3rd Model Validation for Propulsion Workshop Overview and Validation Cases

Contact Information: Adam Comer (aiaa.mvpws@gmail.com)
Last Updated: 8 June 2018 at 1620EST
*Emphasis items or significant updates 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 the Volvo bluff-body premixed flame validation case 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 1 and MVP 2 proceedings. For convenience, a brief summary of the challenges and findings from the technical sessions can be found in Appendix A.

2 MVP 3 Organization and Logistics

The format, timing, and submission process of the MVP 3 workshop have changed from the previous workshops. Please read this section carefully to find key deadlines, requirements, and travel considerations.

2.1 Pre-SciTech 2019 MVP 3 Workshop

The workshop will be held Sunday, 6 January 2019, prior to the AIAA SciTech 2019 workshop. The location will be announced soon; venues close to the Manchester Grand Hyatt, San Diego (SciTech site) will be prioritized.

Technical presentations at the workshop must be based on at least one of the validation cases and focus areas 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 11 June 2018, 8PM EST. These abstracts will be reviewed by the organizing committee, and the submitter will be notified by 31 August 2018. 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 2019, in addition to the workshop, and providing an additional SciTech presentation are highly encouraged but not required.

Participation in the workshop will also require submission of a subset of results prior to the workshop. Your submitted results may be used in summary plots alongside results from other groups; however, in the interest of anonymity and a cooperative environment, all of these plots will be non-attributional (no group names will be used to identify the source of the results). Details on the required submission will be provided at a later date, but the selection will be a subset of the items in Sections 5.6 and 6.6 (depending on your selected test case).

2.2 MVP 3 Workshop Technical Paper Session(s) at SciTech 2019

Although a technical paper submission to SciTech 2019 is no longer an MVP workshop requirement, you are highly encouraged to submit your MVP contribution to SciTech 2019. To ensure your SciTech paper and presentation are placed in an appropriate session, please complete the following steps:

- Submit abstract via the SciTech 2019 website by the SciTech deadline of 11 June 2018, 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 4 December 2018, 8PM EST, USA

2.3 Registration Process for Pre-SciTech 2019 MVP 3 Workshop

Registration is required to attend the Pre-SciTech 2019 MVP 3 Workshop for planning purposes. Priority will be given to those working on topics directly relevant to one or more objectives of the MVP Workshop series as space will be limited. Please register for the Pre-SciTech 2019 MVP 3 Workshop by sending an email to aiaa.mvpws@gmail.com by 31 August 2018. Please include "MVP 3 Registration" in the subject line and include your name, affiliation, and email address in the email.

2.4 MVP 3 Workshop Overview Session at SciTech 2019

Even if you are not able to participate in the MVP Workshop on Sunday, please consider attending the overview and summary session during SciTech 2019. This session will summarize the workshop findings and 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.

2.5 Pre-Workshop Conference Call Discussions

Prior to SciTech 2019, we plan to hold online conferences to discuss the validation cases and preliminary results. If you received the MVP 2 proceedings via email, then you will receive the invitations to the first event. Otherwise, please email aiaa.mvpws@gmail.com to ensure that you receive an invitation or monitor the MVP website for details.

3 MVP 3 Focus Areas

In light of its history and feedback from participants, the workshop is soliciting presentations featuring simulation results from at least one of the MVP 3 validation cases (see Section 4, Section 5, and Section 6) and an approach and analysis based one or more of the following areas of interest:

- **Grid Convergence** – There was consensus from past MVP workshops that achieving grid convergence is imperative to make valid assessments of modelling and simulation results. Previous work by several groups has shown that large, computationally expensive grids are required to show grid independence for the MVP validation cases for implicitly filtered LES. The development and demonstration of novel methods for (a) producing grid independent results or (b) quantifying the sensitivity of simulation results to grid resolution is highly encouraged. Even if novel methods for producing grid independent results are not pursued, some quantification of the sensitivity of the results to grid resolution is required.
- **Explicit Filtering** – Explicit filtering may be useful (a) to separate physical model errors from numerical errors and (b) to enable more definitive statements about model accuracy. A computationally affordable explicit filtering approach was demonstrated in MVP 2 as one methodology to produce grid independent results. In addition to efforts to show grid independence with explicit filtering, presentations investigating best practices for grid-to-filter ratios, comparing physical models on a grid-independent basis, and exploring the costs and benefits of explicit filtering with reference to more traditional, implicit approaches are encouraged.
- **High-Order Methods** – There was consensus from past MVP workshops 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. The development and demonstration of novel methods utilizing high-order numerical schemes for turbulent reacting flow simulations is highly encouraged.
- **Unsteady Metrics** – With the introduction of a new validation case and the potential for future unsteady experimental data, the application of unsteady metrics and techniques (e.g., POD, DMD, Lyapunov exponent, etc.) to the MVP validation case(s) is highly encouraged. Such contributions are likely to influence future workshop recommendations for required simulation results and metrics. In the absence of experimental data, these metrics may pair well with grid convergence or sensitivity analyses for quantitative assessment of changes in flow and flame dynamics.
- **Unit Physics Problems** – The workshop is actively considering the potential introduction of a suitable unit physics problem with relevance to the turbulent premixed, bluff-body validation cases studied in this workshop. Unit physics problems that can be simulated via both DNS and LES in a computationally affordable manner provide the possibility of (a) performing a larger number of computational parametric studies aimed at evaluating the interactions between numerical error and physical modeling effects and (b) eliminating uncertainties in boundary conditions and chemical kinetics that complicate current comparisons with experiments. Linking the proposed unit physics efforts to the more applied validation cases of MVP is a key requirement. Any thoughts or proposals for unit physics problems can be sent to aiaa.mvpws@gmail.com and could be included in a modified version of this document.
- **Sensitivity Analyses of Boundary Conditions –** There was consensus from past MVP workshops 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 the inlet turbulence intensity boundary condition, the flameholder and wall thermal boundary conditions, and exit boundary condition. Sensitivity to exit boundary conditions has been identified as a potential leading contributor to the variation in results from different groups.

- **Sensitivity Analyses of Modeling Approaches –** There was consensus from past MVP workshops 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 cases to contribute to one or more objectives of the MVP Workshop.

4 MVP 3 Validation Cases

Two separate bluff-body-stabilized turbulent premixed flame experiments have been selected for MVP 3. First, the Volvo validation case from MVP 1 and 2 is described, and updated guidelines are provided, particularly for the exit boundary condition. A second option is a similar bluff-body-stabilized turbulent premixed flame experiment from the Air Force Research Laboratory (AFRL). Specifications are provided for the inflow and outflow boundary conditions consistent with ongoing experiments, but experimental data (e.g., PIV, OH PLIF, and CH_2O PLIF) in the region of the flame will not be available until the time of the workshop due to the experimental campaign schedule. In order to get an early start on this case for future workshops, the AFRL experiment has been included as an option for MVP 3. At least one of the two experiments must be simulated and presented in order to participate in MVP 3.

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.

5 Volvo Bluff-Body Stabilized Turbulent Premixed Flame Validation Case

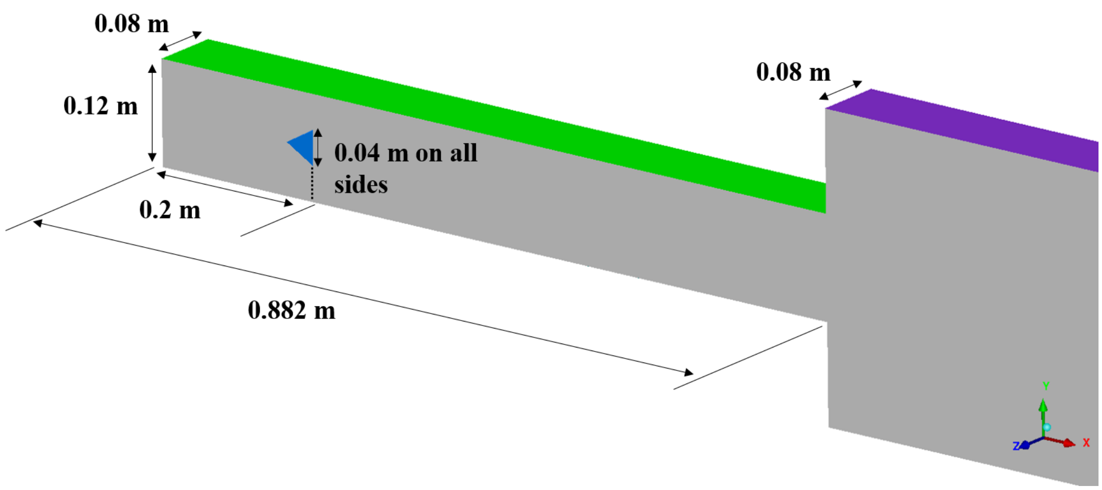
Two conditions have been selected for the Volvo bluff-body-stabilized turbulent premixed flame:

- **Required Condition** – If selecting the Volvo case, the required condition is the flame with an **inlet temperature of 288 K**. This required condition for the Volvo experiment includes updated recommendations for boundary conditions. Red text is utilized to indicate the updated recommendations that are being made for the MVP 3 Workshop.
- **Optional Condition** – The optional condition features is the flame with an **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.

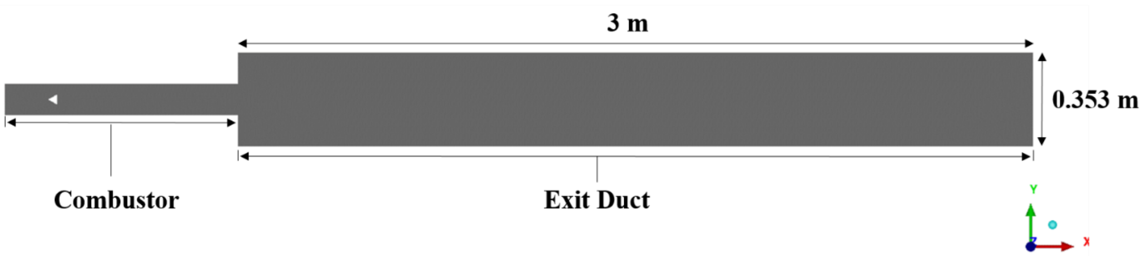
Case-specific guidance can be found in this section, and general modeling guidance can be found in Section 7.

5.1 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 combustor flow exhausts to a sudden expansion. In the experiment, this exit duct is cylindrical but for the workshop, a rectangular exit duct is recommended in order to enable the use of periodic boundary conditions and a reduced domain size in the spanwise direction (along the z-axis in Figure 1). 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 duct 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 duct and, in turn, placement of the exit boundary condition 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 (see Section 3). The use of grid stretching in the exhaust to reduce computational cost and to minimize reflections from the outlet is also suggested. Additional details of the Volvo bluff-body-stabilized premixed flame can be found in Refs. [1-2].



(a)



(b)

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

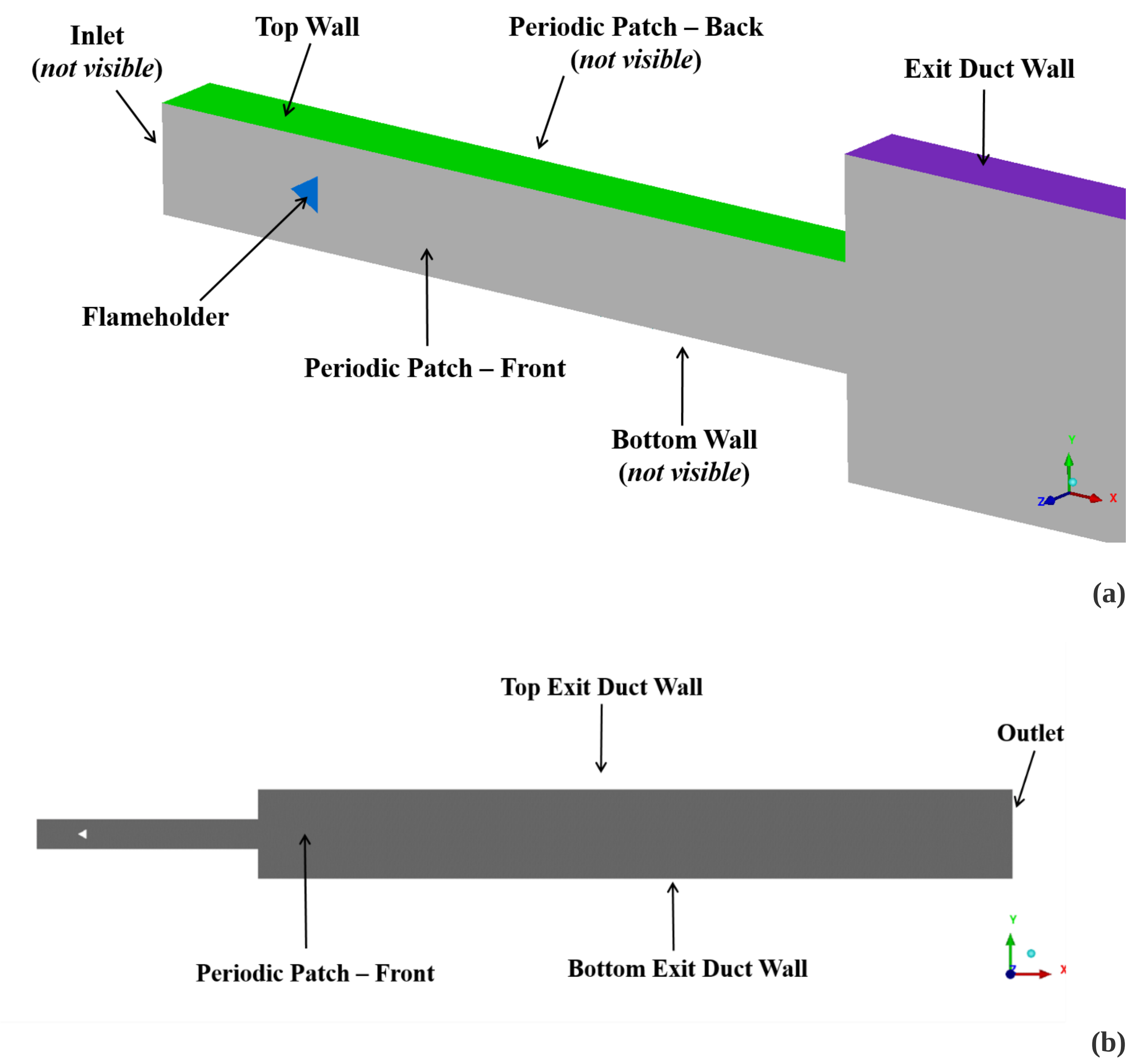


Figure 2. Boundaries for the Volvo bluff-body-stabilized premixed flame. (a) Isometric view and (b) spanwise normal view.

5.2 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.

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 (0.16 m), whereas we have recommended a shorter domain depth (0.08 m) in consideration of computational cost (see Figure 1).

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

5.3 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 rates have 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

5.4 Boundary Conditions

Table 3 summarizes the recommended boundary conditions for the Volvo bluff-body-stabilized premixed flame validation case. All exceptions to these boundary treatments should be emphasized in your 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 & Bottom Combustor Wall Temperature	Adiabatic	Adiabatic
Top & Bottom Combustor Wall Velocity	No-Slip	No-Slip
Exit Duct Walls Temperature	Adiabatic	Adiabatic
Exit Duct Walls Velocity	Slip	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)

5.5 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]. Please note that the figure quality limited the precision of the extracted data. Formatting details can be found in the header of each file.

- 288K Inlet:
  Volvo_Exp_Data_Non-Reacting_20160922.zip
  Volvo_Exp_Data_Reacting_20160922.zip
  Volvo_Exp_Data_Reacting_CARS_20171116.zip

- 600K Inlet:
  Volvo_Exp_Data_Reacting_600Kinlet_20171208.zip

5.6 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 previously 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. A grid convergence or sensitivity study is required but does not need to be the main focus of your work. See Section 3 for MVP 3 focus areas.

Nomenclature and Definition of Coordinate System

Nomenclature is listed in 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)

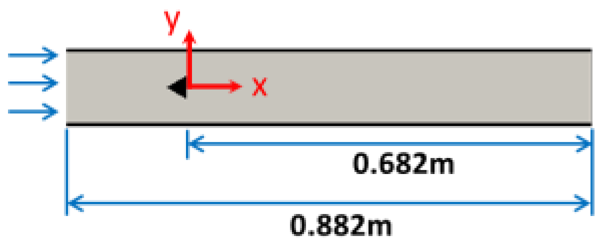


Figure 3. Definition of coordinate system for the Volvo bluff-body-stabilized premixed flame. The figure depicts the z = 0 plane, which is parallel to and centered between the periodic patches of the computational domain.

Values of Interest (φ)

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

Instantaneous and Time-Averaged Distributions

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

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, & x/D = 0 to 10)

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

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)

Consider using the Wasserstein metric [7] for comparing PDFs. A sample code can be found at the following link: https://github.com/IhmeGroup/WassersteinMetricSample

Unsteady Metrics

The application of unsteady metrics, such as PSDs, modal decomposition techniques, and others, are highly encouraged. Although unsteady experimental data are not available for comparison, these techniques could be readily applied to grid convergence assessments or sensitivity analyses.

6 AFRL Bluff-Body Stabilized Turbulent Premixed Flame Validation Case

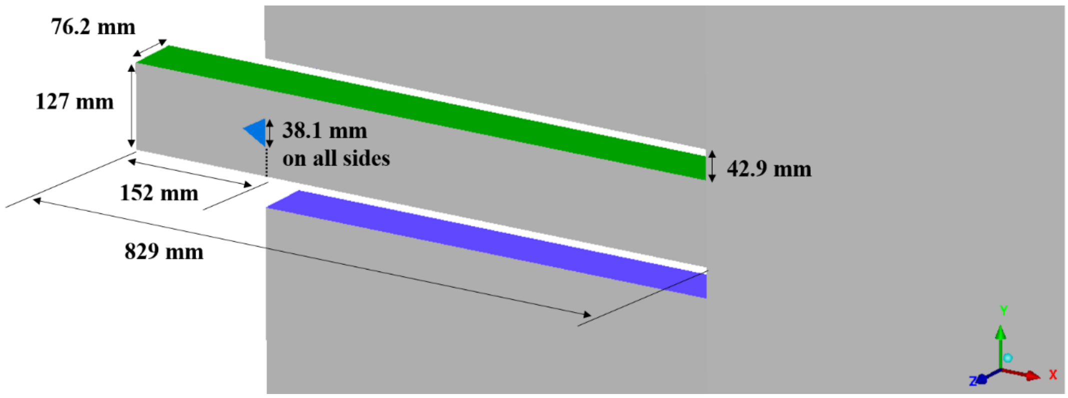
Two conditions have been selected as a starting point for the AFRL bluff-body-stabilized turbulent premixed flame:

- **Required Condition** – If selecting the AFRL case, the required condition is the flame with an **inlet temperature of 310 K**. Blue text is utilized to indicate differences between the AFRL case and Volvo case.
- **Optional Condition** – The optional condition is the flame with an **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.

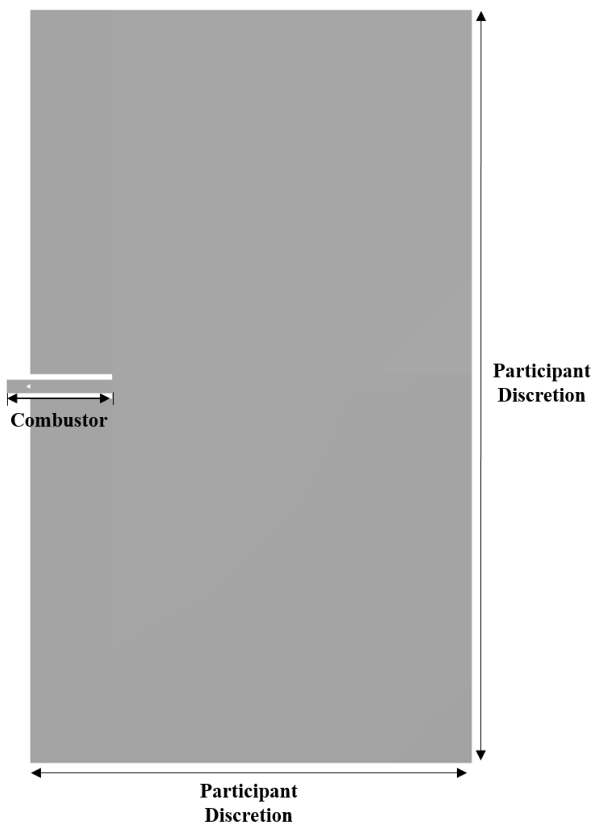
Case-specific guidance can be found in this section, and general modeling guidance can be found in Section 7.

6.1 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 4 and the boundaries labeled in Figure 5. 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 (see Section 3). The use of grid stretching in the exhaust to reduce computational cost and to minimize reflections from the outlet is also suggested.



(a)



(b)

Figure 4. Computational domain for the AFRL bluff-body-stabilized premixed flame. (a) Isometric view and (b) spanwise normal view.

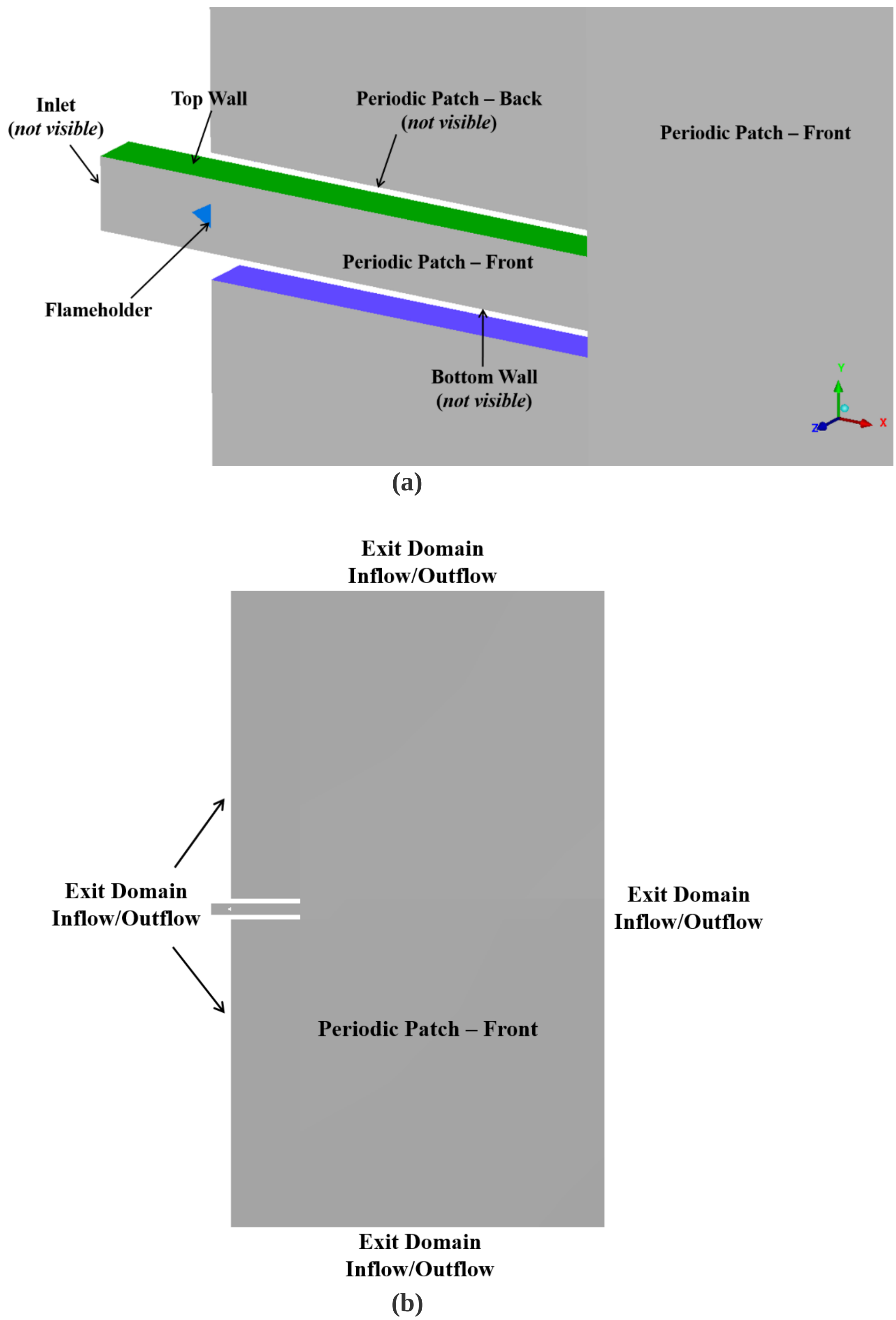


Figure 5. Boundaries for the AFRL bluff-body-stabilized premixed flame. (a) Isometric view and (b) spanwise normal view.

6.2 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.

6.3 Operating Conditions

Table 6 summarizes the operating conditions for the AFRL bluff-body-stabilized premixed flame validation case.

Table 6. 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.

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	0.1746 kg/s *	0.1746 kg/s *
Bulk Velocity	15.9 m/s	30.7 m/s
Bulk Mach Number	0.045	0.063
Bulk Reynolds Number	36,000	23,000
Unburned / Burned Density Ratio	5.9	3.4

6.4 Boundary Conditions

Table 7 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 7. Boundary conditions for the AFRL 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	0.65	0.65
Inlet Stagnation Temperature	310 K	600 K
Inlet Mass Flow Rate	0.1746 kg/s *	0.1746 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

6.5 Experimental Data

Experimental data from the non-reacting and reacting bluff-body experiments conducted at AFRL are unavailable at this time due to the experimental campaign schedule. Time-dependent and time-averaged distributions, profiles, and flowfield statistics of u_x, u_y, OH, and CH_2O are expected to be available by the time of the MVP 3 workshop. The operating conditions and boundary conditions previously described will not be changed.

6.6 Required Results

Participants are required to present 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. 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 required but does not need to be the main focus of your work. See Section 3 for MVP 3 focus areas.

Nomenclature and Definition of Coordinate System

Nomenclature is listed in Table 8, and the coordinate system is defined in Figure 6.

Table 8. 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)

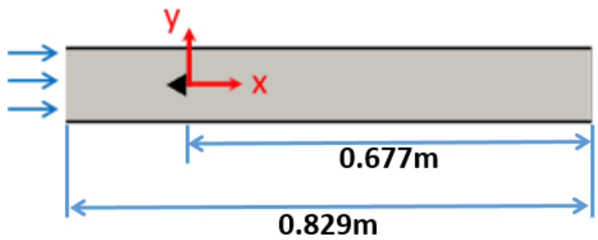


Figure 6. Definition of coordinate system for the AFRL bluff-body-stabilized premixed flame. The figure depicts the z = 0 plane, which is parallel to and centered between the periodic patches of the computational domain.

Values of Interest (φ)

- Velocity components (u_x, u_y)
- Spanwise Vorticity (ω_z)
- Temperature (T)
- Species mass fraction of OH (if available from the computational results)
- Species mass fraction of CH_2O (if available from the computational results)

Instantaneous and Time-Averaged Distributions

Plot at least one instantaneous distribution and the time-averaged distribution in the z/D = 0 plane of the following:

- Temperature
- Vorticity
- Axial velocity
- Heat release
- OH (if available)
- CH_2O (if available)

Experimental Data Comparisons

Plot the following profiles of the values of interest.

- **Mean – Transverse Profiles:**
  - 310 K Case – (u_x, u_y): z/D = 0 & x/D = 0.5, 1.0, 1.5, 3.0, 10.0, 15.0
  - 310 K Case – (T): z/D = 0 & x/D = 0.5, 1.0, 1.5, 3.0, 10.0, 15.0
  - 600 K Case – (u_x, u_y): z/D = 0 & x/D = 0.5, 1.0, 1.5, 3.0, 10.0, 15.0
  - 600 K Case – (T): z/D = 0 & x/D = 0.5, 1.0, 1.5, 3.0, 10.0, 15.0

- **Mean – Axial Profile of u_x Only:** (z/D = 0, y/D = 0, and x/D = 0 to 10)
- **RMS – Transverse Profiles:**
  - 310 K Case – (u_x, u_y): z/D = 0 & x/D = 0.5, 1.0, 1.5, 3.0, 10.0, 15.0
  - 310 K Case – (T): z/D = 0 & x/D = 0.5, 1.0, 1.5, 3.0, 10.0, 15.0
  - 600 K Case – (u_x, u_y): z/D = 0 & x/D = 0.5, 1.0, 1.5, 3.0, 10.0, 15.0
  - 600 K Case – (T): z/D = 0 & x/D = 0.5, 1.0, 1.5, 3.0, 10.0, 15.0

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

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

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

<u>Probability Density Functions</u>

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

- **Axial Positions** (x/D = 0.5, 1.0, 1.5, 3.0, 10.0, 15.0)
- **Transverse Positions** (y/D = 0, 0.5)

Consider using the Wasserstein metric [7] for comparing PDFs. A sample code can be found at the following link: https://github.com/IhmeGroup/WassersteinMetricSample

<u>Unsteady Metrics</u>

The application of unsteady metrics, such as PSDs, modal decomposition techniques, and others, are highly encouraged. Although unsteady experimental data are not available for comparison at this time, these techniques could be readily applied to grid convergence assessments or sensitivity analyses.

7 Modeling Suggestions

The 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. [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

7.2 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 the results of MVP 1 and MVP 2, the use of a turbulent combustion closure can facilitate grid convergence and is recommended for this session.

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Appendix A

A brief summary of key findings and challenges from the Volvo validation case are presented below.

Grid Convergence:

- A computationally feasible explicit filtering approach was demonstrated on the Volvo validation 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 also computationally efficient.
- 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.
- Laminar combustion closure has demonstrated significant grid sensitivity, whereas the use of certain turbulent combustion closure models appeared to reduce this sensitivity and aid grid convergence.
- Comparisons of PDFs and unsteady metrics for grid convergence assessment have been limited.

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.
- 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.

New Metrics for Comparison:

- 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.
- 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.

Numerics:

- Even for large meshes (over 60 million cells), the numerics can have a noticeable impact on the solution of the Volvo validation case.
- The use of upwinding has a noticeable effect on reacting solutions. One group applied upwinding throughout the domain and noted an overwhelming, adverse effect, 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:

- 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.
- Multiple groups have 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.