Proceedings of the Second Model Validation for Propulsion (MVP 2) Workshop

2018 AIAA Science and Technology (SciTech) Forum and Exposition
January 8 - 12, 2018
Kissimmee, Florida

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Abstract

The purpose of this report is to document the Proceedings of the Second Model Validation for Propulsion (MVP) Workshop which was held at the 2018 AIAA SciTech Forum from January 8 - 12 in Kissimmee, Florida. 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 2 Workshop was attended by approximately 50 researchers. There were seven technical papers and corresponding presentations at the workshop sessions representing contributions from 15 organizations and three countries. The workshop sessions consisted of two technical paper sessions focused on the Volvo bluff-body premixed flame validation case and one invited presentations session. The invited presentations session focused on a summary of outcomes from the MVP 2 Workshop, recent findings in the physics of reactive turbulence, interactions between turbulent combustion experiments and computations in relevant regimes, challenges facing embedded direct numerical simulations (DNS) of turbulent combustion, and the path forward for the MVP Workshop series. These proceedings summarize the objectives, final program, discussion topics, and conclusions for the MVP 2 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, University of Michigan
- Matthias Ihme, Stanford University
- Chiping Li, Air Force Office of Scientific Research
- Suresh Menon, Georgia Institute of Technology
- Joseph Oefelein, Georgia Institute of Technology
- Brent Rankin, Air Force Research Laboratory
- Vaidyanathan Sankaran, United Technologies Research Center
- Venkateswaran Sankaran, Air Force Research Laboratory

Objectives of MVP 2 Workshop

Technical papers featuring simulations of the Volvo bluff body test case were solicited. To align MVP 2 with the workshop series goals, the following topics were proposed as focus areas for technical paper submissions:

- Grid Convergence – Most MVP 1 participants were unable to obtain grid-independent results for the reacting Volvo bluff body test case. Participants were requested to focus on achieving grid-converged LES or DES solutions.
- High-Order Methods – The demonstration of higher-order methods and their potential merits on the provided test case were encouraged. A desired outcome was to gain insights into the impact of these methods on grid convergence and computational cost for a specified level of accuracy.
- Explicit Filtering – The application and development of explicit filtering to separate physical model errors from numerical errors and to enable more definitive statements about model accuracy were requested.

- Sensitivity Analyses– To aid in the identification of the largest sources of error and to guide potential future experiments, sensitivity studies of the boundary conditions were suggested as useful technical paper topics. Additionally, sensitivity analyses of model parameters and choices were encouraged to help identify leading order effects on simulation accuracy.

Invited sessions featured an MVP 2 summary and the solicitation of feedback for future workshops. Additionally, overviews of current activities in turbulent combustion research, as well as a more detailed talk on embedded DNS, were presented with the goal of identifying ways of better aligning the workshop with current turbulent combustion research efforts.

Planning for MVP 3 Workshop

Based on workshop feedback, the dates and venue for the Third Model Validation for Propulsion Workshop are under consideration. Options include the 2019 AIAA SciTech Forum and the 2019 AIAA Propulsion and Energy Forum and Exposition. Conducting the workshop during the weekend before the conference is also being considered. The exact dates and times of the workshop will be determined over the coming months.

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 2 WORKSHOP

Technical Papers Session I

Monday, January 8, 2018, 9:30AM-10:30AM

Chaired by Adam Comer and Joseph Oefelein

- **C. Fureby**, "The Volvo Validation Rig – A Comparative Study of Large Eddy Simulation Combustion Models at Different Operating Conditions," AIAA-2018-0149.
- **V. Hasti**, J.P. Gore, G. Kumar, S. Liu, "Comparison of Premixed Flamelet Generated Manifold Model and Thickened Flame Model for Bluff Body Stabilized Turbulent Premixed Flame," AIAA-2018-0150.

Technical Papers Session II

Monday, January 8, 2018, 2:00PM-4:30PM

Chaired by Brent Rankin and Venke Sankaran

- **A.L. Comer**, S.V. Sardeshmukh, B.A. Rankin, M.E. Harvazinski, "Effects of Turbulent Combustion Closure on Grid Convergence of Bluff Body Stabilized Premixed Flame Simulations," AIAA-2018-0439.

- **H. Wu**, P.C. Ma, Y. Lv, M. Ihme, "Lyapunov exponent and Wasserstein metric as validation tools for assessing short-time dynamics and quantitative model evaluation of large-eddy simulation," AIAA-2018-0440.
- **T.P. Gallagher**, V. Sankaran, "Explicitly filtered LES of Bluff Body Stabilized Flames," AIAA-2018-0441.
- B. Rochette, O. Vermorel, **L.Y. Gicquel**, T. Poinsot, D. Veynante, "ARC versus two-step chemistry and third-order versus second-order numeric schemes for Large Eddy Simulation of the Volvo burner," AIAA-2018-0442.
- **G.V. Candler**, A. Kartha, P. Subbareddy, P. Dimotakis, "LES of the Volvo Combustion Experiment with an Ignition-Delay Variable," AIAA-2018-0443.

Invited Presentations Session and Discussion
Tuesday, January 9, 2018, 9:30AM-12:30PM

- **A. Comer**, "Summary of MVP-II"
- **A. Steinberg**, "Recent Findings in the Physics of Reactive Turbulence"
- **B. Rankin**, "Interactions between Experiments and Computations for Turbulent Combustion Research in Relevant Regimes"
- **A. Kerstein**, "Challenges facing embedded DNS of turbulent combustion and strategies for addressing them"
- **V. Sankaran**, "Model Validation for Propulsion Workshop: Looking Ahead"

SUMMARY OF MVP 2 WORKSHOP

Volvo Bluff-Body Premixed Flame Validation Case

Two technical paper sessions were organized in which seven 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** – Non-reacting simulation results generally demonstrate grid convergence across all mean and root mean square statistics. Reacting simulations require significantly higher mesh resolutions to demonstrate convergence of the mean and root mean square statistics, but multiple groups were still able to show reasonable levels of reacting solution convergence with these statistics. It should be noted that very few groups showed PDFs in their grid convergence studies, and this metric might show discrepancies in cases in which mean and root mean square statistics agree. Laminar combustion closure demonstrated significant grid sensitivity, whereas the use of certain turbulent combustion closure models appeared to reduce this sensitivity and aid grid convergence. Explicit filtering was demonstrated to provide grid independence at a much lower grid resolution than implicitly filtered approaches.

- **Flame Topology** – A variety of flame topologies were observed across the simulation results. Due to a lack of standardization, it is difficult to ascertain the source of these differences. Moreover, a lack of high speed planar imaging makes it difficult to know the actual flame's shape and dynamics. Potential discrepancies include the implementation and nature of selected boundary conditions, the nature of the numerical methods employed, and the turbulent combustion model and related inputs.

- **Explicit Filtering** – A novel and computationally feasible explicit filtering approach was demonstrated on the Volvo test case. By fixing the filter width, the method demonstrated grid convergence at much coarser resolutions than previously reported. This approach represents a promising path forward for physical model comparisons that are independent of numerical error and computationally efficient.

- **New Metrics for Comparison** – Applications of the Lyapunov exponent and the Wasserstein metric to the test case demonstrated significant promise in better quantifying the difference between simulations. Through the Lyapunov exponent, the dynamics of a simulation can be expressed as a single value and compared with that of other simulations for grid convergence assessment, model and code comparisons, or other comparisons. Similarly, the Wasserstein metric quantifies the difference between two PDFs using a single value, enabling a more rigorous comparison of two datasets than visual inspection. Since PDFs contain all the statistical information for a given quantity, the Wasserstein metric offers a much more thorough assessment than current approaches based on first and second moment statistical comparisons. These two metrics are appealing candidates for future workshop comparisons.

- **Numerics** – Three of the groups investigated the impact of numerics on the solution. All studies noted an impact from changes in numerical methods, but one group noted more significant effects, which were possibly attributable to the use of a coarser grid. It was demonstrated that the use of upwinding can have a dramatic effect on the solution, which can exceed the impact of changing the order of accuracy of the method. One group applied upwinding throughout the domain and noted the impact was adverse, but results from a different group and code that selectively applied upwinding for stability suggested that the effects were not necessarily negative.

- **Physics and Chemistry Modeling** – Turbulent combustion closure models were shown to influence the grid sensitivity of the solution. Additionally, for the same grid resolution, different turbulent combustion models sometimes produced significantly different results, as expected. However, it is often unclear if these differences are due to a lack of grid convergence (i.e., an effect produced by the interaction of the numerical errors and the model) or if the differences can be attributed to the actual behavior of the models at grid-converged resolutions. In spite of this difficulty, comparisons at resolutions that are not grid-converged are still informative as LES is often conducted at such resolutions due to computational cost. Furthermore, if two models converge to the DNS solution as the grid is refined, then the grid-converged comparison should reveal no difference. Thus, the comparisons of interest for this scenario would be conducted at coarser resolutions in order to ascertain model performance. Within this line of inquiry, multiple groups applied thickened flame models, enabling some analysis of the performance of this model across multiple codes.
  Global chemical kinetics provided reasonable predictions of many mean and root mean square statistics. In fact, reasonable mean CO predictions were even made with a four-step

mechanism. However, skeletal mechanisms are required to capture details, such as temperature PDFs and heat release contours.

Workshop Discussion

Many suggestions for future MVP Workshops and next steps related to the validation case(s) were made throughout the workshop sessions. The suggestions are summarized in this section.

- **Validation Cases**
  - **Bluff-body Premixed Flames** - 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. It was suggested that transitioning from the Volvo bluff-body case to the AFRL bluff-body case is a logical next step considering that new experimental data sets are actively being acquired.
  - **Operating Conditions** - Evaluating the capability of simulations to predict trends over multiple stationary combustion conditions would be a useful next step for additional validation cases. The introduction of additional operating conditions and an assessment of trend prediction capability would be of interest to industry.
  - **Supersonic Cavity-Stabilized Flames** - Supersonic cavity-stabilized flames may serve as a reasonable additional validation case for future workshops considering that experimental data sets are actively being acquired.
  - **Unit Physics Problems** - Developing a framework for model evaluation may be achieved more efficiently on smaller unit physics problems (e.g., freely propagating premixed flame). For the unit physics problem, the objectives would be to (a) verify that DNS results can be achieved with the code and (b) observe the effects of the numerics on the solution as the mesh is coarsened to LES resolutions.

- **Boundary Conditions**
  - **Non-Reflective Boundary Conditions** - The details in the implementation of non-reflecting boundary conditions could be affecting the acoustics of the simulations and thus the solutions observed. Additionally, it was mentioned that we may be observing significant improvement in convergence this year due to the common implementation of non-reflecting boundary conditions.
  - **Exit Boundary Conditions** - Incorporating an exhaust duct downstream of the combustion chamber could be a useful step in reducing sensitivity to the outlet boundary condition.
  - **Inlet Boundary Conditions** - Inflow turbulence was mentioned as a potential improvement to the boundary condition specifications that could improve agreement with the experiment. However, it is not clear that the time is appropriate to pursue more involved inlet boundary conditions considering that different groups have not converged on a result nor have they eliminated numerical error.

- **Models**
  - **Combustion Models** - Separating the effects of numerical errors and models is challenging as certain combustion models enable grid convergence (especially thickened flame) to be achieved more easily. More standardization of modeling

    approaches across the groups could aid in identifying leading order effects. Grouping the presentations by models used might also facilitate comparisons.
  - **Chemistry Models** - The limitations associated with using global kinetics models were pointed out, and it was suggested that we consider implementing more advanced chemistry or at least utilize an improved global mechanism. However, it is not clear that the time is appropriate to move towards more expensive chemistry models given the remaining issues with numerical errors.

- **Future Metrics and Comparisons**
  - **Additional Metrics -** Additional metrics (e.g., POD, PSD) are needed for comparing unsteady flow and flame dynamics to help understand the wide variety of results observed and better quantify their differences.
  - **Post-Processing Tools** - Each research group should be provided with the same post-processing code to minimize differences in how the metrics (e.g. POD, PSD, Wasserstein metric, or Lyapunov exponent) are computed if new metrics are utilized in future workshops.
  - **Comparison of Measurements and Computations** – The general consensus was that there needs to be a new bluff-body premixed flame experiment with dynamic data made publicly available.
  - **Commercial Codes** – Obtaining more results from commercial codes would be useful from an industry perspective since those are the most commonly used codes.
  - **Mesh Generation** – Grid synchronization received mixed reception. It was stated that certain codes are more sensitive to certain grid quality metrics than others; therefore, finding a grid acceptable for all codes would be difficult. It was suggested that the grid generation process was inherently tied to the modeling process of a given code.
  - **Uncertainty Quantification** - Given the motivation of the workshop to look at more realistic problems, we need to incorporate more systematic uncertainty quantification studies. As problems increase in complexity, the level of uncertainty on a number of inputs and parameters grows.

- **Workshop Format and Organization**
  - Conducting the workshop on the weekend before the AIAA SciTech conference was suggested. The weekend workshop format would (a) afford more time for discussion and (b) enable more detailed dialog that is needed to identify the sources of discrepancies in the results from different codes.
  - One session could be held during the AIAA SciTech conference to communicate the outcomes of the weekend workshop and next steps for a future workshop with the broader community.

CONCLUSIONS FOR MVP 2 WORKSHOP

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

- The influence of numerical schemes on reacting LES results was clearly demonstrated, reinforcing the need for grid independent results that separate physical model errors from numerical errors. Multiple groups were able to show reasonable grid convergence for mean and root mean square statistics of the reacting flow with implicitly filtered LES. These results were obtained on meshes with tens of millions of cells and through the use of turbulent combustion closure models. PDFs were only sporadically plotted, so grid convergence could not be assessed on a more detailed and statistically rigorous basis. Future efforts should move beyond the mean and root mean square values through the use unsteady metrics (e.g., PSD, POD, and/or Lyapunov exponent) and PDF-based comparisons—perhaps, via the Wasserstein metric—to assess grid convergence and to evaluate models.

- In spite of improved convergence on mean and root mean square statistics, significant variation remains in the flame topology predicted by the many groups, even on the finest grids. Unfortunately, a lack of standardization of the boundary conditions and models made it difficult to determine the source of these discrepancies. Future workshops should consider requesting greater standardization in modeling approaches and possibly grouping the papers by selected models in order to facilitate comparisons.

- A computationally tractable explicit filtering approach was developed and demonstrated on the Volvo bluff body test case. Preliminary tests suggest that grid independent solutions can be obtained on coarser grids and with significantly less computational cost than grid independent solutions from implicitly filtered LES. This approach represents a promising path forward for demonstrating grid convergence and evaluating physical models independent of the code and its numerical schemes.

- Global chemical kinetics can provide reasonable predictions of many mean and root mean square statistics for the Volvo test case. However, skeletal mechanisms are required to capture details, such as temperature PDFs and heat release contours.

APPENDIX: MVP 2 Validation Case Guidelines

2nd Model Validation for Propulsion Workshop Validation Case

Contact Information: Adam Comer (aiaa.mvpws@gmail.com)

Last Updated: 19 April 2017 at 1401EST

Abstract Submission Guidelines

Please complete the following steps to submit an abstract for the MVP Workshop and to ensure that the paper is placed in the correct session:

- Submit abstract via the SciTech 2018 website
- Select "Propellants and Combustion" as the topic
- Select "Turbulent Combustion" as the subtopic
- Send an email to aiaa.mvpws@gmail.com with the submission control ID, abstract title, authors, and affiliations

We anticipate that the best papers from this workshop may be considered for publication in a special series of the Journal of Power and Propulsion.

Pre-Workshop Conference Call Discussions

Prior to SciTech 2018, we plan to hold online conferences to discuss the test cases and preliminary results. If you received the MVP-1 proceedings via email, then you will receive the invitations to these events. Otherwise, please email aiaa.mvpws@gmail.com to ensure that you receive an invitation or monitor the MVP website for details.

1.0 Validation Cases Overview

The validation cases for the MVP 2 Workshop are based on the bluff-body-stabilized premixed flame experiments conducted by Volvo. Participation in the workshop is open, and participants can contribute by performing reacting flow simulations of the selected cases. Two validation cases have been selected for the MVP 2 Workshop:

- **Required Case** – The required case is the Volvo bluff-body-stabilized premixed propane/air flame with an **inlet temperature of 288 K**. The required case is similar to the one used for the MVP 1 Workshop, and it is being repeated for the MVP 2 Workshop primarily because grid convergence was not demonstrated by most simulations performed for the MVP 1 Workshop. The required case for the MVP 2 workshop includes updated recommendations for grid resolution, operating and boundary conditions, model settings, and required results. Red text is utilized to indicate the updated recommendations that are being made for the MVP 2 Workshop.
- **Optional Case** – The optional case is the Volvo bluff-body-stabilized premixed propane/air flame with an **inlet temperature of 600 K**. The optional case is selected as an initial step towards evaluating the capability of different modeling and simulation approaches to accurately capture trends in relevant operating conditions such as density ratios across the flame.

Several specific areas of interest have been identified based on discussions during the MVP 1 Workshop. Interested participants are encouraged to use the validation case to explore one or more of the following areas:

- **Grid Convergence** – There was consensus from the MVP 1 Workshop that achieving grid convergence is imperative to make valid assessments of modelling and simulation results.
- **High-Order Methods** – There was consensus from the MVP 1 Workshop that high-order methods are useful (a) to enable more computationally efficient simulations given the same accuracy requirements and (b) to reduce numerical dissipation and dispersion errors.
- **Explicit Filtering** – There was consensus from the MVP 1 Workshop that explicit filtering is useful (a) to separate physical model errors from numerical errors and (b) to enable more definitive statements about model accuracy.
- **Sensitivity Analyses of Boundary Conditions –** There was consensus from the MVP 1 Workshop that computational sensitivity analyses of boundary conditions are useful (a) to identify the largest sources of error and (b) to guide potential future experiments. Several examples include examining the sensitivity of the simulation results to inlet turbulence intensity boundary condition, flameholder and wall thermal boundary condition, and exit boundary condition.
- **Sensitivity Analyses of Modeling Approaches –** There was consensus from the MVP 1 Workshop that computational sensitivity analyses of model parameters are useful for identifying leading order effects. Several examples include examining the sensitivity of the simulation results to chemistry (i.e., global vs. skeletal vs. detailed), turbulence closure models, and turbulent combustion closure models.
- **Other Areas** – Interested participants are encouraged to discuss with the organizing committee other areas which use the validation case to contribute to one or more objectives of the MVP Workshop.

The computational domain and grids, operating and boundary conditions, recommended model settings, experimental data, and required results are described in the following sections. The guidelines are provided to ensure consistency among the simulations and to facilitate code and model comparisons. The guidelines are not necessarily the best modelling and simulation choices, and the organizing committee does not intend to imply that there is consensus regarding these choices.

2.0 Computational Domain

The Volvo bluff-body-stabilized premixed flame experimental arrangement consists of a flameholder centered in a rectangular duct. The flameholder 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. Additional details of the Volvo bluff-body-stabilized premixed flame can be found in Refs. [1-2].

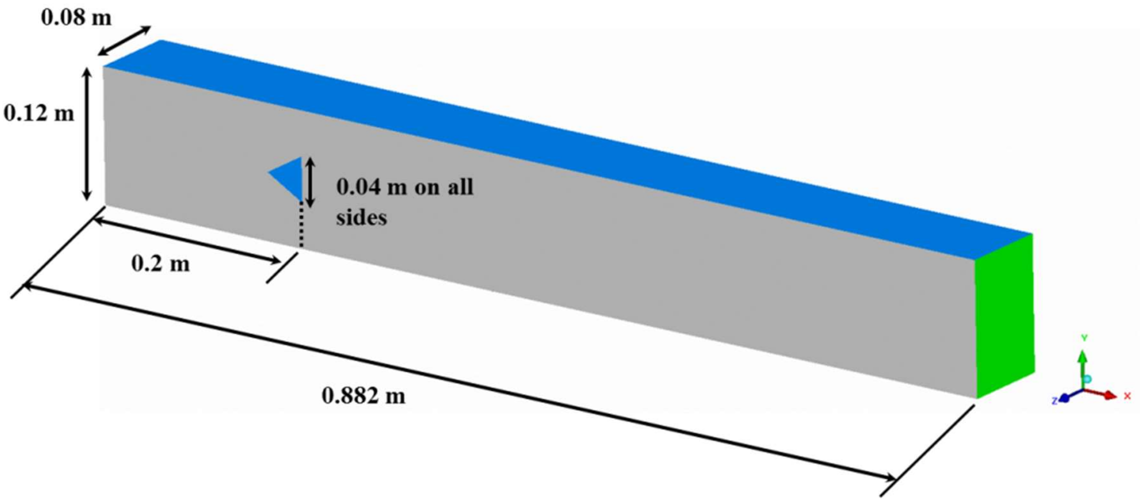

Figure 1. Computational domain for the Volvo bluff-body-stabilized premixed flame.

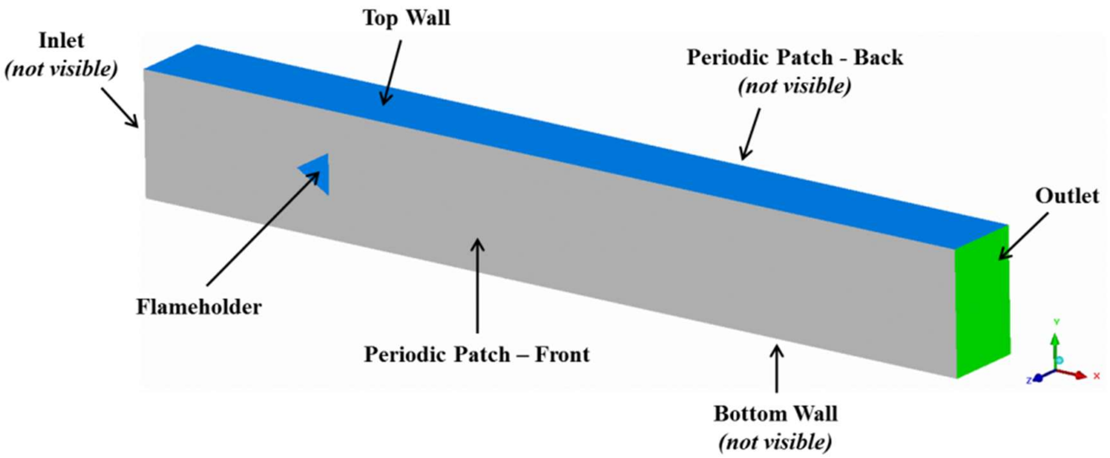

Figure 2. Boundaries for the Volvo bluff-body-stabilized premixed flame.

3.0 Computational Grids

Grid convergence with a sequence of mesh resolutions should be demonstrated. In addition to overall cell count, the details of grid topology (e.g., the use of clustering and associated growth rates) and the overall approach to refinement (e.g., preferentially refining certain regions or directions) should be provided in your paper. The intention is to enable interested participants to reproduce your grid arrangement. Additionally, more rigorous methods of achieving grid convergence/independence, including the use of explicit filtering, are highly encouraged.

As a general guideline, key parameters from a successful grid convergence study presented at MVP-1 are shown in Table 1. The parameters suggest the use of clustering to capture critical regions of the flow, while minimizing overall cell count. Note that the cell counts are for a spanwise domain depth of four bluff dimensions (4D), whereas we have recommended a shorter domain depth (2D) in consideration of computational cost (see Section 2.0).

Participants are expected to demonstrate grid convergent LES solutions using a set of at least 3 progressively refined meshes. Grid convergence is defined here as a consistent convergence to the same answer (even if it is different from the target experimental data). We understand that that there may be fundamental difficulties with ensuring consistent results in the LES context. Therefore, unique approaches designed to shed light on these issues and/or demonstrate grid convergence for LES are also welcome. An example of such an approach is the use of constant LES filter-width (i.e., explicit filtering) for the sequence of meshes.

Table 1. Summary of approximate spatial resolutions from a successful MVP-1 grid convergence study Ref [3]. The cell counts are for a depth of 4 bluff body dimensions.

Grid Description	Min Cell Size (mm)	Mean Cell Size (mm)	Max Cell Size (mm)	Total Grid Size (M cells)
Coarse	0.5	1.3	2.7	3.7
Medium	0.4	1.0	2.1	12.5
Fine	0.3	0.7	1.6	29.5
Very Fine	0.2	0.5	1.1	99.6

4.0 Operating Conditions

Table 2 summarizes the operating conditions for the Volvo bluff-body-stabilized premixed flame validation case.

Table 2. Operating conditions for the Volvo bluff-body-stabilized premixed flame validation case. *The mass flow rate has been adjusted to account for the reduced depth of the computational domain.

Operating Condition	Required Case	Optional Case
Premixed Fuel / Oxidizer	Propane / Air	Propane / Air
Equivalence Ratio	0.62	0.62
Pressure	100 kPa	100 kPa
Inlet Temperature	288 K	600 K
Mass Flow Rate	0.2079 kg/s *	0.2079 kg/s *
Bulk Velocity	17.6 m/s	36.6 m/s
Bulk Mach Number	0.053	0.077
Bulk Reynolds Number	47,000	28,000
Unburned / Burned Density Ratio	5.9	3.1

5.0 Boundary Conditions

Table 3 summarizes the boundary conditions for the Volvo bluff-body-stabilized premixed flame validation case. All other boundary treatments should be described in detail in the paper and presentation.

Table 3. Boundary conditions for the Volvo bluff-body-stabilized premixed flame. *The mass flow rate has been adjusted to account for the reduced depth of the computational domain.

Boundary Condition	**Required Case**	**Optional Case**
Inlet Premixed Fuel / Oxidizer	Premixed Propane / Air	Premixed Propane / Air
Inlet Equivalence Ratio	0.62	0.62
Inlet Stagnation Temperature	288 K	600 K
Inlet Mass Flow Rate	0.2079 kg/s	0.2079 kg/s
Inlet Velocity Profile	Uniform Steady Flow	Uniform Steady Flow
Inlet Turbulence Intensity	0 %	0 %
Flameholder Surface Temperature	Adiabatic	Adiabatic
Flameholder Surface Velocity	No-Slip	No-Slip
Top and Bottom Wall Temperature	Adiabatic	Adiabatic
Top and Bottom Wall Velocity	No-Slip	No-Slip
Front and Back Patches	Periodic	Periodic
Outlet Static Pressure	Characteristic/ Transmissive BC recommended (Target P = 100 kPa, describe/ provide any tuned parameters)	Characteristic/ Transmissive BC recommended (Target P = 100 kPa, describe/ provide any tuned parameters)

6.0 Chemical Mechanisms

Specific chemical mechanisms are recommended to ensure consistency among the simulations and to facilitate code and model comparison. Table 4 summarizes the recommended global, skeletal, and detailed chemical mechanisms for propane / air.

Table 4. Summary of recommended chemical mechanisms for propane / air.

Mechanism	**Reactions**	**Species**	**Reference**
Global	2	5	Ghani et al. [3]
Skeletal	66	24	Zettervall et al. [4]
Detailed	235	50	UCSD [5]

For global chemistry, the mechanism from Ref. [4] is recommended. The global chemical mechanism is described in more detail at the following link (Note: The link below features a corrected activation energy due to an error in Ref. [4]):
https://community.apan.org/wg/afrlcg/mvpws/p/global-mech-propane

For skeletal chemistry, the mechanism from Ref [5] is recommended. The skeletal chemical mechanism can be found at the following link:
http://doi.org/10.1016/j.combustflame.2016.12.007

For detailed chemistry, the UC San Diego mechanism from Ref. [6] is recommended. The detailed chemical mechanism, thermophysical properties, and transport properties can be found at the following link:
http://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html

7.0 Turbulence and Turbulent Combustion Models

The turbulence and turbulent combustion models can be selected at the discretion of the participant. The use of standard values for turbulence model constants is recommended in order to facilitate comparisons between codes. For instance, if the model requires a turbulent Schmidt number, a value of 0.7 is recommended. Based upon the results of MVP-1, the use of a turbulent combustion closure can facilitate grid convergence and is recommended for this session.

8.0 Experimental Data

Experimental data from the non-reacting and reacting bluff-body experiments conducted by Volvo [1-2] can be downloaded from the links listed below. The data have been extracted from the figures in the publicly available papers [1-2,5] describing the experiments and providing simulation comparisons. Please note that the figure quality limited the precision of the extracted data. Formatting details can be found in the header of each file.

Volvo_Exp_Data_Non-Reacting_20160922.zip
Volvo_Exp_Data_Reacting_20160922.zip
Volvo_Exp_Data_Reacting_600K – Not Yet Available

9.0 Required Results

Participants are required to present data comparisons with the provided experimental data and detailed flowfield statistics as described in this section. All results should be presented for a sequence of meshes with different spatial resolutions in order to evaluate grid convergence of the results. Although the requisite data were not reported in every paper, a rough estimate of the flow through times (based on domain length and cold bulk velocity) used in MVP-1 were as follows: 3-5 flow through times for the initial transient and an additional 3-5 flow through times for sampling statistics. Papers presenting a more precise and reliable method of assessing temporal convergence are encouraged.

9.1 Nomenclature and Definition of Coordinate System

Nomenclature is listed Table 5, and the coordinate system is defined in Figure 3.

Table 5. List of nomenclature.

φ	generic scalar (or vector component) value of interest
$\langle\varphi\rangle$	mean (temporal) value
φ'	fluctuation about the mean value
U_{bulk}	bulk inlet velocity
D	bluff-body dimension (40 mm)

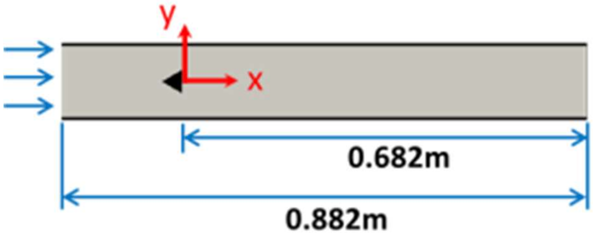

Figure 3. Definition of coordinate system for the Volvo bluff-body-stabilized premixed flame. The figure depicts the z = 0 plane, which is parallel to and centered between the periodic patches of the computational domain.

9.2 Values of Interest (φ)

- Velocity components (u_x, u_y)
- Spanwise Vorticity (ω_z)
- Temperature (T)
- Species mass fraction of CO

9.3 Instantaneous and Time-Averaged Distributions

Plot several instantaneous distributions and the time-averaged distribution of vorticity and temperature for the z/D = 0 plane.

9.4 Experimental Data Comparisons

Plot the following profiles of the values of interest along with the corresponding experimental data.

- **Mean – Transverse Profiles:**
  - 288 K Case – (u_x, u_y): z/D = 0 & x/D = 0.375, 0.95, 1.53, 3.75, 9.40
  - 288 K Case – (T): z/D = 0 & x/D = 0.95, 3.75, 8.75, 9.40, 13.75
  - 288 K Case – (CO): z/D = 0 & x/D = 3.75, 8.75, 13.75
  - 600 K Case – (u_x, u_y): z/D = 0 & x/D = 0.95, 3.75, 9.40
  - 600 K Case – (T): z/D = 0 & x/D = 0.95, 3.75, 9.40
  - 600 K Case – (CO): z/D = 0 & x/D = 0.95, 3.75, 9.40

- **Mean – Axial Profile of u_x Only:** (z/D = 0, y/D = 0, and x/D = 0 to 10)

- **RMS – Transverse Profiles:**
  - 288 K Case – (u_x, u_y): z/D = 0 & x/D = 0.375, 0.95, 1.53, 3.75, 9.40
  - 288 K Case – (T): z/D = 0 & x/D = 0.95, 3.75, 9.40
  - 600 K Case – (u_x, u_y): z/D = 0 & x/D = 0.95, 3.75, 9.40
  - 600 K Case – (T): z/D = 0 & x/D = 0.95, 3.75, 9.40

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

- **Turbulence Intensity – Axial Profile:** (z/D = 0, y/D = 0.0, & x/D = 0 to 10)

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

9.5 Probability Density Functions

Plot probability density functions of temperature at the following locations on the z/D = 0 plane.

- **Axial Positions** (x/D = 0.95, 3.75, 9.40)
- **Transverse Positions** (y/D = 0, 0.5)

10.0 References

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