2nd Model Validation for Propulsion Workshop Validation Case

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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].

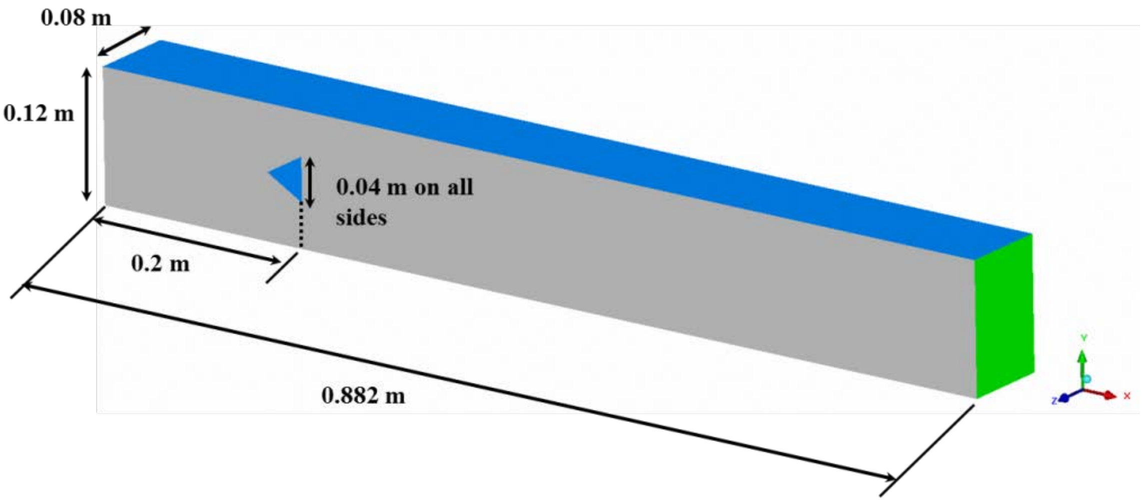

Figure 1. Computational domain for the Volvo bluff-body-stabilized premixed flame.

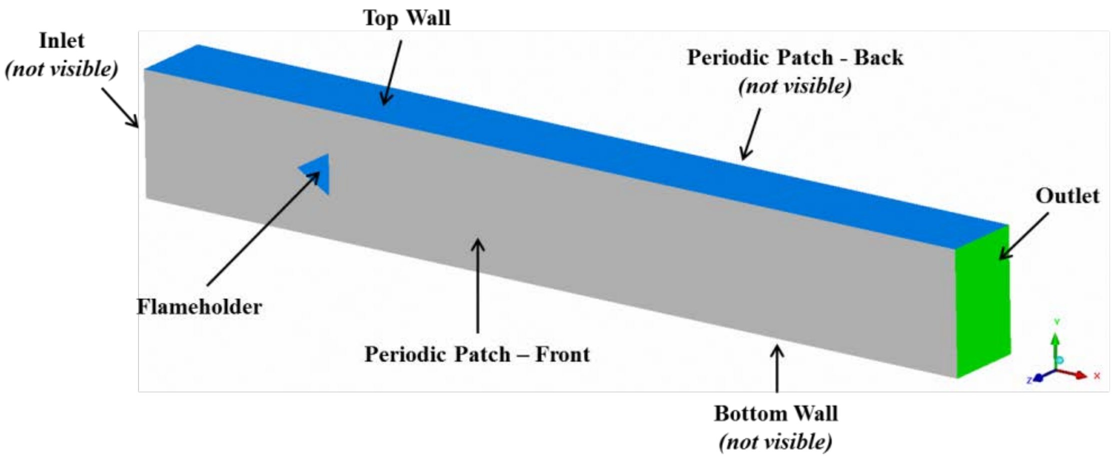

Figure 2. Boundaries for the Volvo bluff-body-stabilized premixed flame.

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)

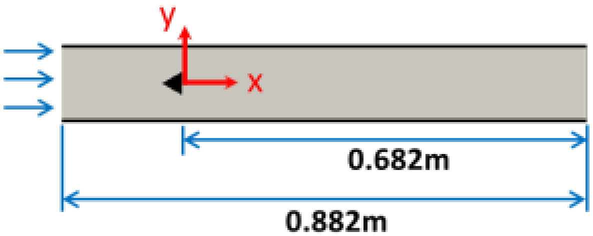

Figure 3. Definition of coordinate system for the Volvo bluff-body-stabilized premixed flame. The figure depicts the z = 0 plane, which is parallel to and centered between the periodic patches of the computational domain.

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

1. Sjunnesson, A., Olovsson, S., and Sjöblom, B. “Validation Rig – A Tool for Flame Studies”, International Society for Air-breathing Engines Conference, ISABE-91-7038, Nottingham, United Kingdom, 1991.

2. Sjunnesson, A., Nelsson, C., and Max, E. “LDA Measurements of Velocities and Turbulence in a Bluff Body Stabilized Flame”, Fourth International Conference on Laser Anemometry – Advances and Application, ASME, Cleveland, OH, 1991.
3. Fureby, C. “A Comparative Study of Large Eddy Simulation (LES) Combustion Models applied to the Volvo Validation Rig,” 55th AIAA Aerospace Sciences Meeting, AIAA SciTech Forum, AIAA 2017-1575, Grapevine, TX, 2017.
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).