of different resolutions, coarse, medium and fine are provided. Participants are not obligated to use the meshes provided, although they may provide some guidelines to grid resolution levels. Please note that workshop participation requires the submission of a full SciTech 2017 paper that contains all model details and the requested solution data.

Computational Domain:

Details of the Volvo test case can be found in Refs. [1-2]. The combustor is a rectangular duct with a flameholder centered in the duct. The flameholder's cross section is a 40 mm equilateral triangle. The computational domain should consist of the dimensions shown in Figure 1 and the boundaries labeled in Figure 2:

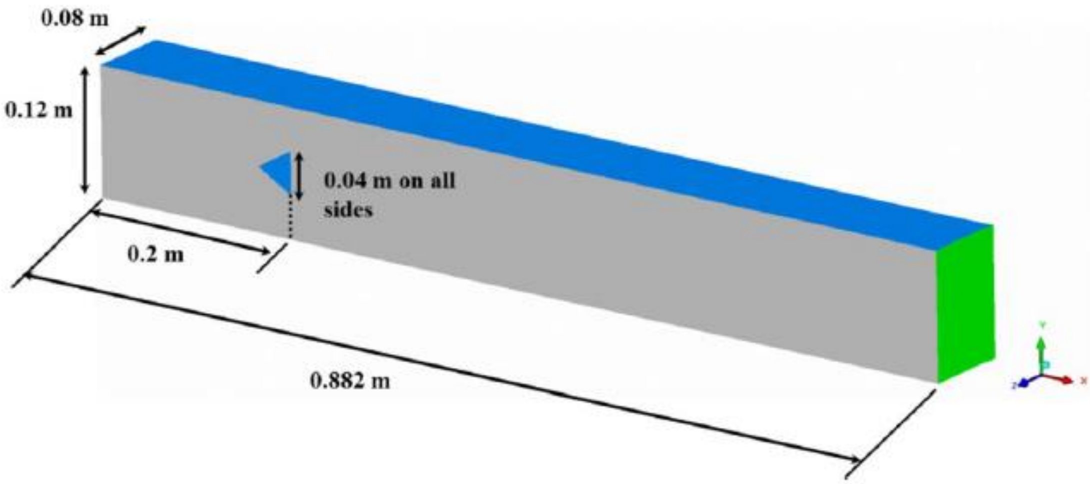

Figure 1. Computational domain dimensions for the Volvo test case.

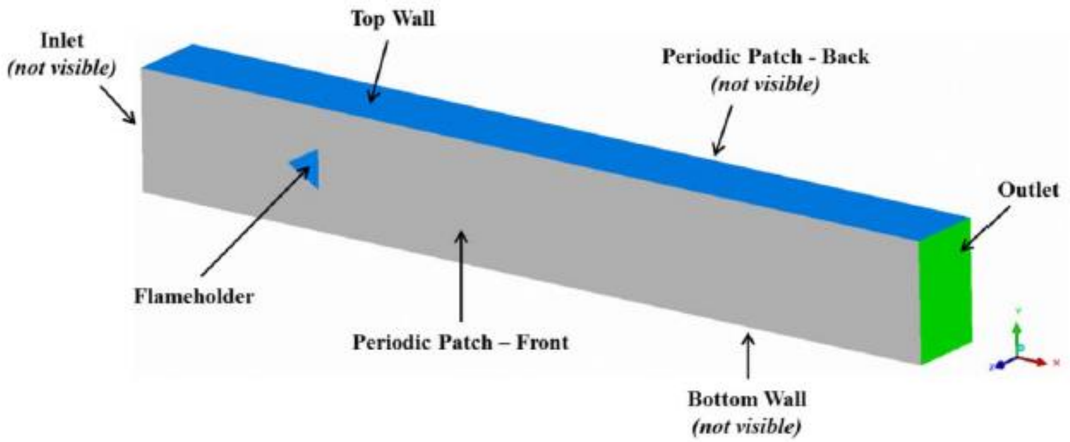

Figure 2. Volvo test case boundaries.

Table 1 summarizes the conditions to be simulated and considered for comparisons:

Table 1. Operating conditions to be simulated.

Fuel	Propane
Oxidizer	Air
Mass Flow Rate	0.2083 kg/s
Inlet Temperature	288 K
Equivalence Ratio	0.65

Boundary Conditions:

Please use the boundary conditions summarized below (reference Figure 2 for labels):

Inlet:

- Fixed mass flow rate of 0.2083 kg/s (adjusted for shortened domain depth and fuel flow rate)
- Fixed stagnation temperature = 288.2 K
- Zero inlet turbulence, i.e., no velocity fluctuations
- Bulk flow, without prescribed velocity profile
- Premixed propane-air at an equivalence ratio of 0.65

Top and Bottom Walls and Flameholder:

- No-slip
- Adiabatic

Front and Back Patches: periodic boundaries

Outlet: Fixed static pressure of 100kPa

All other boundary treatments such as characteristic variable extrapolation or zero-gradient variables must be explicitly summarized in the paper. Likewise, the use of modeled or resolved boundary layers is at the discretion of the modeler but should be described in the paper.

Grid:

The grids provided at the links below feature the recommended domain described in "Computational Domain" and are provided for your convenience. A sequence of coarse, medium and fine meshes are provided with approximate length-scale resolutions of 4 mm, 2 mm and 1 mm respectively in the flame region. If you choose to use these grids, please specify which grid(s) you used in your presentation of the results. If you do not use one of the grids below, please present and discuss your grid, including resolutions throughout the domain and the grid topology (e.g., the clustering of nodes near the bluff body shear layer). The intention is to enable interested participants to reproduce your mesh arrangement.

Grid convergence with a sequence of mesh resolutions should be demonstrated using the mean and RMS data provided in the section "Experimental Data." Thus, the mesh resolutions suggested are simply guidelines, and we recommend even finer resolutions if needed to achieve convergence. In addition to these comparisons, turbulence statistics (also specified below) should be presented at multiple grid resolutions to show convergence.

Volvo_Grids

Combustion Model and Mechanisms:

The chemical mechanism and turbulent combustion closure model, to include models that do not require a mechanism, can be selected at the discretion of the participant. However, please be sure to describe the model and any mechanisms in detail. Additionally, we recommend that you present an assessment of the chemical mechanisms used by comparing global properties of interest (e.g., laminar flame speed and ignition delay time) with experimental data or detailed kinetics results. Suggested mechanisms can be found below.

If you plan to use simple chemistry, we recommend the mechanism below from Ref. [3]:

$C_3H_8 + 3.5O_2 \rightarrow 3CO + 4H_2O$

$CO + 0.5O_2 \leftrightarrow CO_2$

The reaction rates are calculated using the following:

$$q_1 = A_1 \left(\frac{\rho Y_{C_3H_8}}{W_{C_3H_8}}\right)^{0.9028} \left(\frac{\rho Y_{O_2}}{W_{O_2}}\right)^{0.6855} exp\left(\frac{-E_1}{RT}\right)$$

$$q_2 = A_2 \left[\left(\frac{\rho Y_{CO}}{W_{CO}}\right)^{1.0} \left(\frac{\rho Y_{O_2}}{W_{O_2}}\right)^{0.5} - \frac{1}{K}\left(\frac{\rho Y_{CO_2}}{W_{CO_2}}\right)^{1.0}\right] exp\left(\frac{-E_2}{RT}\right)$$

where $A_1 = 2.0\text{x}10^{12}$cgs, $A_2 = 4.5\text{x}10^{10}$cgs, $E_1 = 3.3\text{x}10^4$cal/mol, and$E_2 = 1.2\text{x}10^4$cal/mol. The value of the equilibrium constant is given by Kuo in Ref [4].

If you plan to simulate this case with detailed chemistry, we recommend the UC San Diego mechanism [5]. The mechanism and associated thermophysical and transport properties files can be found at the link below:

http://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html

Turbulence Model Constants and Properties:

We recommend (but do not require) the use of standard values for turbulence model constants in order to facilitate comparisons between codes. For instance, if the model requires a turbulent Schmidt number, we recommend a value of 0.7.

Experimental Data:

Data have been extracted from the figures in the publicly available Volvo papers (NOTE: figure quality limited the precision of the data extracted). Text files containing the relevant data have been provided below for your convenience. Formatting details can be found in the header of each file.

Volvo_Exp_Data_Reacting_20160922

Volvo_Exp_Data_Non-Reacting_20160922

Required Results and Turbulence Statistics:

Participants are required to present data comparisons with the provided experimental data and detailed flowfield statistics as specified below. We further request that all data be presented for different grid sizes in order to test and verify grid convergence of the statistical data.

I. Nomenclature

φ = generic scalar (or vector component) value of interest

$\langle\varphi\rangle$ = mean (temporal) value of φ

φ' = fluctuation about the mean value of φ

U_{bulk} = bulk inlet velocity (17.3 m/s)

D = bluff body dimension (40 mm)

II. Values of Interest (φ)

Velocity components (u_x, u_y)
Temperature (T)
Species mass fractions (CO_2, CO)

III. Definition of Coordinate System

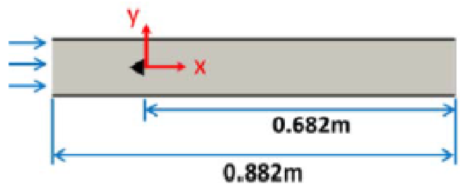

Figure 3. Coordinate system for Volvo case. The depicted plane corresponds to the z = 0 plane, which is parallel to and centered between the periodic patches of the computational domain.

IV. Experimental Data Comparisons – Axial and Transverse Profiles

Plot the following profiles of the values of interest (see Section II above) along with the corresponding experimental data, if available. NOTE: Not all experimental values of interest are available at every requested location.

1. **Mean – Transverse Profiles** (z/D = 0 and x/D = 0.375, 0.95, 1.53, 3.75, 8.75, 9.40, 13.75)
2. **Mean – Axial Profile** (z/D = 0, y/D = 0, and x/D = 0 to 10)
3. **Root Mean Square of Fluctuation – Transverse Profiles** (z/D = 0 and x/D = 0.375, 0.95, 1.53, 3.75, 8.75, 9.40, 13.75)

$$\varphi'_{RMS} = \sqrt{\left\langle (\varphi - \langle \varphi \rangle)^2 \right\rangle}$$

4. **Turbulence Intensity – Axial Profile** (z/D = 0, y/D = 0.0, and x/D = 0 to 10)

$$TI_{2D} = \frac{\sqrt{\left(u'_{x,RMS}\right)^2 + \left(u'_{y,RMS}\right)^2}}{U_{bulk}}$$

V. One-Point Temporal Statistics

The temporal statistics should be computed at the positions listed below (normalized by D):

(x/D, y/D, z/D) = (0.375, 0.0, 0.0); (0.95, 0.0, 0.0); (1.53, 0.0, 0.0); (3.75, 0.0, 0.0); (9.40, 0.0, 0.0)

(x/D, y/D, z/D) = (0.375, 0.5, 0.0); (0.95, 0.5, 0.0); (1.53, 0.5, 0.0); (3.75, 0.5, 0.0); (9.40, 0.5, 0.0)

(x/D, y/D, z/D) = (0.375, 1.0, 0.0); (0.95, 1.0, 0.0); (1.53, 1.0, 0.0); (3.75, 1.0, 0.0); (9.40, 1.0, 0.0)

1. **Temporal Correlations**

$$\varphi'(\vec{x}, t) = \varphi(\vec{x}, t) - \langle \varphi(\vec{x}, t) \rangle$$

$$\vec{x} = (x, y, z)$$

$$\rho(\vec{x}, \Delta\tau) = \frac{\langle \varphi'(\vec{x}, t)\varphi'(\vec{x}, t+\Delta\tau) \rangle}{\left\langle \varphi'(\vec{x}, t)^2 \right\rangle}$$

2. **Integral Time Scales**

$$\tau_I(\vec{x}) = \int_0^\infty \rho(\vec{x}, \Delta\tau) d\Delta\tau$$

VI. Grid Convergence

We request that all data be presented for a sequence of meshes of different resolutions in order to test and verify grid convergence of the statistical data.

References:

1. Sjunnesson A., Olovsson S. and Sjöblom B., "Validation Rig – A Tool for Flame Studies", *International Society for Air-breathing Engines Conference*, ISABE-91-7038, Nottingham, United Kingdom, 1991.
2. Sjunnesson A., Nelsson C and Max E., "LDA Measurements of Velocities and Turbulence in a Bluff Body Stabilized Flame", *Fourth International Conference on Laser Anemometry – Advances and Application*, ASME, Cleveland, OH, 1991.
3. Ghani, A., Poinsot, T., Gicquel, L., and Staffelbach, G. "LES of longitudinal and transverse self-excited combustion instabilities in a bluff-body stabilized turbulent premixed flame," Combustion and Flame, Vol. 162, 2015, pp. 4075-83.
4. Kuo, K. K. Principles of Combustion, John Wiley, New York, 1986.
5. "Chemical-Kinetic Mechanisms for Combustion Applications", San Diego Mechanism web page, Mechanical and Aerospace Engineering (Combustion Research), University of California at San Diego (http://combustion.ucsd.edu).

Recent SciTech Papers for this Case:

Cocks, P. A. T., Sankaran, V., and Soteriou, M. C. "Is LES of reacting flows predictive? Part 1: Impact of numerics," *51st AIAA Aerospace Sciences Meeting*, AIAA 2013-0170, Grapevine, TX, 2013.

Sardeshmukh, S. V., Huang, C., Harvazinski, M., Sankaran, V., and Anderson, W. "Impact of Chemical Kinetics Mechanisms on the Predictions of Bluff Body Stabilized Flames," *54th AIAA Aerospace Sciences Meeting*, San Diego, CA, 2016

Comer, A. L ., Huang, C., Rankin, B., Harvazinski, M., and Sankaran, V. "Modeling and Simulation of Bluff Body Stabilized Turbulent Premixed Flames," *54th AIAA Aerospace Sciences Meeting*, San Diego, CA, 2016