# NUMERICAL SIMULATION OF A DRY LOW NO<sub>X</sub> – LPP COMBUSTOR OPERATING WITH LPG FUEL

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Abstract. Last years new technologies in gas turbines involve the use of lean premixed prevaporized (LPP) combustors for achieving new restrictions on emission levels. The main advantage of LPP combustors is the small emission of  $NO_x$ , avoiding the high temperatures of near stoichiometric operation, largely responsible for  $NO_x$  production, designated thermal  $NO_x$ . The design of LPP combustors is a complex task and, nowadays, has employed Computational Fluid Dynamics (CFD) codes in the flow field study and reaction process, although reduced mechanisms are used due to the required computational effort for carrying out turbulent 3D simulations with available detailed mechanisms. Also interactions between turbulent flow field and chemical kinetics require an accurate model to obtain good prediction about flow field and reaction rates. Model limitations like that are responsible by great difficulties for predicting pollutants emissions in modern combustors of low emission level, considering relative importance of diverse pathways. So choice of appropriate models is a key point to obtain relative consistency of results and to validate any simulation. This paper presents the simulation of a real LPP combustor with combustion at two stages built at University of Brasília for small plants operating with liquefied petroleum gas (LPG) fuel at full load. Different combustion models of a commercial CFD code are tested and, by means of comparisons between available experimental data and numerical results, a combustor model is investigated to be used in prediction and developments of LPP combustors.

### **1** INTRODUCTION

The combustors design has as main objectives high combustion efficiency, easy ignition, a large range of operation and minimal pollutant emissions [1]. In the design of modern combustion systems, control of pollutant emissions is a major factor due to stringent emission standards to reduce air pollution and its harmful effects.

Oxides of nitrogen are one of the most important pollutants produced from fossil fuel combustion which notedly consist of nitric oxide (NO) and nitrogen dioxide (NO<sub>2</sub>), so those are referred under the general designation of  $NO_x$ . Emissions of  $NO_x$  are directly responsible for the photochemical smog, acid precipitation, deterioration of the ozone layer and human health problems.

In the traditional combustors with diffusion flames, targets of reduction of fuel consumption and CO and UHC emissions are in conflict with  $NO_x$  emissions, because the major mechanism for NO formation is the oxidation of  $N_2$  by the  $O_2$  at high temperature and sufficient residence time, named thermal NO. Strategies to control  $NO_x$  emission act mainly reducing peak temperature and oxidation of organically bound nitrogen in the fuel.

Among the technologies for low  $NO_x$  emission, it's possible to make staged combustion with zones designed to optimize different combustion aspects. At small partial loads a primary zone may be operated with equivalence ratio around 0.8 to obtain minimal CO and UHC emission. That zone, at power conditions works as a pilot flame to provide heat for the main zone of lower equivalence ratio, operating with premixture and equivalence ratio around 0.6 to reduce  $NO_x$  emissions. Staged combustion has been successfully used to reach  $NO_x$  restriction rules at industrial plants without the use of steam or water.

The LPP technology is used for low-  $NO_x$  combustors operating with liquid or gas fuels. Such technique consists in vaporizing the fuel and carry out a homogeneous mixture with air at low equivalence ratio before the combustion. So it's possible to avoid high  $NO_x$  emissions of droplet burning due to high temperatures at regions of high equivalence ratio. The main drawbacks concern the possibility of self ignition and flame return at high pressures and full load conditions. LPP technology can be used together variable geometry and staged combustion to solve main difficulties.

Another option of low-  $NO_x$  characteristic is RQL (Rich-burn/Quick-quench/Leanburn) combustion. That technology involves combination of two combustion zones: the primary one rich in fuel and the secondary one of low equivalence ratio. Afterwards the primary zone, additional air sufficient to complete the combustion and to lower temperature is injected at a manner to promote a fast and uniform mixture with primary gases. That fast mixture is essential to avoid thermal NO formation [2].

Other technology adopted is that of catalytic combustion for LPP combustors. Air and fuel are mixed at extremely low equivalence ratio then it flows for a catalyst that allows combustion can occurs at a condition out of flammability limit for gas combustion. But the materials used in catalyst are expensive and its durability must be considered due to high temperatures and rough ambient involving combustion. Drop pressure must be taken in account too for those systems because the inevitable flow obstruction imposed by catalyst [3]. Those technologies described above don't use water or steam, so are designated Dry Low-  $NO_x$  (DLN). Low  $NO_x$  emissions could be obtained with the injection of water or steam in the flow. Water injection is responsible for decreasing temperature and alters chemical kinetics, mainly O radical concentration for  $NO_x$  production [4]. The injection of water or steam can be made before the swirlers for good homogeneity and atomization (for water) or in combustion zone with injectors well positioned. The water amount required is considerable, around 40% of fuel mass flow at liquid phase (for steam the amount required can be 60% greater because the lower capability to absorb heat) and must be of great quality to avoid corrosion and deposit formation. Therefore, adoption of that technology is restricted to places where pure water is available. Other problems are related with flame oscillation and increase in CO emission with temperature reduction [4].

In this paper we present the analysis of a LPP turbine combustor based on CFD modeling. More specifically, the combustor flow is investigated by the FLUENT 6.3 code according operations conditions at full load with LPG fuel used in an experimental work from laboratory LEA at University of Brasília [5]. Pollutant emissions are used to compare different combustion models to obtain better agreement to experimental data.

### 2 THE DLN LPP COMBUSTOR

As development for a micro turbine of research applications at University of Brasília, a combustor LPP was designed, based on General Electric DLN-1 combustor. That is a LPP combustor of staged combustion concept (two stages) for operation in an overall range with natural gas and liquid fuel, as showed in Figure 1.



Figure 1: The DLN LPP Combustor.

It has six radial fuel primary injectors and an adjustable secondary one located in combustor centerline. Each injector has a swirler with 8 blades of 60° and a venturi is responsible for anchoring flame in the secondary combustion zone. A dilution zone is downstream where occurs mixture of dilution air and combustion gas to reduce turbine inlet temperature. According load level, the combustor can operate at three different modes. In the range of load from 0 to around 20%, fuel is injected inside the six radial injectors while air for a diffusion flame is supplied in a bit excess. At partial load in the range close to 20% until 50% the fuel injection is divided between centerline and radial injectors: around 30% of fuel is injected in the center and low equivalence ratio is applied for both combustion zones. Above half load, around 17% of fuel is directed for centerline injector which acts as a pilot flame for the lean fuel-air mixture from radial injectors. That last operation condition, based on LPP and two stage combustion zones is investigated in the present study, according experimental conditions used by Ferreira [5].

#### **3** MATHEMATICAL EQUATIONS

Description of flow field is based on the numerical solution of mass conservation, Navier-Stokes and energy equations, considering production and consumption of the chemical species involved.

Net production/consumption rates of species involved are calculated according Arrhenius model for finite chemical rate and turbulence macroscale mixture process for eddy dissipation model that considers the minimum rate for a species n in the reaction m among the expression (1) involving reactants, R, and expression (2) involving products, P:

$$q_{n,m} = v'_{n,m} (M_w)_n A \rho \frac{\varepsilon}{k} \min_{R} \left( \frac{Y_R}{v'_{R,m} (M_w)_R} \right)$$
(1)

$$q_{n,m} = v'_{n,m} (M_w)_n A B \rho \frac{\varepsilon}{k} \left( \frac{\sum_{p} Y_p}{\sum_{j}^{N} v''_{j,m} (M_w)_j} \right)$$
(2)

### **4** COMPUTATIONAL MODEL

In order to simulate the flow field in the LPP combustor, a computational model with the centerline swirler for pilot flame, the venturi, a dilution air inlet and the six radial inlets for air-fuel premixture, based on combustor geometry, has been constructed using the Gambit 2.4 commercial software. The volume is divided in some portions in order to facilitate following mesh control. A mesh using 594812 elements, mainly hexahedrals, and 467300 nodes was made for running simulations with FLUENT 6.3 commercial package, as presented in figure 2.



Figure 2. Computational mesh

To model the fuel, LPG composition was considered according Brazilian specifications limits. In such way LPG composition can be assumed, in practice, as a mixture of propane and butane whose constitution is found in a range of 30/70 until 60/40 of propane/butane volumetric rate [6]. So, LPG fuel is considered to be formed by only a propane/butane mixture at rate of 50/50, that allows adopt for combustion models the reduced mechanisms available for propane and butane.

Different boundary conditions are considered for the four inlets: central fuel inlet, central air inlet, the six mixture inlets and dilution air, according experimental conditions for premixed mode described by Ferreira [5], based on mass flow. Velocity profile in the model is taken normal to central fuel and central air sections. For the six mixture inlets and dilution air intake the profile has an axial and a tangential component to try to reproduce swirler effect. Time-averaged simulations are considered with  $k - \varepsilon$  turbulence model.

# **5 RESULTS**

Operational condition of DLN LPP combustor used as reference for the computational model is presented in table 1. It's possible to observe lean condition for global operation despite of rich pilot flame.

	Global	Excess air inlet	Pilot inlet	Radial inlets
Air flow [kg/s]	0.200	0.11956	0.011555	0.068885
Fuel flow [g/s]	2.5640	0	1.2405	1.3235
Equivalence ratio	0.48	0	1.62	0.29
Air temperature [K]	-	368.15	323.65	323.65
Pressure [kPa]	-	107.42	107.42	107.42

Table 1: Operational conditions used for the computational model.

# 5.1 Standard eddy dissipation model

Analysis of turbulent flame regime suggests that combustion process is limited by the turbulent mixture process in the DLN LPP combustor. So at the first simulations it was adopted eddy dissipation as combustion model. With standard constants to reaction rates, CO oxidation process was too fast, occurring in a very little zone. By that means temperature prediction was always close to adiabatic flame temperature (much greater than normal LPP maximum temperature) and a very high  $NO_x$  formation was found with thermal path.

	CO [ppm]	<i>CO</i> <sub>2 [%]</sub>	NO <sub>x [ppm]</sub>	<i>O</i> <sub>2 [%]</sub>
Computational model	0	2.47	205	16.6
Experimental data	435	1.35	17	18.6

Table 2: Emissions with standard eddy dissipation combustion model compared to experimental data.

#### 5.2 Finite rate/eddy dissipation model

Due to fast reaction process observed with eddy dissipation model, a new approach was tested with the finite rate/eddy dissipation model. That model uses the lowest reaction rate among chemical kinetics and eddy dissipation model. In that case two step mechanisms were used for propane and butane combustion according simplified reactions proposed by Westbrook and Dryer [7]:

$$C_3H_8 + 3.5O_2 \rightarrow 3CO + 4H_2O \tag{3}$$

$$C_4 H_{10} + 4.5 O_2 \rightarrow 4 CO + 5 H_2 O$$
 (4)

$$CO + 0.5O_2 \rightarrow CO_2 \tag{5}$$

Activation energy for reactions (3) and (4) was modified to 21,7 kcal/mol to anchor the pilot flame at a right position whose was permitted to increase the CO consumption zone but with a high temperature profile (figure 3) and almost no CO emission was observed due to a fast oxidation with the turbulent limited process.



Figure 3. Temperature prediction with finite rate/eddy dissipation model.

Despite of better description of initial reaction phase, concentrated CO consumption implies a low CO emission and high temperature level, responsible for the  $NO_x$  over prediction observed. Emissions results with that model are presented in table 3.

	CO [ppm]	<i>CO</i> <sub>2 [%]</sub>	NO <sub>x [ppm]</sub>	<i>O</i> <sub>2 [%]</sub>
Computational model	5.8	2.47	159	16.6
Experimental data	435	1.35	17	18.6

Table 3: Emissions with finite rate/eddy dissipation combustion model compared to experimental data.

### 5.3 Modified finite rate/eddy dissipation model

In order to obtain a better agreement with experimental data, eddy dissipation model was modified to provide lower rates for initial process of fuel oxidation and  $CO_2$  formation. As characteristic time of turbulence macroscale is function of turbulence model, it was necessary to adjust constants of eddy dissipation model to the simulated flow conditions of DLN LPP combustor with  $k - \varepsilon$  turbulence model.

Reaction	Constant A	Constant B
(1)	2.00	0.25
(2)	2.00	0.25
(3)	3.20	0.40

Empirical model constants that multiplies inverse of big scale characteristic turbulent time were set up according values presented in table 4.

Table 4: Constants used for 2-steps mechanisms with eddy dissipation model.

At this point was possible to obtain a good approximation of CO emission results, and reduced  $NO_x$  emissions avoiding the contribute of high local temperature, as can be seen in figure 4, with the prediction of temperature field for the modified model. Table 5 presents the results for emissions, where can be observed the great  $NO_x$  reduction after the model changes.



Figure 4. Temperature prediction with modified finite rate/eddy dissipation model.

	CO [ppm]	<i>CO</i> <sub>2 [%]</sub>	NO <sub>x [ppm]</sub>	<i>O</i> <sub>2 [%]</sub>
Computational model	408	2.40	2.2	16.7
Experimental data	435	1.35	17	18.6

Table 5: Emissions with modified eddy dissipation combustion model compared to experimental data.

### **6** CONCLUSIONS

A model for the DLN LPP combustor operating at full load with LPG fuel was developed with  $k - \varepsilon$  turbulence and eddy dissipation models. The  $k - \varepsilon$  model was choosen due stability and low computational resources required. With a 2-steps reduced mechanism it's possible to calibrate the model to obtain a good agreement with CO emission experimental data. For others turbulence models it's necessary to alter eddy dissipation constants in order to adjust CO production/consumption rates.

A more accurate experimental investigation of flow with otical access would permit to describe and to adjust better the reacting zone.  $NO_x$  emissions present considerable absolute discrepance but results near operation condition suggest the same trend.

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