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REVIEW OF NUMERICAL STUDIES ON FLAMELESS COMBUSTION OF LIQUID FUELS

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Abstract. *This paper presents a review of the numerical studies in the literature dealing with the flameless combustion of liquid fuels. The focus of this review is to discuss models of combustion and turbulence used by the authors showing their potential in the reproduction of the flameless combustion regime making a comparative analysis between them. Another issue discussed in this review is the modeling of turbulent sprays of liquid fuel, because the fuel injection directly influences the results obtained during the simulation of flameless combustion. The purpose of this review is to obtain the advantages and disadvantages of turbulence and combustion models presented, which are the most appropriate models to simulate the flameless combustion and promote better understanding of the modeling of turbulent sprays. The analyses will provide a database for future numerical simulations on the flameless combustion of biofuels.*

Keywords: *flameless combustion, liquid fuel, combustion models, turbulence models, turbulent sprays*

1. INTRODUCTION

Flameless combustion is a combustion regime where the fuel/air reactant mixture are submitted to a strong flow which results from the recirculation exhaust gas inside the combustion chamber and the appropriate temperature conditions lead to a well-distributed reaction zone with low temperature gradients and low emissions.

The flameless combustion regime receives various denominations in the scientific and industrial environments, these are given according to the parameters used in the process and include: FLOX® - Flameless Oxidation - (Wünning and Wünning, 1997), HiTAC - High Temperature Air Combustion - (Katsuki *et al*., 1998), Mild Combustion (Coelho and Peters, 2001; Kumar et al., 2002) and Colorless Distributed Combustion (Arghode and Gupta, 2009).

Various experimental studies are found in the literature regarding the phenomena involved in this combustion regime evaluating parameters such as temperature preheating of combustion air (Gupta, 2000; Kumar et al., 2005), changes in burner design for reproduction of this regime (Szegö et al., 2009, Arghode and Gupta, 2010) and the influence of the physical state of the fuel used (Derudi and Rota, 2011).

The development of numerical tools such as computational fluid dynamics (CFD) has greatly aided the progress of research on this new regime of combustion. These tools provide a detailed analysis of physical, chemical and thermodynamic phenomena involved in flameless combustion, since the models used in the simulations are properly validated, and is being increasingly applied to this type of study. Furthermore assist in optimizing the performance of combustion systems allowing to investigate the influence of the geometry of fuel nozzles and combustion gas recirculation devices (Galletti et al., 2007).

This paper presents a review of the numerical work in the open literature about the flameless combustion of liquid fuels and has two aims where the first is to assess the potential of turbulence and combustion models in reproducing this regime and the second is to get a improved understanding of modeling turbulent sprays of liquid fuels.

2. NUMERICAL MODELING OF FLAMELESS COMBUSTION OF LIQUID FUELS

The numerical modeling of flameless combustion of liquid fuels is a recent practice and in the literature are found few studies on the subject. Some significant work are Rochaya (2007), Bekdemir (2008), Zhu et al. (2011), Jenny et al. (2012), Li et al. (2014) e Jamali (2014).

An overview of these studies shows that there is no single model of turbulence or combustion that is more adequate for reproduction of flameless combustion regime, there is a dependency between the fuel injector geometry characteristics and operating conditions of the system to select the model to be used. So the development of numerical simulations requires knowledge of the models available in CFD and ability to control the constants that govern turbulent interactions, chemical, heat transfer, and others that appear when studying any type of combustion regime.

In this section we will discuss the models of turbulence and combustion and modeling of sprays used by the authors cited above, in order to evaluate the potential of these models and also the possibility of applying new models available in numerical tool CFD for modeling of the flameless combustion.

2.1 Turbulence models

There are several turbulence models for representing different types of flow and each one has a particular behavior in relation to the type of application. In the case of simulation of combustion systems it is very important to analyze carefully the turbulence models to be used, because they influence the prediction of temperature peaks obtained during the modeling of these regimes (Reitz and Rutland, 1995).

Among the reviewed studies we observed that the turbulence models most used for the flameless combustion of liquid fuels are: k-ε standard, k-ε realizable and the Reynolds Stress Model (RSM).

The k-ε standard model is one of the most common models used in numerical simulations because it is relatively simple to implement, reach convergence simple and quick way and generate reasonable results for different types of turbulent flows. But characteristics such as incorrect prediction for swirling and rotating flows, flows with strong separation, axis symmetric jets, certain unconfined flows and fully developed flows in non-circular ducts make this unfeasible model. In most research it is used as a starting point so that the researcher has his first contact with the modeling of turbulence, afterwards it is replaced by more consistent turbulence models for correct reproduction of the phenomenon being studied. Yang and Błasiak (2006) showed in their work for modeling the flameless combustion that this model is unable to reproduce efficiently the characteristics of the regime such as the areas of recirculation exhaust gas being necessary the application of turbulence models more robust and efficient.

The k-ε realizable model was developed recently and differs from the k-ε standard model for contain a new formulation for the calculation of turbulent viscosity and a new transport equation. The term "realizable" means that the model meets certain mathematical constraints present in Reynolds tensor. This model is more accurate in the reproduction of flows involving rotation, boundary layers under strong adverse pressure gradient, separation and recirculation.

The Reynolds Stress Model (RSM) has superior prediction performance to eddy-viscosity models, the main justification for their performance is that the RSM is based on transport equations for the individual components of the tensor of Reynolds stresses and the dissipation rate. This model is characterized by a high degree of universality and contra entry offers a high degree of complexity. Another feature is the spent computational time by the use of RSM due to increased transport equations to be solved. But what attracts attention for this study is its ability to accurately reproduce the phenomena that occur within combustors.

Rochaya (2007) used the turbulence models k-ε Standard and RSM in your simulation to flameless combustion of biofuels. The k-ε standard model was chosen because of the greater possibility of convergence compared to more sophisticated turbulence models and the RSM model by adapting well for modeling strongly swirling flows. The author showed that both models positively reproduce the experimental results. An analysis of the profiles of axial velocity of the air flow (see Fig. 1) shows that in regions close to the fuel injection point the two turbulence models satisfactorily reproduced the experimental results available for numerical simulations.

Zhu et al. (2011) reported in its conclusions that the components of air velocity measurements at different points of the simulated combustion chamber in his work showed good agreement with the experimental results for the turbulence model k-ε standard with enhanced wall treatment.

Jamali (2014) examined the influence of turbulence models k-ε standard, k-ε realizable and RSM in modeling the flameless combustion to burn ethanol and noted that the distribution of axial and radial velocities are consistent with the experimental values available for simulation, since the temperature distribution is influenced by three models. For the k-ε standard model the temperature peaks inside the combustion chamber is presented below the experimental values while for the k-ε realizable model and RSM the peak temperatures were above experimental data. This behavior is due to scalar dissipation rate which is a function of the mixing ratio between the phases flow (continue (air) and diperse (ethanol droplets)) and turbulence variables that directly affect the temperature range of the flame and its structure.

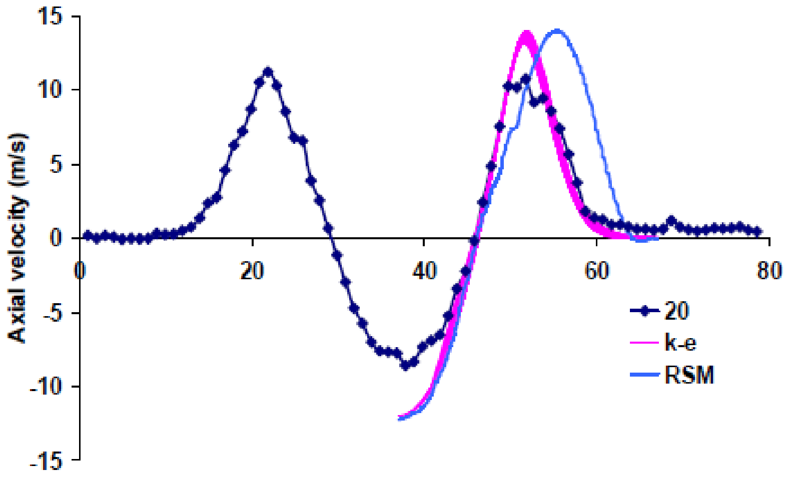

Figure 1 – The distribution of axial velocity inside the combustion chamber. (Rochaya, 2007).

An overview of available works in the literature shows that few are related to flameless combustion, most research involving numerical modeling of liquid fuel sprays is for applications to conventional combustion systems. Therefore more in-depth studies on turbulence modeling are necessaries in order to examine the possibility of applying other turbulence models present in the CFD tool and also aimed to evaluate the constants involved in these models for correct reproduction of the flameless combustion.

2.2 Combustion models

As well as the turbulence models there are several combustion models available in CFD tools for modeling conventional combustion systems and the flameless combustion. For the latter regime numerical simulations for burning liquid fuel sprays is still a little explored area with sparse information.

Among the models used for modeling the combustion of liquid fuel sprays are the steady laminar flamelet model and the Flamelet Generated Manifold (FGM).

The steady laminar flamelet approach models a turbulent flame brush as an ensemble of discrete, steady laminar flames, called flamelets. The individual flamelets are assumed to have the same structure as laminar flames in simple configurations, and are obtained by experiments or calculations. The laminar flamelets are then embedded in a turbulent flame using statistical PDF (probability density function) methods. The advantage of the laminar flamelet approach is that realistic chemical kinetic effects can be incorporated into turbulent flames. The chemistry can then be preprocessed and tabulated, offering tremendous computational savings. However, the steady laminar flamelet model is limited to modeling combustion with relatively fast chemistry. The flame is assumed to respond instantaneously to the aerodynamic strain and thus the model cannot capture deep non-equilibrium effects such as ignition, extinction, and slow chemistry (like NOx).

The Flamelet Generated Manifold (FGM) is a chemistry reduction method that combines the advantages of dimension reduction techniques based on chemical steady-state assumptions and flamelet models. This model assumes that the scalar evolution (that is the realized trajectories on the thermo-chemical manifold) in a turbulent flame can be approximated by the scalar evolution in a laminar flame. Both laminar flamelet and FGM parameterize all species and temperature by a few variables, such as mixture-fraction, scalar-dissipation and/or reaction-progress, and solve transport equations for these parameters in a 3D CFD simulation. Its advantages are the precise modeling of physical and chemical phenomena of flame, the effects of fuel and emissions.

Ma et al. (2013) presented the modeling of flameless combustion from ethanol sprays using the laminar steady flamelet model and noted that there was a failure in the prediction of ignition and the flame extinction in high stress regions, especially near the fuel injector. This model was not able to reproduce the flameless combustion regime as shown in Figure 2, where a high concentration of OH radicals (hydroxyl radical) in the region near the nozzle is noted, representing a concentrated and well-defined flame.

Bekdemir (2008) and Jamali (2014) also modeled the flameless combustion of liquid fuel through the laminar steady flamelet model. Bekdemir (2008) noted that the fuel suffer auto ignition early and very low maximum combustion temperature. Jamali (2014) has shown that the present combustion model generated just a reaction zone with a high concentration of OH radicals in the vicinity of the nozzle, corresponding to the conventional combustion regime.

Jamali (2014) also conducted simulations for the flameless combustion regime applying in combustion modeling the FGM. The numerical results were compared to experiments and its conclusions the author states that FGM reproduced correctly two combustion zones with homogeneous distribution of OH radicals which characterizes the flameless combustion (See Fig. 3).

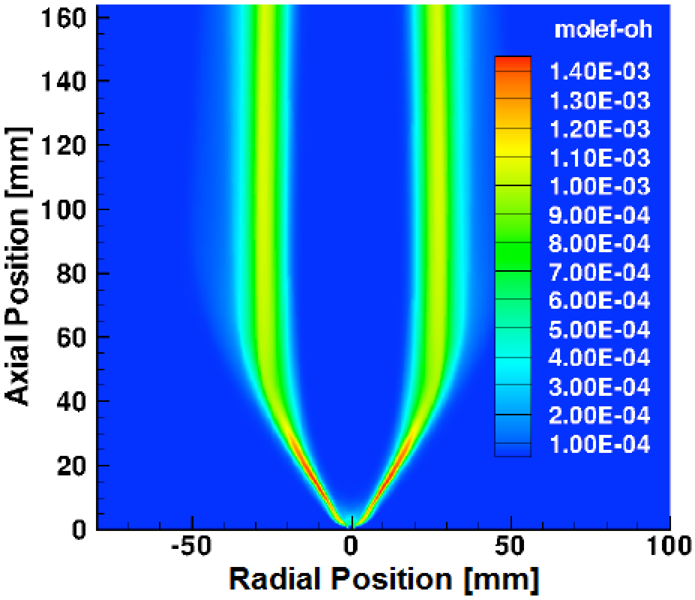

Figure 2 – Distribution of hydroxyl radical, OH, using the laminar steady flamelet model (Ma *et al.* 2013).

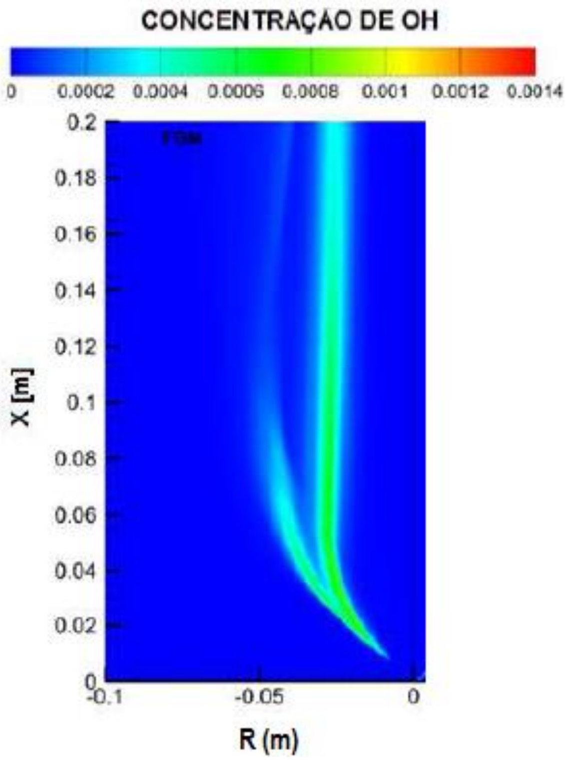

Figure 3 – Distribution of OH radicals in the flame obtained through combustion model FGM (Jamali, 2014).

The modeling of flameless combustion of liquid fuel is still little explored and as previously seen the most widely used models are the steady laminar flamelet and FGM, so further studies should be conducted addressing the other models available on CFD in order to analysis its viability in the reproduction of this new combustion regime.

2.3 Modeling of turbulent sprays

A spray is considered a multiphase flow where are found in the domain a dispersed liquid phase in the form of drops and a gaseous continuous phase (Sirigano, 2010). The formation and development of a spray involves transport and dynamic fluid phenomena fairly complicated as heat transfer, mass transfer and momentum transfer between droplets that are formed in the spray and droplets vaporization rate. The combustion sprays is a very complex subject to discuss because of the presence of a spatial distribution of temperature, concentration gradients, internal circulation of liquid and also the interaction between drops.

The modeling of multiphase flows in CFD environment can be performed by the Eulerian-Eulerian multiphase model or through the Lagrangian Particle Tracking the multiphase model also known as Discrete Phase Model. The latter model is more used because it provides more completes information about the behavior of particles, turbulence modeling can be added automatically and the computational time involved is much lower compared to the Eulerian-Eulerian multiphase model. The discrete phase modeling allows simulating a wide variety of problems involving discrete phases such as spray drying, dispersion aerosol coal combustion and liquid fuel combustion.

The sprays liquid fuel combustion is directly affected by the interaction between the liquid phase and the gas. The liquid phase is that provides fuel to the development of combustion and is also responsible for adding momentum to the flow within the chamber to accelerate the gas phase. The most important phenomena that occur in turbulent combustion is spray atomization, the turbulent dispersion, evaporation, micro-mixing and combustion (Jamali, 2014).

Atomization is not well understood yet because of the difficulty of access to the densest region of the spray both experimentally and numerically. Most numerical simulations begin with the already atomized spray with an initial distribution of droplets defined by experimental tests (Gutheil, 2011).

When working with CFD tools are available various types of spray injection, as an example are mentioned: single, group, hollow cone, solid cone and surface. Each of these types requires some initial input conditions such as position, speed, droplet diameter and mass flow. During the atomization of liquid fuel also occur phenomena such as break-up and the collision of drops and both can be modeled. Modeling drops break-up is common in most found work and the collision between droplets can be neglected when the spray is already considered in atomized form.

For the drops break-up modeling are also found several models in CFD tools, an analysis of available works in the literature involving the combustion of sprays shows that one of the most used models is the Linearized Instability Sheet Atomization, LISA, which simulates the break-up effects in primary pressure-swirl atomizers. Other models like Blob Method, Enhanced Blob Method and Turbulence Induced Atomization are also available for the primary break-up modeling, but in order to apply them must take into account the type of injector being simulated.

Ma et al. (2013) has used the LISA model to simulate the ethanol injection and spray atomization in a combustion chamber. The author showed that for several axial positions in the combustion chamber the numerical results of the Sauter mean diameter showed good agreement with the experimental values and the same was observed for the axial velocity distribution of the droplets, as shown in Figure 4.

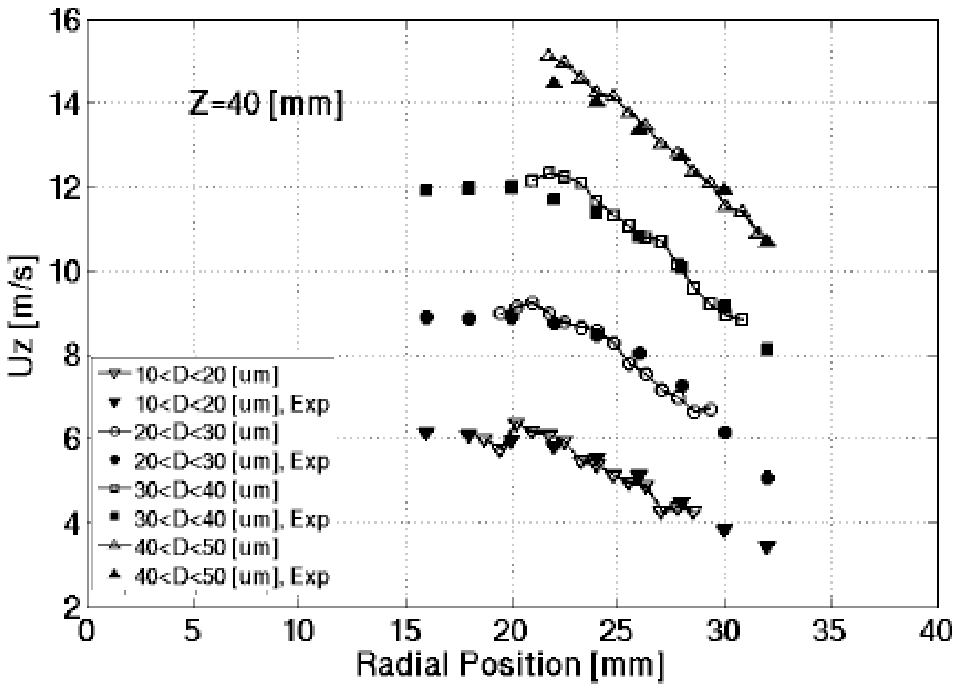

Figure 4 – The distribution of axial velocity of the droplets within the combustion chamber (Ma et al. 2013).

Jamali (2014) also applied the LISA model in their simulations to ethanol spray combustion based on the type of injector modeled in their work which is of type pressure-swirl atomizer. In Figure 5 are compared to the axial velocity profiles obtained experimentally and in numerical simulations which have a very next behavior, then it is concluded that this model is satisfactory to atomization modeling.

In the CFD tool are available models for droplets secondary break-up such as Reitz and Diwakar Break-up Model and Taylor Analogy Break-up (TAB) Model. However, due to combustion the majority of authors despise the secondary break that comes not happen because of the high temperatures involved in these processes.

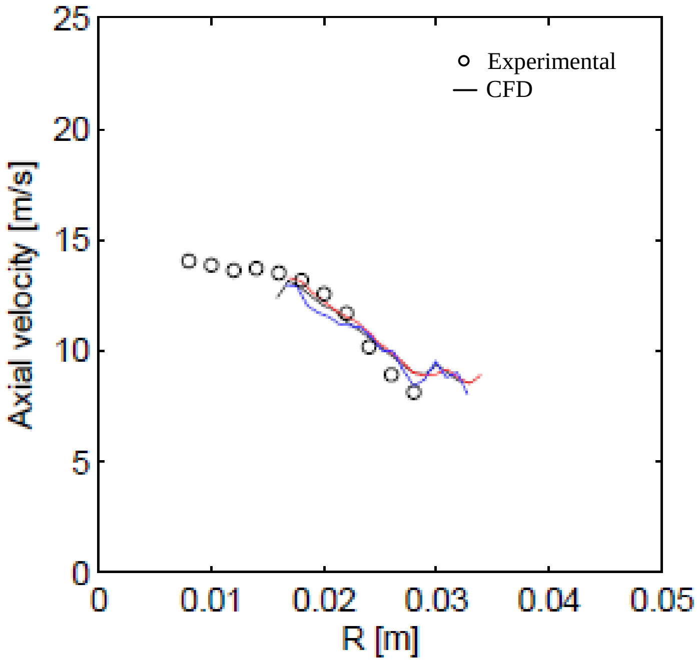

Figure 5 – Axial velocity distribution of the spray droplets to the LISA model (Jamali, 2014).

3. CONCLUSIONS

As discussed in this paper the flameless combustion of liquid fuels modeling is not trivial because of the large number of parameters and phenomena involved in this process.

An overview of current work on the literature shows that research into the flameless combustion of ethanol are recent, unlike what happens with gaseous fuels where the studies are at an advanced stage.

In this study, given the word limit, it was presented only the most relevant numerical researches available in the literature for flameless combustion of ethanol, in which the main models of turbulence, combustion and modeling of turbulent sprays are highlighted.

Among the turbulence models studied RSM model has greater potentiality in representing the flameless combustion of turbulent sprays, promoting better distribution of the fuel within the combustion chamber. But new models need to be investigated even the RSM model that presents extra equating resulting in sub-models that are better suited to the type of spray that is intended to simulate.

Regarding combustion models, the authors highlighted in present work and also in the literature emphasize the use of laminar steady flamelet models and FGM. The conclusions show that the laminar steady flamelet can be discarded to simulate the flameless combustion for liquid fuels for failing to flame prediction, because the fuel enters into self-ignition early and temperatures in the combustion atmosphere are very low. But the FGM model appears very effective in representing the temperature field generating very accurate results. But researchers from the area of combustion encourage the implementation of combustion models such as the Finite Rate Chemistry and Finite Rate / Eddy dissipation that have a more robust equating for representing combustion regimes like flameless.

Finally, the modeling of sprays is an issue that depends on the type of spray to be modeled. Until now the sprays use the swirl mechanism and the LISA model has generated very precise results and promotes a good distribution of the fuel droplets in the spray area.

The general conclusion of this study shows that there is much to study for modeling the flameless combustion of liquid fuels from the standpoint of numerical models used, for although some models stand out, there is a wide range of numerical models available in CFD numerical tool that can reproduce efficiently this regime involving less computational time and generating accurate results.

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