

ENCIT-2018- FLAMES DYNAMICS OF BLUFF-BODY-STABILIZED IN LEAN PREMIXED STOICHIOMETRIC SYNGAS/AIR

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Abstract. *Large-eddy simulations (LES) are conducted through a Computational Fluid Dynamics (CFD) using Fluent code to investigate the general insights of the responsible variables in this harmful phenomenon which affect many thermal applications and known the bluff-off limits working in stoichiometric conditions. The flow was simulating in two dimensions with a square flame such holder are adopted in the model configuration using syngas mixture with 1 ratio of CO:H₂ and equivalence ratio of one is considered. First, simulations of the non-reacting mixture at 80 m/s were performed. The velocities were increased in each group of simulations in such a way that each time step was 0.01 s, and 200 time step numbers were made and iterated 200 times for each time step. The method of turbulence chemistry interaction was Eddy dissipation, it was used for the reactive fluid simulations to be able to ignite the mixture. The Blow off event started when the speed reached 85 m/s, showing an increase and decrease behavior of the temperature downstream, near the 4 mm location. The results showed that the blow-off events were generated by an excessive amount of eddies registered in the zones of low temperatures.*

Keywords: *Bluff-body-stabilized flames, Premixed flames, Blow-off limits, Syngas, Large Eddy simulation.*

1. INTRODUCTION

Bluff-body is usual utilized to stabilize the diffusion and premixed flames in many industrial applications, such as in gas turbines, ramjets and furnaces. The bluff-body provides a recirculation zone downstream the fluid to improve the mixing of fuel and air and bring back the hot combustion products to ignite the reactants. Hence, the flame is stabilized by the recirculation vortex creating a short flame attached in this zone. Besides, the emission levels of NO_x and CO get altered by the use of a bluff-body or swirl flow. An easy control is achieved in the flame by utilization of a bluff-body (Gubernov et al., 2017).

A good understanding of the dynamics for flame stabilization around a bluff-body has long been a basis of many investigations to know the practical significance in combustion devices. Different types of studies have been carried out, either numerical or experimental, to provide new ideas on this topic. Nevertheless, due to the difficult turbulence-chemistry interactions occurring at a wide range of time and length scales, it is difficult to obtain detailed physics data that occurs, using either advanced laser diagnostic techniques or high-quality computational tools in the macro-scale combustors. Further investigations are necessary to reveal the details of intricate dynamics at the exact onset of the extinction and blow-off events. This study examine the characteristics of syngas/air flames in a micro-combustor. Consideration of syngas mixture is a practical interest in terms of bio- or coal-driven alternative fuel utilization, and the results are anticipated to serve as guidance to the micro-combustor applications utilizing similar configurations. In addition, one of the main motivations of this work is to demonstrate that using a cheap numerical simulation method, in terms of time, can provide important ideas and results in the combustion of syngas (Lee and Im, 2017).

Investigate the combustion of syngas is important as H₂ and CO form building blocks for all hydrocarbon combustion. For this reason, many numerical and experimental studies were carried out to understand the dynamic close to blow-off limit: Recently (Lee et al., 2015a) studied a two-dimensional direct numerical simulations using micro combustor and a square bluff-body to stabilize the flame of a lean hydrogen/air mixture at near-blow off conditions in a mesoscale channel. These simulations were carried out by increasing the inflow velocity in order to reach the blow off limit. This novel study show a full demonstration and a detailed visualization of the near blow off flame characteristics. As the inflow velocity achieves blow off limit, the flame dynamics exhibit a complex sequence of events, such as periodic local extinction and recovery, and regrowth of the bulk flame by the flame segments attached behind the bluff-body. The total extinction of the flame as the attached flames shrink down and are no longer able to regrow the bulk flames. Despite the disparity in the physical scale under study, the observed sequence of the extinction pathway shows a strong similarity with experimental observations at larger scale combustion systems. The recent work by (Askari et al., 2017) have been investigated fundamental properties such as flame structure and laminar burning speed of syngas with O₂ and He premixed flames. Synthetic gas, also known as syngas, is a mixture of hydrogen and carbon monoxide that been used in

the present study. The next mole fractions 5%, 10% and 25% of hydrogen in the syngas were used in the investigation. The experiment were carried out in a cylindrical and spherical chamber. The cylindrical vessel was coupled with a Z-shape schlieren system, equipped with a high speed camera, which has the capability of capturing pictures up to 40,000 frames per second, to study flame instability. They found some discrepancies between the experimental laminar burning speeds of H₂/CO/O₂/He mixtures compared with numerical values calculated by free flat flame simulation using two chemical kinetics mechanisms for equivalence ratios greater than two. (Brambilla et al., 2014) made a numerical investigation about the dynamics and stabilization of fuel lean premixed CO/H₂/air atmospheric pressure flames in mesoscale channels, using detailed gas phase transport and chemistry. They detected chemiluminescence of the flame by OH radical doing many experiments carried out in a channel flow reactor allowed for model validation. The numerical results revealed different flame modes, which included oscillatory ignition, random ignition spots, as well as steady weak and V-shaped flames. The physicochemical process was studied by Computational Singular Perturbation (CSP) to obtain insights regarding the weak flames, which were found at relatively high inflow velocities compared to previous studies, and V-shaped flames. (Tong et al., 2018) studied on his paper the flow structure and flames stabilized by combinations of swirl flow and bluff-body. The numerical study was based on the CFD software OpenFOAM. They took experimental data using high-speed PIV to make the validation of the numerical model. High-speed CH₂O PLIF, CH* chemiluminescence and broadband chemiluminescence, visualized the flame structures. Experimental data and results from the simulations have the same behavior, especially in predicting the spatial distribution of CH₂O. Their results achieved two relevant conclusions in flame dynamics: using a larger bluff-body positions the air driven recirculation more upstream close to the burner exit and when the burner uses a larger bluff body and/or stronger swirl number the flame prone to be more stable. (Fan et al., 2014) carried out a numerical study in a micro-combustor with a bluff body using the Fluent code to solve the mass, momentum, energy and species conservation equations as well as the conjugated heat conduction in solid materials, this model demonstrated 3- to 5-time extension in the blow-off limit. They studied the blockage ratio with a detailed H₂/O₂ reaction mechanism. And (Yilmaz et al., 2017) shows results obtained from modelling of hydrogen/air combustion in micro-combustor. They carried out many simulations using different turbulence models to appreciate performance of these models and its behavior in the micro-combustor simulations by using Fluent code. The model implemented in this study are Standard k- ϵ , Realizable k- ϵ , Renormalization Group k- ϵ and Reynolds Stress Transport. A detailed combustion reaction scheme with 9 species and 19 steps using Eddy Dissipation Concept model was used. The numerical results showed that the turbulence models give consistent simulation results with published experimental data by means of trend and value. The numerical results obtained from the simulations, show a lot of concordance in terms of trend and values with the experimental data. It does conclude that the fluent code applied to previous works is a good tool to model the combustion of premixed flames; this tool was used in this work since most of previous validations with experimental works show great relationship.

In the present study, the transient characteristics of bluff-body-stabilized lean premixed syngas flames near the blow-off conditions are investigated in detail by Large Eddy simulations, which is a mathematical model for turbulence used in (CFD). This model works solving the Navier–Stokes equations and requires resolving a very wide range of time and length scales, all of which affect the flow field. One of the main reasons for using this model is the short time and amount of memory it requires to simulate turbulent flows, in addition to previous work was used to obtain results very consistent with reality.

2. METOLOGY

The simulation is based on the well-known Large Eddy Simulation working with CFD, which solves fully compressible multispecies reacting Navier–Stokes equations with a Finite Volume Method (FVM). A two-dimensional computational domain Fig. 1 is considered for a rectangular channel of height at $D = 1$ mm and the length at $10D$, it was built and simulated using Ansys/Fluent CFD code. A bluff-body flame stabilizer is represented by a square block of size $0.5D$ by $0.5D$, whose center is located at $2.25D$ downstream of the inflow boundary on the left. For Syngas/air mixture with the equivalence ratio of 1 and CO:H₂ ratio of 1, a simple reaction with (H₂ , O₂ , OH, H₂O , CO, CO₂ , N₂) is employed. Chemical kinetics, thermodynamics, and transport properties are calculated using the subroutine modules adapting the Fluent libraries.

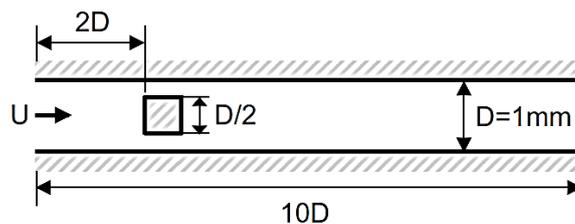


Figure 1. Configuration of a two-dimensional channel with a square-cylinder flame stabilizer (Lee et al., 2015b; Lee and Im, 2017).

Transient state forms of the momentum, continuity, species and energy equations are solved using finite volume method. The mentioned equations were discretized by second order upwind scheme. For pressure-velocity coupling, SIMPLE algorithm is chosen. The gas phase Syngas/air is modelled using Eddy Dissipation model, this model was used in a previous study by (Cam et al., 2017) they made a validation of the model applied in a micro-combustor, the numerical results were very similar to the experimental data.

A premixed Syngas/air mixture enters the combustor at atmospheric conditions. A fully developed velocity profile of the flow solution is imposed at the inflow boundary, at a temperature of 298 K and atmospheric pressure. Throughout the series of simulations, the mean inflow velocity was ramped up from a previously set value to a target value then was held constant to investigate the subsequent temporal evolution of the flame dynamics at the target value, thereby suppressing the transient characteristics directly caused by the abrupt inflow acceleration. The applied methodology is similar to previous numerical investigations (Lee et al., 2015b; Lee and Im, 2017), however in this investigations we applied a different solver method. The equivalence ratio was registered joined with the inlet velocity, entering the moles fractions of the reactants (including the fuel and oxidizer species). Hydraulic diameter and turbulence intensity (5%) are specified at the combustor inlet and outlet. Convergence criteria for continuity, momentum and species equations are $10e-3$ and $10e-6$ for energy equation. Mixture physical properties such as density, specific heat, thermal conductivity, viscosity and mass diffusivity are calculated using incompressible ideal gas law, mixing law, mass weighted mixing law, mass weighted mixing law and kinetic theory, respectively.

2.1 Governing equations

The system state is described by the conservation equations for mass, momentum, energy and species in the low-Mach-number limit. Therein, acoustic waves are neglected, allowing for larger integration times steps, while compressibility effects due to heat release and density variations are fully accounted for.

Continuity

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (1)$$

Momentum

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p_1 + \nabla \cdot (\mu \mathbf{S}) \quad (2)$$

$$\mathbf{S} = \nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I}$$

Energy

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = \nabla \cdot (\lambda \nabla T) - \sum_{i=1}^{N_g} h_i \dot{\omega}_i - \rho \left(\sum_{i=1}^{N_g} C_{p,i} Y_i V_i \right) \cdot \nabla T \quad (3)$$

$$C_p = \sum_{i=1}^{N_g} C_{p,i} Y_i$$

Species

$$\rho \left(\frac{\partial Y_i}{\partial t} + \mathbf{u} \cdot \nabla Y_i \right) = -\nabla \cdot (\rho Y_i V_i) + \dot{\omega}_i \quad i = 1, \dots, N_g \quad (4)$$

with N_g the total number of gaseous species.

Equation of state (ideal gas)

$$p_0 = \frac{\rho R T}{\bar{w}} \quad (5)$$

$$\bar{w} = \left(\sum_{i=1}^{N_g} \frac{Y_i}{W_i} \right)^{-1} \quad (6)$$

The leading order term p_0 is the thermodynamic pressure, while the first order term p_1 appearing in the momentum equation is the hydrodynamic pressure.

Standard $\kappa - \varepsilon$ turbulence model

This model including in the Fluent code solves the Reynold stress such:

$$-\rho \overline{u_i u_j} = \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \rho \kappa \delta_{ik} \quad (7)$$

where k represent the turbulence kinetic energy, and μ_t is the turbulence viscosity given by

$$\mu_t = \frac{\rho C_\mu \kappa^2}{\varepsilon} \quad (8)$$

C_μ is a constant and ε is the dissipation rate of kinetic energy. The turbulence kinetic energy and its dissipation rate are following as

$$\frac{\partial}{\partial x_i} (\rho u_i \kappa) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_\kappa} \right) \frac{\partial \kappa}{\partial x_i} \right] + G_\kappa - \rho \varepsilon \quad (9)$$

$$\frac{\partial}{\partial x_i} (\rho u_i \varepsilon) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + C_{1\varepsilon} G_\kappa \frac{\varepsilon}{\kappa} - C_{2\varepsilon} G_\kappa \frac{\varepsilon^2}{\kappa} \quad (10)$$

In previous equations, G_κ is the generation of turbulence kinetic energy due to the mean velocity gradient. Turbulent heat flux and mass flux can be modelled with the turbulent heat conductivity (λ_t) and the turbulent diffusion coefficient (D_t), respectively.

$$\rho C_p \overline{u_i T} = -\lambda_t \frac{\partial T}{\partial x_i} = -C_p \frac{\mu_t}{Pr_t} \frac{\partial T}{\partial x_i} \quad (11)$$

$$\rho \overline{u_i C} = -\rho D_t \frac{\partial C}{\partial x_i} = -\frac{\mu_t}{Sc_t} \frac{\partial C}{\partial x_i} \quad (12)$$

The values of the constants $C_{1\varepsilon}$, $C_{2\varepsilon}$, C_μ , σ_κ , and σ_ε , used are 1.44, 1.92, 0.09, 1.0, and 1.3, respectively.

Eddy dissipation model

Most fuels are fast burning, and the overall rate of reaction is controlled by turbulent mixing. In premixed flames, the turbulence slowly convects/mixes cold reactants and hot products into the reaction zones, where reaction occurs rapidly. In such cases, the combustion is said to be mixing-limited, and the complex and often unknown, chemical kinetic rates can be safely neglected.

The Fluent code provides a turbulence-chemistry interaction model, based on the work of (Magnussen and Hjertager, 1977), called the eddy-dissipation model. The net rate of production of species i due to reaction r , $R_{i,r}$, is given by the smaller (i.e., limiting value) of the two expressions below:

$$R_{i,r} = \dot{v}_{i,r} M_{w,i} A \rho \frac{\varepsilon}{\kappa} \min_R \left(\frac{Y_R}{\dot{v}_{R,r} M_{w,R}} \right) \quad (13)$$

$$R_{i,r} = \dot{v}_{i,r} M_{w,i} A B \rho \frac{\varepsilon}{\kappa} \frac{\sum Y_P}{\sum_j^N \dot{v}_{j,r} M_{w,j}} \quad (14)$$

where Y_P is the mass fraction of any product species, Y_R is the mass fraction of a particular reactant, A and B are empirical constants equal to 4 and 0.5 respectively.

In the previous equations the chemical reaction rate is governed by the large-eddy mixing time scale, κ/ε , as in the eddy-breakup model of (Spalding, 1971). Combustion proceeds whenever turbulence is present $\kappa/\varepsilon > 0$, and an ignition source is not required to initiate combustion.

The 2-D mesh was generated in the Workbench of Ansys 2017. In order to obtain accurately results, the meshing was performed with the inclusion of sizing in the walls of the micro combustor, inlet and outlet. In addition, a method was added using triangles on the fluid domain, fig 2, shows the mesh made.

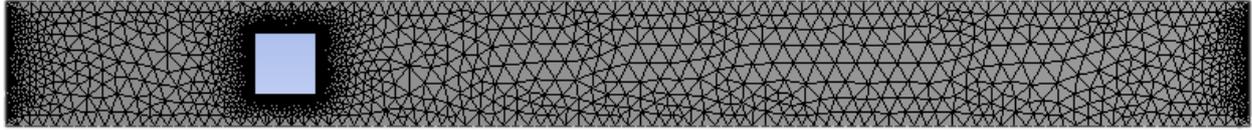


Figure 2. Mesh of the micro combustor using all method triangles on the surface.

The quality of the mesh is reported below.

Minimum Orthogonal Quality = 2.86078e-01
 Maximum Ortho Skew = 5.07938e-01
 Maximum Aspect Ratio = 7.13018e+00

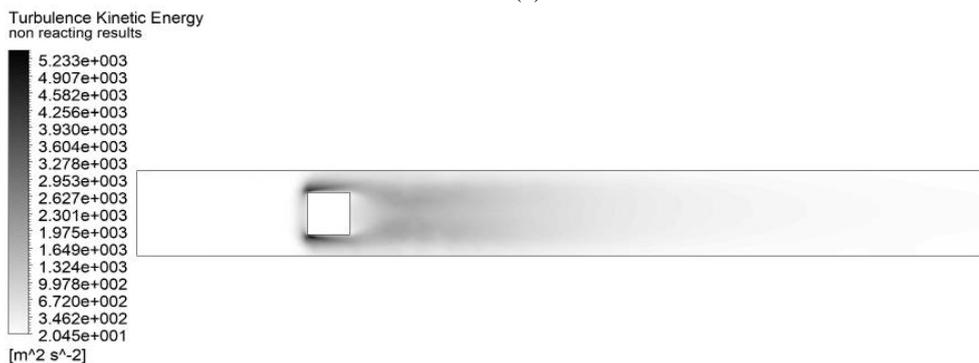
3. RESULTS

As an initial idea of the behavior of the flow, simulations were carried out without applying the eddy dissipation analyses, rather the flow is non-reactive. The input velocity is 80 m/s, and there are three graphs of speed, turbulence kinetic energy and H₂ mass fraction in the fig.3.

The simulations carried out without reaction flow, show the velocity field when a constant speed of 80 m/s is applied, the flow passing through the narrowing generated by the Bluff body increases the speed reaching maximum values of 200 m/s in the side. The high speeds generated by the presence of the Bluff bod are normalized when reaching the end of the combustor with speeds of the order of 90 m/s. It is important to highlight the presence of zero velocities located in the center and downstream of the bluff body, those values represented by a white spot denote the presence of recirculation on the fluid.



(a)



(b)



(c)

Figure 3. Isocontours of the velocity (a), turbulence kinetic energy (b) and H2 mass fraction (c) for nonreacting flow simulations at 80 m/s at $t = 0.5$ s

The presence of the bluff body generates turbulence around the square; the maximum values reached are $5396 \text{ m}^2 \cdot \text{s}^{-2}$. The simulations without reaction of the mass fraction of H₂, shows how the whole surface of the flow is almost covered by the same amount of hydrogen, which is interpreted in the non-reaction of the hydrogen with air.

In this section, the simulations are carried out in reactive flows. The Turbulence chemistry interaction method chosen to activate the mixture was Eddy dissipation. When the simulations is initialize the solution for steady flows, Fluent sets all species mass fractions to a maximum of the user specified initial value and 0.01. This amount was enough to start the reaction in each simulation.

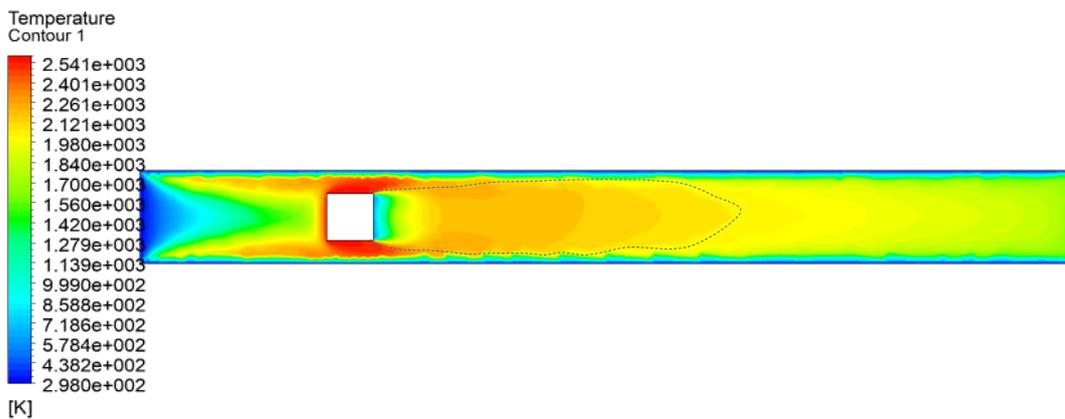


Figure 4. Temperature isocontours for the syngas flames at $U = 80$ m/s, at $t=0.5$ s.

Fig. 4 shows the results of the temperature inside the combustor at the speed of 80m/s a 0.5 s. In fig.4 the temperatures reach the 2000 K, these values are obtained on the lateral sides of the Buff-body, the generated flame located downstream is between temperatures of 1800 K. The gases that are removed from the combustor are around of 1400 K.

Simulations were performed as in fig.4 consecutively increasing 0.5 m/s the speed in order to reach the blow off event. The event was reported reaching the speed 85 m/s. In each group of simulations was carried out a time step size of 0.01 s, it was used to observe in detail the flame behavior, a total of 200 numbers of time steps, with each time steps of a maximum of 200 iterations converging in most the cases were carried .

When the speed reaches 85 m/s the temperatures of the gases and of the flames experienced event of blow off. These events were characterized by increasing and decreasing the temperature downstream. In Fig. 5, this behavior plotted. The first observed image captured at $t = 0.25$ s shows how the temperatures increase along the combustor reaching temperatures of 1800 K at the 2 mm location. In the image (b) it captures the temperatures in the same as when it was taken for 80 m/s, $t = 0.5$ s, here it is observed that the temperatures take to reach the same values obtained in the same time in fig.4 . Continuing with the remaining time intervals, it can be seen that at the time $t = 0.73$ s the temperatures fall downstream of the bluff body, dotted lines highlight the zone where the temperatures decreases close to location at 4mm.

This behavior continues until the time $t = 0.9$ s when the flame vanishes completely and the total extinction of the flame occurs in ms later.

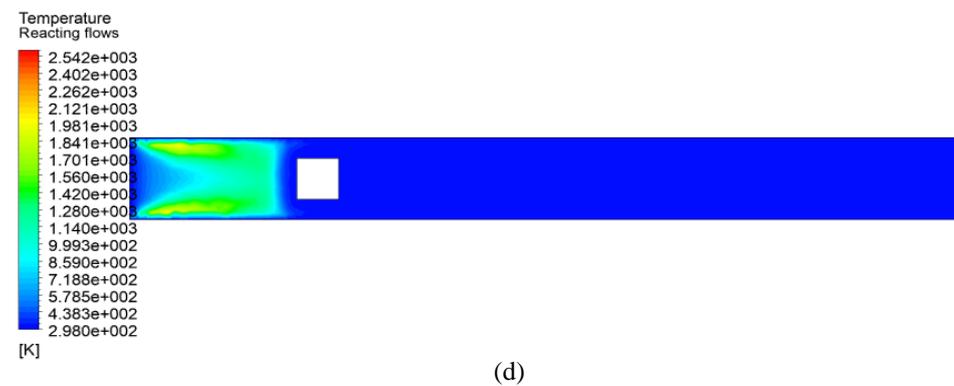
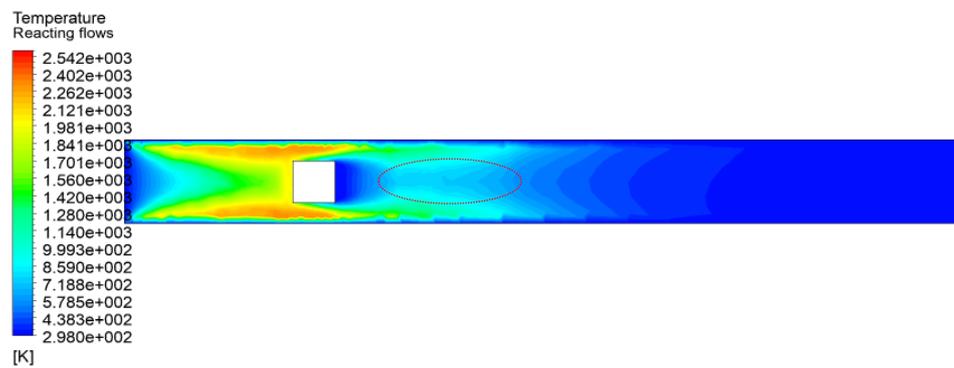
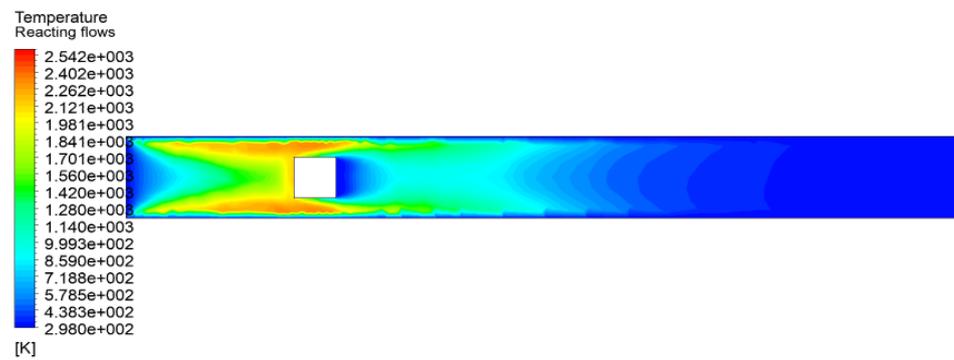
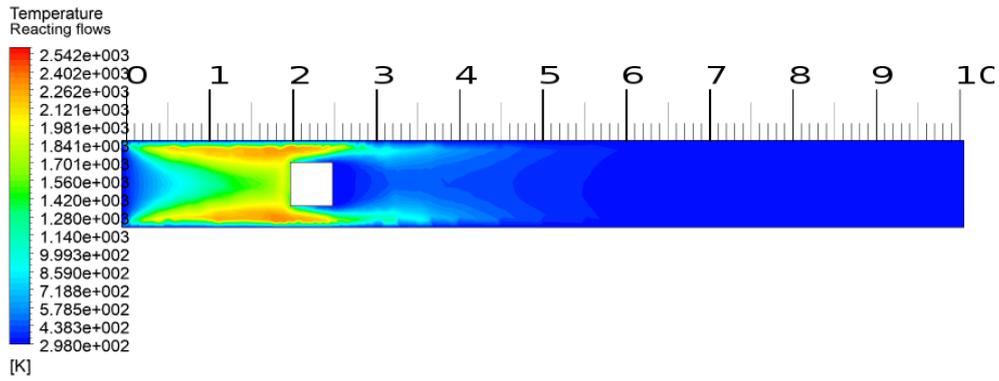
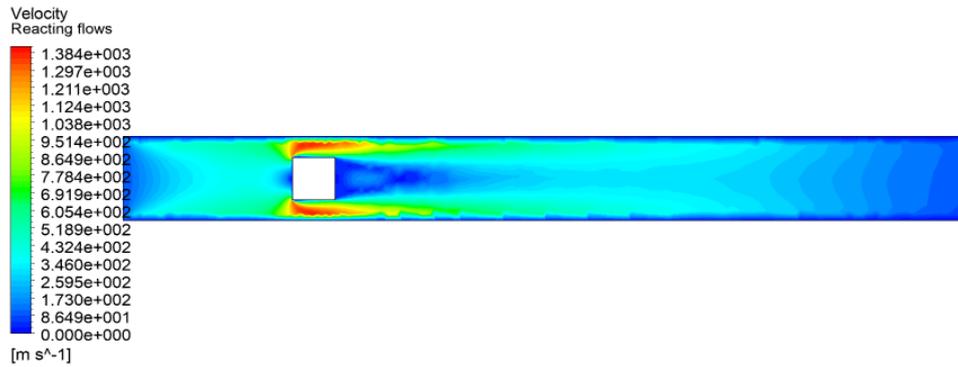
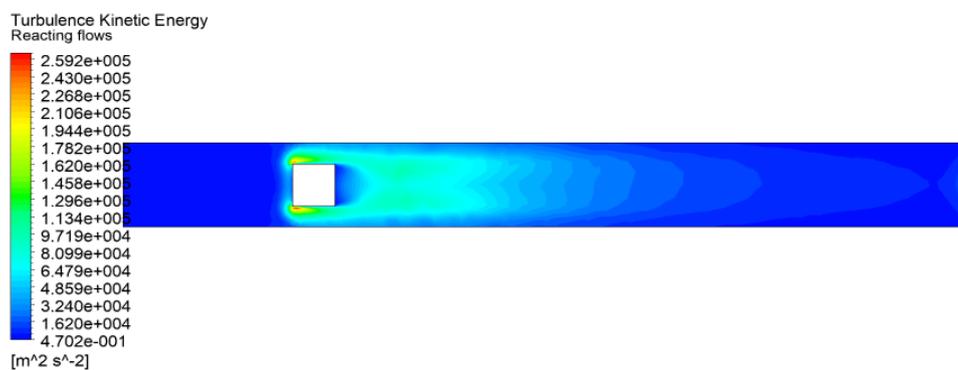


Figure 5. Temperature isocontours for the syngas flames at $U = 85$ m/s, a (a) $t = 0.25$ s, (b) $t = 0.5$, (c) $t = 0.73$, (d) $t = 0.90$ s



(a)



(b)

Figure 6. Temperature isocontours for the syngas flames at 85 m/s and $t = 0.9$ s ; (a) velocity, (b) Turbulence kinetic energy

The fig. 6 shows some characteristics of the flow in conditions close to Blow off at time $t = 0.9$ s, in image (a) the velocity field is appreciated. Very similar when the temperatures in Fig.5 (c) fall, the speeds fall exactly in the same area close to 4mm. Fig.6 (b) presents the behavior of the turbulence kinetic energy, this magnitude measures the kinetic energy associated with the eddies and fluctuations of the velocity. According to what has been shown there is a great activity of eddies in the area where there is flame extinction, which makes the flame banish.

4. CONCLUSIONS

Large Eddy simulations were performed for bluff-body-stabilized syngas/air premixed flames. Despite the short time compared with methods such as DNS that require large capacity memories to obtain detailed simulations, the results were consistent with previous work observing the flame behavior near the Blow off conditions. Initially the same geometry used by (Lee et al., 2015a) was replicated, applying a mesh of minimum orthogonal quality = $2.86078e-01$, which helped to appreciate the intricate physics of the events. First, the fluids without reaction were studied, and then the reactive flows were simulated. Simulating the reactive flows with 80 m/s, temperatures close to 2000 K were obtained, and combustion gases were expelled at 1400 K. The on-off behavior was achieved by increasing the entry speed, the value that began this behavior is 85 m / s. When the speed reached the aforementioned value, the temperatures experienced variations over time, such that when $t = 0.73$ s, the temperatures registered a decrement at 4mm downstream. This event continued until the flame was extinguished at near $t = 0.9$ s. This type of simulation, helped to observe in a general way the behavior of blow off in stoichiometric concentrations, however it did not help to reveal the frequency when these events occurred, besides not being able to register the flame front due to the lack of a detailed mechanism chemistry, therefore no flame was observed coming out of the combustor as is the natural behavior of this event.

5. ACKNOWLEDGEMENTS

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