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URANS SIMULATION OF TURBULENT NON-PREMIXED AND NON-REACTING PROPANE JET FLOW

Valdson Henrique Prado Gonçalves
Gabriel Marcos Magalhães
João Marcelo Vedovoto
Federal University of Uberlandia, Fluid Mechanics Laboratory-MFLab
Av. João Naves de Ávila, 2121, 38400-902, Uberlândia-MG
vhpgoncalves@gmail.com
gabrielmarcosmag@gmail.com
vedovoto@ufu.br

Abstract. *In the present work, numerical simulations of a turbulent non-premixed and non-reacting propane jet flow, in presence of co-flowing air, were made. Unsteady Reynolds Averaged Navier-Stokes modeling was applied on the simulations of propane jet using standard k-ϵ model. Furthermore, an adaptive refinement was used in the mesh domain to reduce the computational cost. Results for velocity and mixture fraction at jet center line were obtained and compared with experimental data for validation. The simulations were realized using the MFSim code, developed on the Federal University of Uberlandia at Fluid Mechanics Laboratory - MFLab.*

Keywords: *URANS, non-premixed jet, mixture fraction, adaptive refinement*

1. INTRODUCTION

In recent years, the simulation of combustion in transient, turbulent and gaseous jets has been a significant topic of research, motivated by the development and commercialization of new technologies involving the use of fossil and alternative fuels (Wu *et al.*, 2010). In terms of industrial applications, non-premixed jets are used because of their simplicity to design and build besides they are safer to operate, for reacting cases. For this reason, recent works has analyzed flow interactions in turbulent non-premixed jets, mainly on the presence of flow stabilization (Abubakar *et al.*, 2018).

The study of turbulent flows in inert environments is a key point to understand the fuel-air mixing process, and some works dedicated to investigate several applications that involve non-reacting turbulent flows (Banaeizadeh *et al.*, 2013; Yang and Kær, 2012). The inert study of non-premixed helps to focus only on the problem of turbulence, which is one of the most influential phenomena in combustion (Payri *et al.*, 2016). Turbulence increases the mixing process an enhances combustion. For this reason, non-reacting flows calculations are the first step before simulating reactive flows.

The present work aims simulate a non-premixed and non-reacting turbulent jet of propane into coflowing air using URANS model for turbulence analysis. The results obtained on simulations is compared with experimental data computed by Schefer (2001).

2. METHODOLOGY

2.1 Numerical model

The set of equations used to model for mass and momentum conservation of non-reacting flows was based in conservative form for these equations, given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial (\rho u_i)}{\partial x_i} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu\frac{\partial u_i}{\partial x_i}\delta_{ij}\right] \tag{2}$$

where ρ is the density of mixture, u_i is the flow velocity field, p is the pressure, mu is the viscosity and δ_{ij} is the Kronecker delta.

For the present work, it was used the standard $k-\epsilon$ model, proposed by Launder and Spalding (1972) and, also the

two-layer wall treatment model to simulate internal flows. The standard $k-\epsilon$ model requires two more transport equations besides the Navier-Stokes equations and the continuity equation.

The first equation of this model transports the turbulent kinetic energy, k [m^2/s^2], and it is given by

$$\frac{\partial(\rho k)}{\partial t} + \bar{u}_j \frac{\partial(\rho k)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + \mu_t S^2 - \rho\epsilon \tag{3}$$

where μ and μ_t are the molecular and the turbulent dynamic viscosities, respectively, $\sigma_k = 1.0$ is the model constant and $S = \sqrt{S_{ij}S_{ij}}$, in which S_{ij} represents the strain rate tensor components.

For the MDF (Multi-Direct Forcing) method, it is necessary to force a value for the turbulent kinetic energy at the body boundary. As the velocity at a wall is null, the boundary condition of the immersed boundary for the turbulent kinetic energy is also null.

The second equation transports the dissipation rate, ϵ [m^3/s^2], and it is given by

$$\frac{\partial(\rho\epsilon)}{\partial t} + \bar{u}_j \frac{\partial(\rho\epsilon)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon}{\partial x_j}\right] + C_{\epsilon 1}\frac{\epsilon}{k}\mu_t S^2 - \rho C_{\epsilon 2}\frac{\epsilon^2}{k} \tag{4}$$

where $\sigma_\epsilon = 1.3$, $C_{\epsilon 1} = 1.44$ e $C_{\epsilon 2} = 1.92$ are the model constants.

To describe the gas mixture, the equation of mass conservation of the species was used and it is given by

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho u_i Y_k)}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(\rho D + \frac{\mu_t}{Sc_t}\right)\frac{\partial Y_k}{\partial x_i}\right] + \dot{\omega}_k \tag{5}$$

where Y_k is the mass fraction of species k, D is the coefficient of diffusion, Sc_t is the turbulent Schmidt number and it is equal to 0.7. The last term on the right hand side represents the reaction rate of species k, and for non-reacting flows is equal to zero.

2.2 Computational simulations

The proposed methodology was implemented in a in-house code developed at Fluid Mechanics Laboratory (MFLab), located in Federal University of Uberlandia (UFU), the MFSim code.

The MFSim is based in an adaptive block-structured regular and cartesian mesh which reduces the computational cost. Using this code, it is possible to simulate fluid-structure, multi-phase, reactive and turbulent flows with Large Eddy Simulation (LES) and URANS considering 3D domains and parallel processing (Neto *et al.*, 2019; Melo *et al.*, 2018; Denner *et al.*, 2014; Gasche *et al.*, 2012).

The MFSim has some temporal and advective discretization schemes and the possibility of using the SIMPLE method or fractional-step method for the pressure-velocity coupling.

Simulation was based on experimental analysis of Schefer (2001), which tested a non-premixed and non-reactive turbulent round jet of propane at gas phase into coflowing air. The tests were realized in a forced-draft vertical wind-tunnel with an axisymmetric fuel jet located at the upstream of the test section, which has a 20-cm-square cross section and is 200-cm long. The computational domain is defined with dimensions of $40D \times 80D \times 40D$, where D is the jet nozzle diameter $D = 5.2 \times 10^{-3} m$.

The mesh base used is composed by $32 \times 64 \times 32$ elements plus three physical levels with adaptive refinement, and the finest mesh level has a element dimension $\Delta x = 8.124 \times 10^{-4}$ m, which guarantees at least six elements located in nozzle exit, as shown in Fig. 1. Refinement criteria is based on density, vorticity and turbulent viscosity gradients.

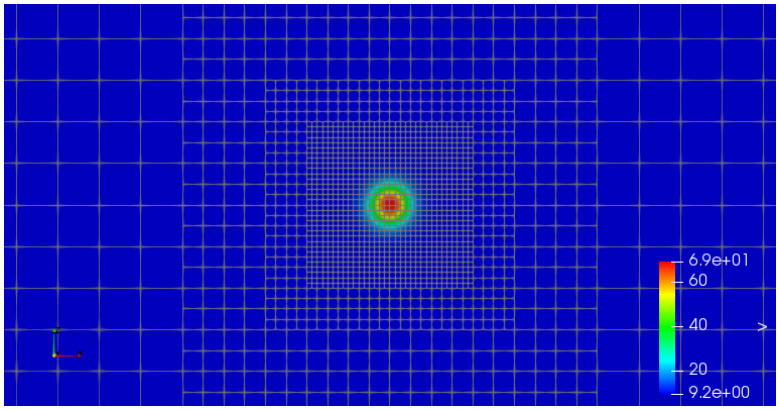

Figure 1. Block-structured refinement at jet nozzle

Inlet conditions for velocity are zero for x and z velocity components. In y-direction, the velocity profile is defined as:

$$v = \frac{1.28v_0 + v_1}{2} - \left(\frac{1.28v_0 - v_1}{2}\right) \tanh\left[r_\theta \left(\frac{r_j}{r_0} - \frac{r_0}{r_j}\right)\right] \tag{6}$$

where $r_j = \sqrt{(x - 0.5D_1)^2 + (z - 0.5D_2)^2}$, $v_1 = 9.2m/s$ and $v_0 = 53m/s$ are the coflow and main jet velocities, respectively, r_0 is the nozzle radius, D_1 and D_2 are dimensions of computational domain in x and z coordinates. Advection condition was chosen for outlet and Neumann condition was used at the other faces.

Mass fractions of fuel jet and coflow air substances is described at Tab.1. Since there are different substances involved in the simulations, it was used a hyperbolic tangential function to represent density and viscosity distributions over computational domain, defined as:

Table 1. Mass fractions of fuel jet and coflow air

	Substances	Mass fraction
Fuel Jet	C_3H_8	1,000
Coflow	N_2	0,767
	O_2	0,233

$$\rho = \frac{\rho_0 + \rho_1}{2} - \frac{\rho_0 - \rho_1}{2} \tanh\left[r_\theta \left(\frac{r_j}{r_0} - \frac{r_0}{r_j}\right)\right] \tag{7}$$

$$\mu = \frac{\mu_0 + \mu_1}{2} - \frac{\mu_0 - \mu_1}{2} \tanh\left[r_\theta \left(\frac{r_j}{r_0} - \frac{r_0}{r_j}\right)\right] \tag{8}$$

where ρ_0 and rho_1 are the main jet and coflow specific masses of the main jet and coflow, respectively, and mu_0 and mu_1 are the main jet and coflow molecular dynamic viscosities, respectively.

Inlet turbulence intensity was defined as 1% at main jet exit.

3. RESULTS

The jet velocity at central plane normal to z-direction is observed in Fig. 2. The mean velocity on flow direction decay in jet center line as far as the two gases are mixing. The decrease of the velocity is consequence of variation of all jet parameters by action of density variation, since the flow is treated as isothermal at jet and coflow regions.

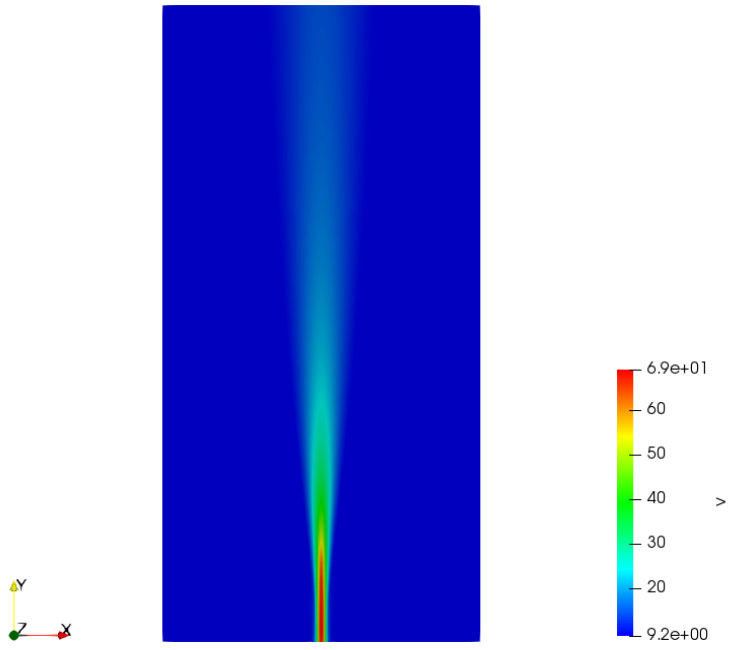

Figure 2. Jet velocity on y-direction observed at central plane normal to z-direction

Numerical and experimental results for mean velocity decay in jet central line is observed in Fig.3. Velocity decay on simulations has closer values compared with experimental data, despite the number of elements that fills nozzle diameter

is less than recommended in literature (Boersma *et al.*, 1998; De *et al.*, 2011). This may be observed in Fig. 3 for values of $y/D < 20$, which there was a small deviation between numerical and experimental results.

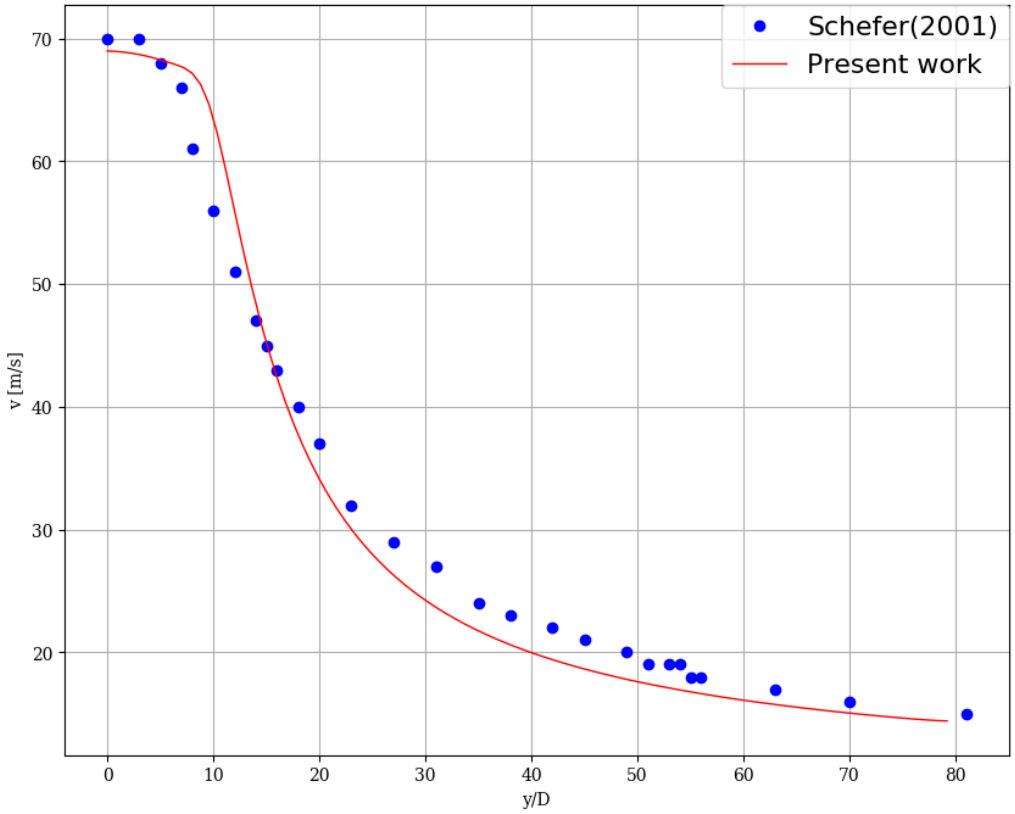

Figure 3. Jet center line velocity profile

Furthermore, the numerical results in Fig. 3 reveal the mean jet velocity begins to decay at location $y/D = 10$, differently of experimental data, where it may be observed at $y/D = 5$. The reason for that is the density variations caused by mixing on the experiments are stronger close to nozzle exit and the numerical model used on the simulations are not able to predict exactly these changes. On the other hand, from $y/D > 15$, the model performs better the velocity prediction.

Figure 4 exhibits mixture fraction decay on jet center line. Mixture fraction was obtained using the expression:

$$z = \frac{sY_F - Y_O + Y_O^0}{sY_F + Y_O^0} \tag{9}$$

where $Y_F^0 = 1.000, Y_O^0 = 0.233$, which represents the initial values for propane and oxygen mass fractions, respectively, and s is the mass stoichiometric ratio and it is equal 3.63 for propane combustion reaction. At locations near to jet nozzle exit there are agreement between experimental and numerical results for mixture fraction. Same remarks about these values may be viewed on the far field flow. These results, moreover, prove the numerical model predicts gas mixing very well.

4. CONCLUSIONS

Simulation of a non-premixed and non-reacting turbulent propane jet flow into coflowing air was performed using k-ϵ turbulence model in order to compare the results of velocity and mixture fraction with profiles obtained through experimental data. Analyzing the results, it was observed that the turbulence model and the formulation for mixing presented satisfactory performance to predict velocity and mixture fraction profiles at jet center line.

For future works is suggested to analyze the jet flow using different turbulence models, such as hybrid URANS-LES models and LES models, and the influence of different mesh refinement on simulations results.

5. ACKNOWLEDGEMENTS

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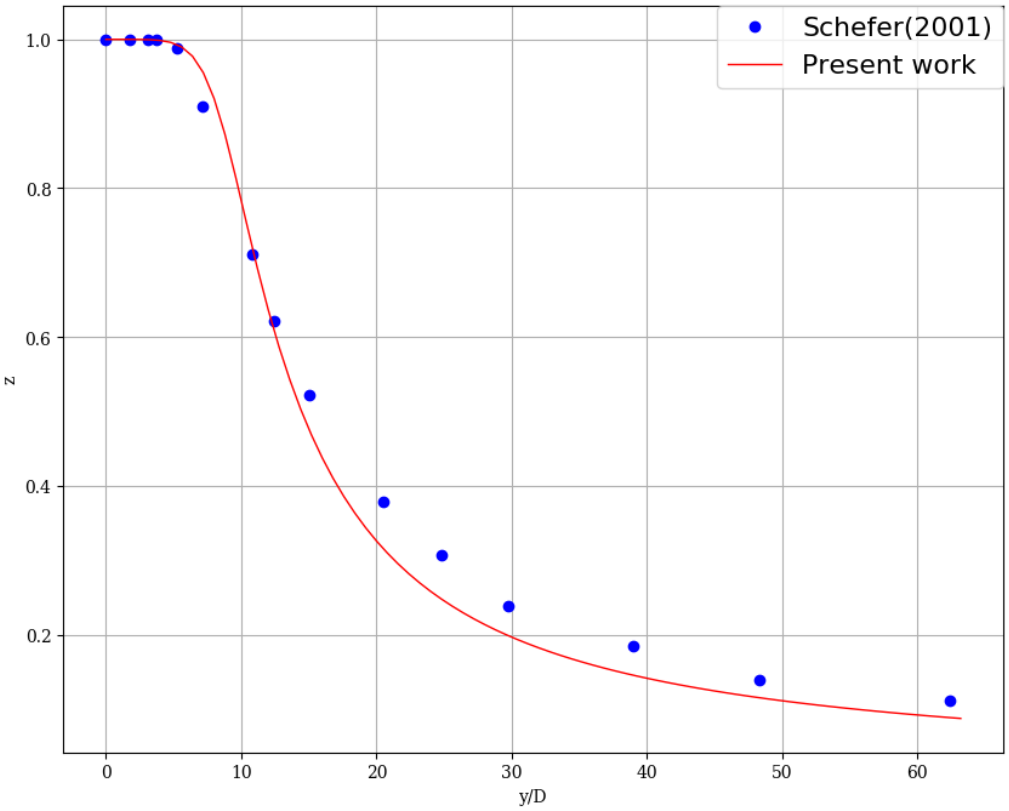

Figure 4. Jet center line mixture fraction profile

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