1st Model Validation for Propulsion Workshop Validation Case

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

MVP 1 Workshop Validation Case Overview:
The first validation case in the MVP Workshop series is the bluff-body premixed flame experiment conducted by Volvo. Participation in the workshop is open, and participants can contribute by performing reacting flow simulations of the selected test case. Non-reacting simulations are highly encouraged but optional. The geometry, conditions, recommended model settings and practices, and experimental data can be found below. The guidelines are provided in order to ensure consistency among the simulations presented and to facilitate code and model comparison. They are not necessarily the best model and simulation choices, and the organizing committee does not intend to imply that there is a consensus regarding these choices. In addition, sample meshes of different resolutions, coarse, medium and fine are provided. Participants are not obligated to use the meshes provided, although they may provide some guidelines to grid resolution levels. Please note that workshop participation requires the submission of a full SciTech 2017 paper that contains all model details and the requested solution data.

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

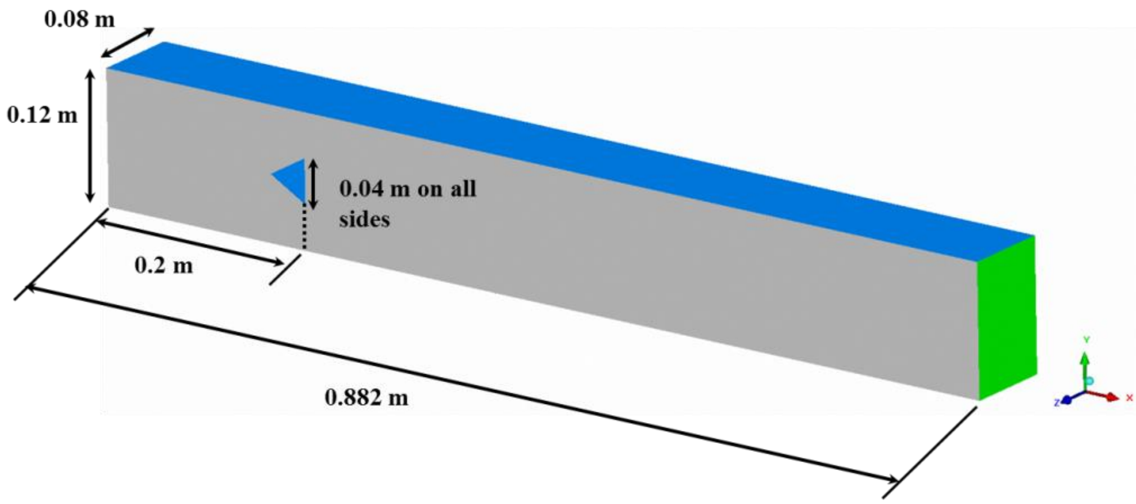

Figure 1. Computational domain dimensions for the Volvo test case.

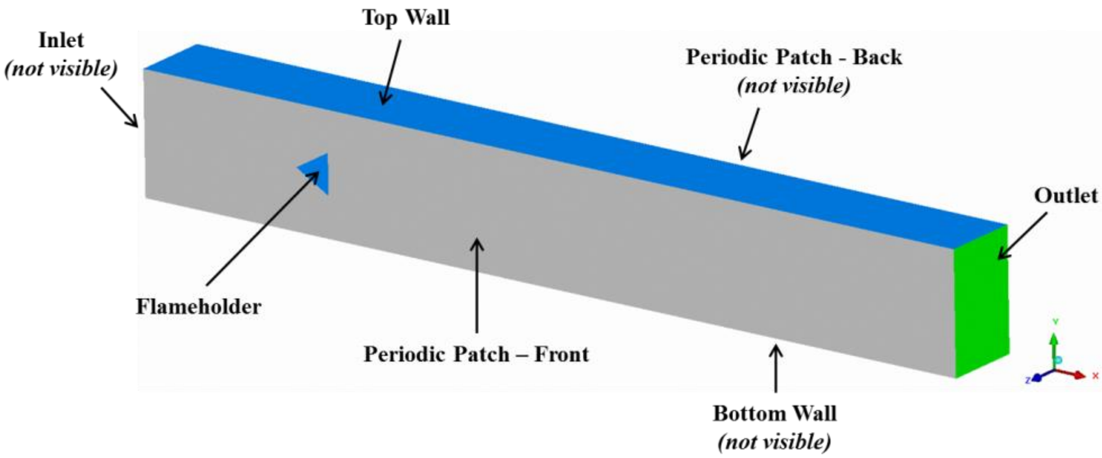

Figure 2. Volvo test case boundaries.

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

Table 1. Operating conditions to be simulated.

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

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

- **Inlet:**
  - Fixed mass flow rate of 0.2083 kg/s (adjusted for shortened domain depth and fuel flow rate)
  - Fixed stagnation temperature = 288.2 K
  - Zero inlet turbulence, i.e., no velocity fluctuations
  - Bulk flow, without prescribed velocity profile
  - Premixed propane-air at an equivalence ratio of 0.65
- **Top and Bottom Walls and Flameholder:**
  - No-slip
  - Adiabatic
- **Front and Back Patches:** periodic boundaries
- **Outlet:** Fixed static pressure of 100kPa

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

Grids:
The grids provided at the links below feature the recommended domain described in "Computational Domain" and are provided for your convenience. A sequence of coarse, medium and fine meshes are provided with approximate length-scale resolutions of 4 mm, 2 mm and 1 mm respectively in the flame region. If you choose to use these grids, please specify which grid(s) you used in your presentation of the results. If you do not use one of the grids below, please present and discuss your grid, including resolutions throughout the domain and the grid topology (e.g., the clustering of nodes near the bluff body shear layer). The intention is to enable interested participants to reproduce your mesh arrangement.
Grid convergence with a sequence of mesh resolutions should be demonstrated using the mean and RMS data provided in the section "Experimental Data." Thus, the mesh resolutions suggested are simply guidelines, and we recommend even finer resolutions if needed to achieve convergence. In addition to these comparisons, turbulence statistics (also specified below) should be presented at multiple grid resolutions to show convergence.
Volvo_Grids

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

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

$$\mathrm{C_3H_8 + 3.5O_2 \rightarrow 3CO + 4H_2O}$$
$$\mathrm{CO + 0.5O_2 \leftrightarrow CO_2}$$

The reaction rates are calculated using the following:

$$q_1 = A_1 \left(\frac{\rho Y_{C_3H_8}}{W_{C_3H_8}}\right)^{0.9028} \left(\frac{\rho Y_{O_2}}{W_{O_2}}\right)^{0.6855} exp\left(\frac{-E_1}{RT}\right)$$
$$q_2 = A_2 \left[\left(\frac{\rho Y_{CO}}{W_{CO}}\right)^{1.0} \left(\frac{\rho Y_{O_2}}{W_{O_2}}\right)^{0.5} - \frac{1}{K}\left(\frac{\rho Y_{CO_2}}{W_{CO_2}}\right)^{1.0}\right] exp\left(\frac{-E_2}{RT}\right)$$

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

If you plan to simulate this case with detailed chemistry, we recommend the UC San Diego mechanism [5]. The mechanism and associated thermophysical and transport properties files can be found at the link below:
http://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html

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

Experimental Data:
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] describing the experiments. 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

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

A. Nomenclature

φ	= generic scalar (or vector component) value of interest
$\langle\varphi\rangle$	= mean (temporal) value of
φ'	= fluctuation about the mean value of
U_{bulk}	= bulk inlet velocity (17.3 m/s)
D	= bluff body dimension (40 mm)

B. Values of Interest (φ)

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

C. Definition of Coordinate System

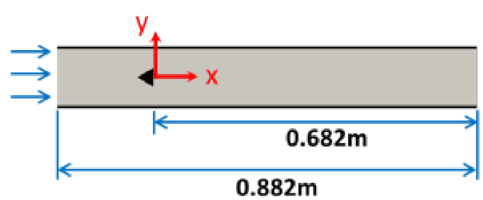

Figure 3. Coordinate system for Volvo case. The depicted plane corresponds to the z = 0 plane, which is parallel to and centered between the periodic patches of the computational domain.

D. Experimental Data Comparisons – Axial and Transverse Profiles
Plot the following profiles of the values of interest (see Section II above) along with the corresponding experimental data, if available. NOTE: Not all experimental values of interest are available at every requested location.

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

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

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

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

E. One-Point Temporal Statistics

The temporal statistics should be computed at the positions listed below (normalized by D):
(x/D, y/D, z/D) = (0.375, 0.0, 0.0); (0.95, 0.0, 0.0); (1.53, 0.0, 0.0); (3.75, 0.0, 0.0); (9.40, 0.0, 0.0)
(x/D, y/D, z/D) = (0.375, 0.5, 0.0); (0.95, 0.5, 0.0); (1.53, 0.5, 0.0); (3.75, 0.5, 0.0); (9.40, 0.5, 0.0)
(x/D, y/D, z/D) = (0.375, 1.0, 0.0); (0.95, 1.0, 0.0); (1.53, 1.0, 0.0); (3.75, 1.0, 0.0); (9.40, 1.0, 0.0)

1. **Temporal Correlations**

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

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

2. **Integral Time Scales**

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

F. Grid Convergence

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

References:

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

Recent SciTech Papers for this Case:

- Cocks, P. A. T., Sankaran, V., and Soteriou, M. C. "Is LES of reacting flows predictive? Part 1: Impact of numerics," *51st AIAA Aerospace Sciences Meeting*, AIAA 2013-0170, Grapevine, TX, 2013.
- Sardeshmukh, S. V., Huang, C., Harvazinski, M., Sankaran, V., and Anderson, W. "Impact of Chemical Kinetics Mechanisms on the Predictions of Bluff Body Stabilized Flames," *54th AIAA Aerospace Sciences Meeting*, San Diego, CA, 2016.
- Comer, A. L ., Huang, C., Rankin, B., Harvazinski, M., and Sankaran, V. "Modeling and Simulation of Bluff Body Stabilized Turbulent Premixed Flames," *54th AIAA Aerospace Sciences Meeting*, San Diego, CA, 2016.