4th Model Validation for Propulsion Workshop Overview and Validation Case

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*Emphasis items are in red text.

1 MVP Workshop Overview

The Model Validation for Propulsion (MVP) 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. Past MVP workshops have focused on bluff-body premixed flame validation cases and have featured invited sessions on a broad range of topics in turbulent reacting flows. 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.

Findings, accomplishments, and outstanding challenges from past MVP workshops are discussed in the MVP proceedings.

2 MVP 4 Organization and Logistics

Please read this section carefully to find key deadlines, requirements, and travel considerations.

2.1 Pre-SciTech 2019 MVP 4 Workshop

The workshop will be held in Orlando, FL, on Sunday, 5 January 2020, prior to the AIAA SciTech 2020 workshop. The exact location will be announced at a later date; venues close to or within the Hyatt Regency Orlando (SciTech site) will be prioritized.

Technical presentations at the workshop must be based on the Air Force Research Laboratory (AFRL) validation case and apply the unsteady metrics outlined in this document. To be considered for a technical presentation slot, a one-paragraph (minimum) abstract describing the presentation and objectives must be submitted to aiaa.mvpws@gmail.com by 1 August 2019, 8PM EST. These abstracts will be reviewed by the organizing committee, and the submitter will be notified by 31 August 2019. Full papers are no longer required for participation in the MVP workshop, but the presentations will *not* be part of the AIAA SciTech proceedings unless you also follow the SciTech submission process for your MVP contribution. Submitting your MVP work as a technical paper to SciTech 2020, in addition to the workshop, and providing an additional SciTech presentation are highly encouraged but not required.

2.2 MVP 4 Workshop Technical Paper Session(s) at SciTech 2020 (OPTIONAL)

Although a technical paper submission to SciTech 2020 is no longer an MVP workshop requirement, you are highly encouraged to submit your MVP contribution to SciTech 2020. To ensure your SciTech paper and presentation are placed in an appropriate session, please complete the following steps:

- Submit abstract via the SciTech 2020 website by the SciTech deadline of 11 June 2019, 8PM EST, USA
- Select "Propellants and Combustion" as the topic
- Select "Turbulent Combustion" as the sub-topic
- Send an email to aiaa.mvpws@gmail.com with the submission control ID, abstract title, authors, and affiliations
- Submit your technical paper by the required deadline of 2 December 2019, 8PM EST, USA

2.3 Registration Process for Pre-SciTech 2020 MVP 4 Workshop

Registration is required to attend the Pre-SciTech 2020 MVP 4 Workshop for planning purposes. Priority will be given to those working on topics directly related to one or more objectives of the MVP Workshop series as space may be limited. Please register for the Pre-SciTech 2020 MVP 4 Workshop by sending an email to aiaa.mvpws@gmail.com by 1 October 2019. Please include "MVP 4 Registration" in the subject line and include your name, affiliation, and email address in the email.

2.4 MVP 4 Workshop Overview Session at SciTech 2020

Even if you are not able to participate in the MVP Workshop on Sunday, please consider attending the invited session during SciTech 2020. This session will feature invited talks on topics relevant to the workshop objectives. The exact time and room for this session will be assigned at a later date.

3 MVP 4 Focus Area

The workshop is soliciting presentations featuring simulation results on the AFRL test case presented in Section 4 and based on the application of the unsteady metrics outlined in Section 5. The focus of MVP 4 is the application of the metrics in Section 5 with the goal of fostering a community effort to explore the utility of these metrics and to gain insights beyond those provided by mean and RMS statistics. We encourage the use of these metrics to compare simulation results with experimental data (see Section 6) and/or to perform numerical studies to include grid convergence, explicit filtering, high-order methods, sensitivity analyses of boundary conditions, sensitivity analyses of modeling approaches, or other areas (see past MVP proceedings and the MVP 3 guidance for summaries of findings on these topics).

4 MVP 4 Validation Case - AFRL Bluff-Body Stabilized Turbulent Premixed Flame Validation Case

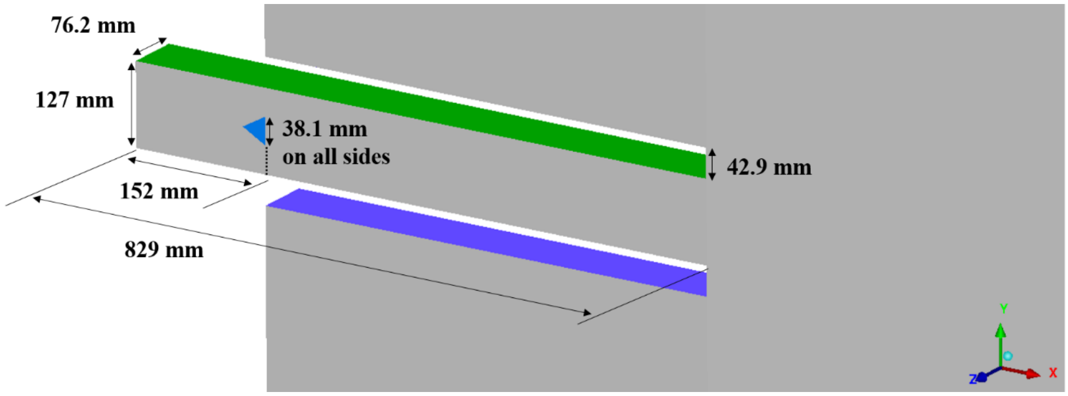
The computational domain and grids, operating and boundary conditions, experimental data, required results, and suggested model settings are described in the following sections. The guidelines are provided to ensure consistency among simulations and to facilitate code and model comparisons. The guidelines 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. Two conditions have been selected for the AFRL bluff-body-stabilized turbulent premixed flame:

- **Required Condition**: Inlet temperature of 310 K.
- **Optional Condition:** Inlet temperature of 600 K. The optional case is selected to assess the capability of different modeling and simulation approaches to capture trends in relevant operating conditions such as density ratios across the flame.

Case-specific guidance can be found in this section, and general modeling guidance can be found in Section 7.

4.1 Computational Domain

The AFRL bluff-body-stabilized turbulent premixed flame experimental arrangement consists of a flameholder centered in a rectangular duct. The flameholder cross section is a 38.1 mm equilateral triangle. The premixed fuel and air enter through a choked perforated plate, and the combustor exhausts to an atmospheric pressure environment. A rectangular exit domain is recommended. The computational domain should consist of the dimensions shown in Figure 1 and the boundaries labeled in Figure 2. In previous workshops, the simulation of the exhaust was not recommended, but sensitivities to the exit boundary condition have been noted and warrant a more realistic treatment of the exit. To mitigate these sensitivities, the inclusion of the exhaust and, in turn, placement of the exit boundary conditions far from the domain of interest are recommended. Please note that these recommendations are not intended to discourage the investigation of other methods of modeling the exit and associated sensitivity analyses with respect to various approaches. The use of grid stretching in the exhaust to reduce computational cost and to minimize reflections from the outlet is also suggested.



(a)

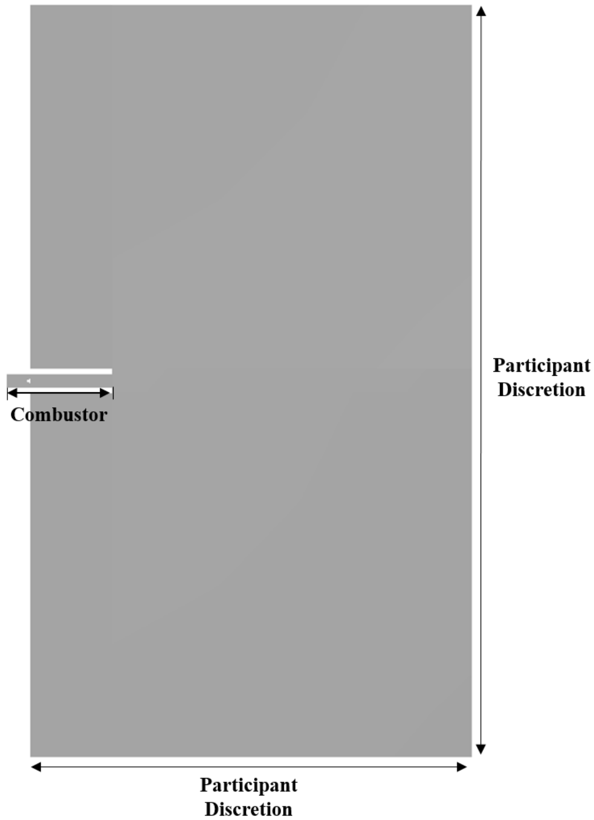


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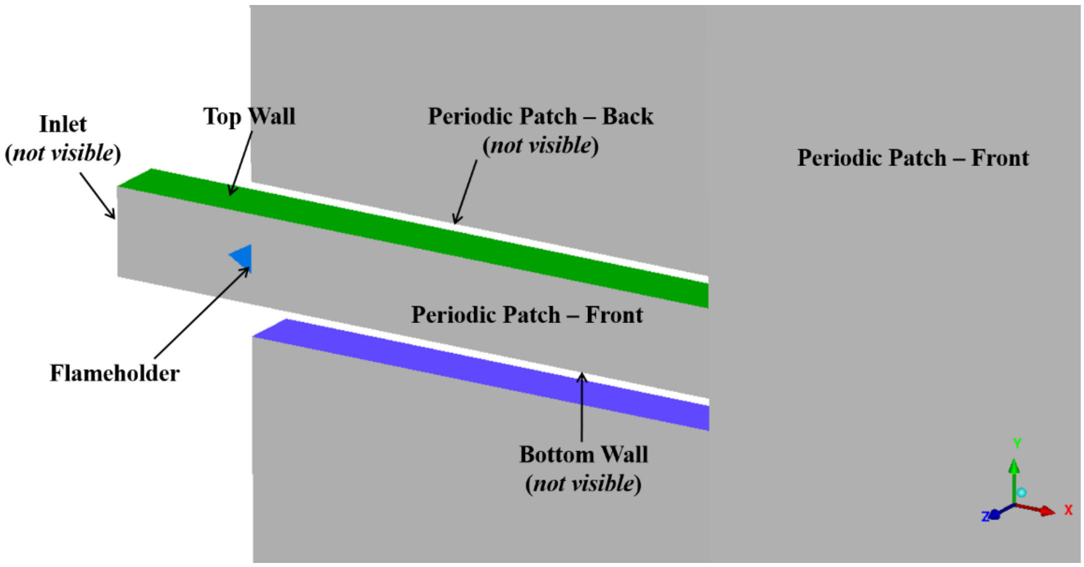
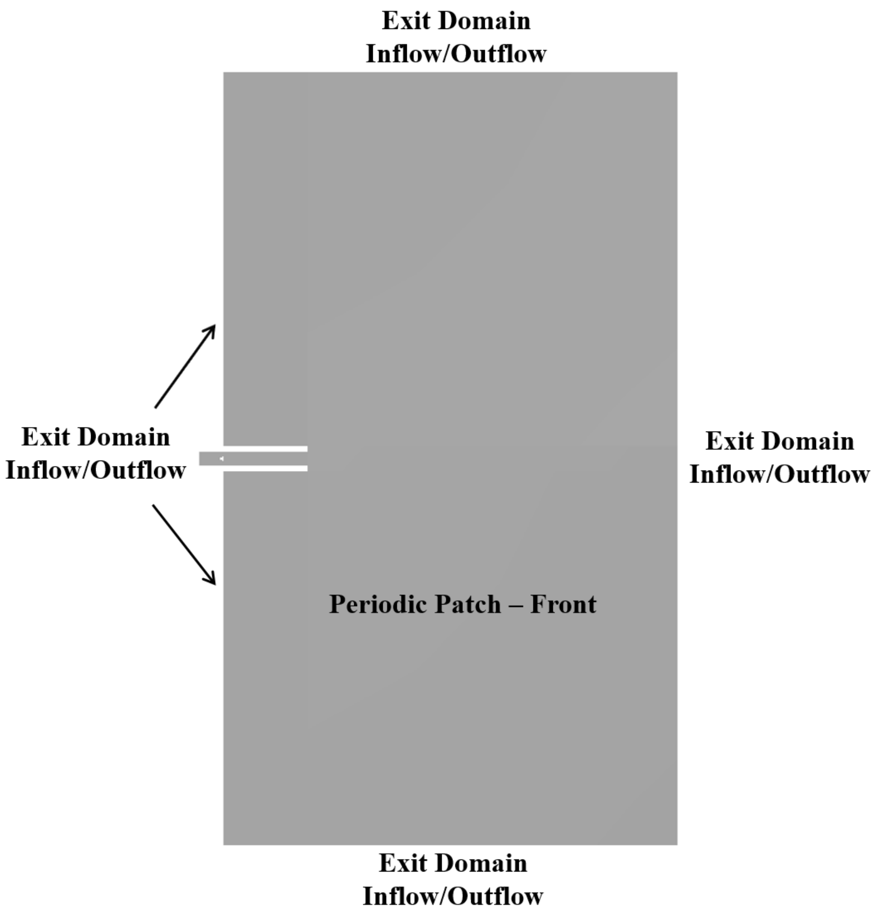
Figure 1. Computational domain for the AFRL bluff-body-stabilized premixed flame. (a) Isometric view and (b) spanwise normal view.



(a)



(b)

Figure 2. Boundaries for the AFRL bluff-body-stabilized premixed flame. (a) Isometric view and (b) spanwise normal view.

4.2 Computational Grids

Grid convergence with a sequence of mesh resolutions should be attempted. 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.

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.

4.3 Operating Conditions

Table 1 summarizes the operating conditions for the AFRL bluff-body-stabilized premixed flame validation case. (updates in red)

Table 1. Operating conditions for the AFRL bluff-body-stabilized premixed flame validation case. *The mass flow rates have been adjusted to account for the reduced depth of the computational domain and to include fuel flow rate.

Operating Condition	Required Case	Optional Case
Premixed Fuel / Oxidizer	Propane / Air	Propane / Air
Equivalence Ratio	0.65	0.65
Pressure	100 kPa	100 kPa
Inlet Temperature	310 K	600 K
Mass Flow Rate (including fuel)	0.1819 kg/s *	0.1819 kg/s *
Bulk Velocity	16.562 m/s	32.051 m/s
Bulk Mach Number	0.048	0.067
Bulk Reynolds Number	39,000	24,000
Unburned / Burned Density Ratio	6.0	3.5

4.4 Boundary Conditions

Table 2 summarizes the recommended boundary conditions for the AFRL bluff-body-stabilized premixed flame validation case. All exceptions to these boundary treatments should be emphasized in your presentation.

Table 2. Boundary conditions for the AFRL bluff-body-stabilized premixed flame. *The mass flow rates have 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	0.65	0.65
Inlet Stagnation Temperature	310 K	600 K
Inlet Mass Flow Rate	0.1819 kg/s *	0.1819 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 & Bottom Combustor Wall Temperature	Adiabatic	Adiabatic
Top & Bottom Combustor Wall Velocity	No-Slip	No-Slip
Front and Back Patches	Periodic	Periodic
Exit Domain Far Field Total Temperature	300 K	300 K
Exit Domain Far Field Total Pressure	100 kPa	100 kPa
Exit Domain Inflow/Outflow Boundaries	Characteristic / Transmissive BC with reverse/back flow conditions from far field stagnation values	Characteristic / Transmissive BC with reverse/back flow conditions from far field stagnation values

5 Results and Unsteady Metrics

Participants are required to present detailed statistics and metrics as described in this section. The various subsections below represent a hierarchy of metrics that should be pursued whether comparing with the experiment or contrasting results from different simulations (e.g., model comparison study). A rough estimate of the flow through times (based on domain length and cold bulk velocity) used in previous MVP sessions is 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. A grid convergence or sensitivity study is requested (if not presented in a previous MVP workshop) but does not need to be the main focus of your work.

Nomenclature and Definition of Coordinate System

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

Table 3. 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 (38.1 mm)

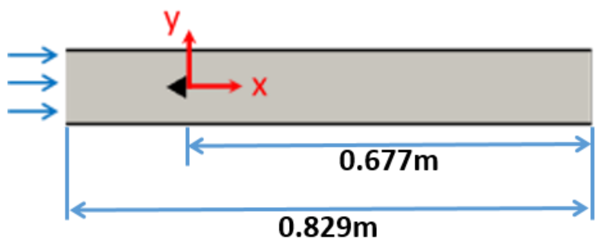


Figure 3. Definition of coordinate system for the AFRL bluff-body-stabilized premixed flame. The figure depicts the z = 0 plane, which is parallel to and centered between the periodic patches of the computational domain.

Values of interest include (φ):

- Axial velocity (quantitative experimental data available)
- Transverse velocity (quantitative experimental data available)
- OH (optional – qualitative experimental data available)
- CH_2O (optional – qualitative experimental data available)
- Heat release (optional – qualitative experimental data available)
- Temperature (optional – no experimental data available)

5.1 Point-Based Statistics

Mean and RMS

From the z/D = 0 plane, present a selection of the mean and RMS profiles below. Rather than present a comprehensive set of results, please select a subset of representative results and any profiles that highlight differences with experimental data and/or between simulations in a numerical study. The RMS should be computed as follows:

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

- Mean & RMS Transverse Profiles: z/D = 0 and x/D = 0.5, 1.5, 3.0, 5.0, 10.0
- Mean Axial Profile of Axial Velocity Only: z/D = 0, y/D = 0, and x/D = 0 to 10

Probability Density Functions (PDFs)

The Wasserstein metric and Earth Mover's Distance (EMD) quantify differences between two PDFs or histograms via a single number representing a "distance" between them. This quantity is provided via the solution of an optimal transport problem. Use the Wasserstein metric or Earth Mover's Distance described in [1] to compare PDFs of the values of interest listed above at the positions described below. The PDFs
should be constructed from time series point data with sample sizes of approximately 1000 for each PDF in order to keep computational cost reasonable. MATLAB software and examples can be found at the following link:

https://github.com/IhmeGroup/WassersteinMetricSample

Locations: x/D = 1.5, 3.0, 5.0, z/D = 0, and y/D = Various; consider constructing profiles of the Wasserstein metric/Earth Mover's Distance from comparisons of PDFs at multiple points in the transverse direction

5.2 Point-Based Spectra

At the locations selected for the PDFs, use the time series data to construct the power spectral densities of the values of interest. Due to the lower computational cost, please consider using a much larger sample size (i.e., high sampling frequency). Please select a subset of representative results and any spectra that highlight differences with experimental data and/or between simulations in a numerical study. More sophisticated metrics such as two-point correlations are encouraged but optional.

5.3 Time Lag Phase Portraits (TLPPs)

TLPPs provide insights into system dynamics from time series point data. Through noise-reduction techniques, turbulence effects can be removed and coherent signals revealed. Whereas averaging or calculating the RMS at a point can eliminate dynamic content, TLPPs offers a way to reconstruct dynamic content from point data.

Using the same time-series data collected for Sections 5.1 and 5.2, construct and compare time lag phase portraits using the method presented in [2]. Compare numerical to experimental portraits (or multiple numerical portraits to each other) at the same spatial locations. An outline of the phase portrait construction process is provided in Figure 3. Python software and an example will be uploaded to the following link at a future date: MVP 4 - Tools

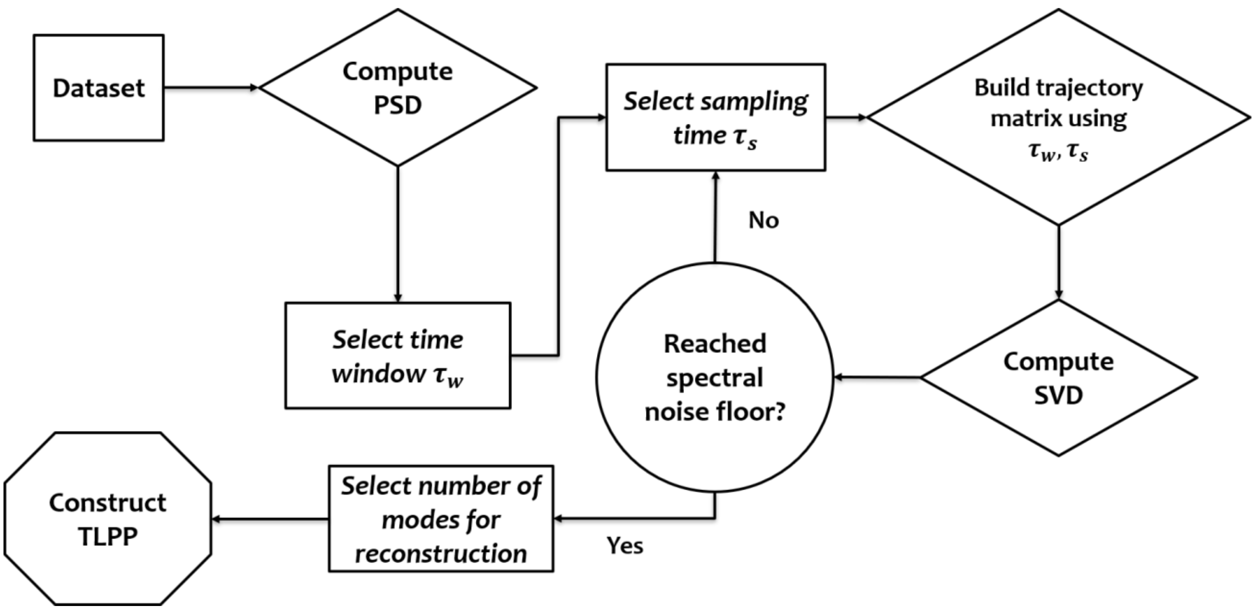


Figure 3. Diagram outlining the TLPP method.

5.4 Dynamic Mode Decomposition (DMD)

DMD decomposes the dynamics of an unsteady flow into different spatial modes at specific frequencies, providing detailed information about coherent structures in the flow. In addition to frequency, DMD provides growth/decay rates of the spatial modes, as well as ways to quantify the spatial mode power or the extent to which a particular mode represents the time-varying data.

Perform DMD on a slice in the z/D=0 plane of the simulation(s). For experimental comparisons, consider a 2D x 5D rectangular slice with the left edge centered on the bluff body trailing edge (see [3] for details). Although not required, interpolation and/or filtering to the PIV resolution may be necessary for a more accurate comparison with experimental velocity modes. Please present the following results:

- DMD power spectrum (see provided software for details and example)
- Mode shapes and frequencies at peaks in DMD power spectrum
- Characterization of mode shapes mentioned above. For example, comment on symmetry and potential physical sources of the mode and its associated frequency (e.g., von-Karman shedding, shear layer instability, acoustics etc.)

Python software and an example are available at the following link: MVP 4 - Tools

6 Experimental Data

Simultaneous 10-kHz CH2O-PLIF, OH-PLIF, PIV, and OH* chemiluminescence have been performed [3]. The operating conditions and boundary conditions previously described match the experiment and will not be changed. Experimental data from the bluff-body experiments conducted at AFRL will be provided at a future date.

7 Modeling Suggestions

These guidelines are provided to ensure consistency among the simulations and to facilitate code and model comparisons for both validation cases. 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.

7.1 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. [4]
Skeletal	66	24	Zettervall et al. [5]
Detailed	235	50	UCSD [6]

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

7.2 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 previous MVP results, the use of a turbulent combustion closure can facilitate grid convergence and is recommended for this session.

References

1. Johnson, R., Wu, H., and Ihme, M., "A general probabilistic approach for the quantitative assessment of LES combustion models," *Combustion and Flame*, Vol. 183, 2017, pp. 88-101.
2. Gallagher, T. P., Martin, R., & Sankaran, V. "Unique Identification of Turbulent Reacting System Dynamics with Time-Lag Phase Portraits," 11th U.S. National Combustion Meeting, Pasadena, CA, 2019.
3. Fugger, C. A., Paxton, B., Gord, J. R., Rankin, B. A., & Caswell, A. W. "Measurements and Analysis of Flow-Flame Interactions in Bluff-Body-Stabilized Turbulent Premixed Propane-Air Flames," 57th AIAA Aerospace Sciences Meeting, AIAA SciTech Forum, AIAA 2019-0733, San Diego, CA, 2019. https://doi.org/10.2514/6.2019-0733
4. 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.
5. Zettervall, N., Nordin-Bates, K., Nilsson, E.J.K., Fureby, C., "Large Eddy Simulation of a premixed bluff body stabilized flame using global and skeletal reaction mechanism," *Combustion and Flame*, Vol. 179, 2017, pp. 1-22.
6. "Chemical-Kinetic Mechanisms for Combustion Applications", San Diego Mechanism web page, Mechanical and Aerospace Engineering (Combustion Research), University of California at San Diego (http://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html).