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CFD RE-DESIGN OF A GAS TURBINE CAN-TYPE COMBUSTION CHAMBER HYDROGEN FIRED

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Abstract. *Hydrogen supply in gas turbine requests the development of the combustion chamber to limit the NO_x emissions avoiding flash-back and auto ignition phenomena.*

The object under investigation is a silo combustion chamber installed on a 10 MW class heavy-duty gas turbine. The aim of the work was to investigate some modifications for the combustion chamber 100% hydrogen fired in dry operation, in order to reduce the NO_x production. The investigation was mainly focused on the burner, while the liner was not substantially changed. The swirler and the fuel injection holes were redesigned in order to achieve a better fuel-air mixing and a higher air flow rate in the primary zone of the combustor; each solution maintains a diffusion flame scheme in order to be adopted in industrial solutions.

The proposed modifications were analyzed by a 3D CFD RANS reactive procedure based on commercial codes. The methodology was previously validated by a comparison with the experimental data coming from the full scale tests of the original combustor version. Full scale tests were performed also on the modified version methane fired. In house-codes were developed for the post-processing of the numerical results. The numerical analysis has shown that the modified version allows a reduction of about 30% on the NO_x emissions.

Finally, preliminary considerations related to the fuel injection scheme and to the effect of the main injection condition on the mixing performance, were carried out together with some estimations for NO_x emissions containment.

1. INTRODUCTION

The use of alternative fuels in gas turbine combustion chambers can provide advantages such as lower environmental impact. In particular, the hydrogen's use as fuel is an important research area because no CO, UHC and PAH are produced by hydrogen combustion. Moreover, if hydrogen is produced by renewable energy, the net CO_2 production is zero. However, hydrogen combustion produces much more NO_x than traditional fuels because of its higher flame temperature. Hydrogen has a higher flame propagation velocity and a wider air-fuel ignition range than CH_4, so that its employment in premixed combustion can cause problems of flashback and explosions. So, from an industrial point of view, hydrogen can be used in non-premixed combustion systems and the methods for reducing pollutant emissions can be borrowed from those used in diffusive gas turbine combustion chambers fired with CH_4, with the advantage that for hydrogen, there are no limits due to CO or UHC production.

In this paper, modifications of the silo gas turbine combustion chamber are investigated in order to reduce NO_x emissions with hydrogen operation.

It's of interest to study minor modifications limited to the burner, maintaining unchanged its maximum radial dimension in order to not modify the liner. As shown by numerical simulations performed by Riccio et al. [1], bad fuel-air mixing is a characteristic of the original version of this combustor. Mixing improvement can be achieved by redesigning the swirler and the fuel injection holes in order to increase the airflow rate in the combustor primary zone and to improve the radial and tangential hydrogen distribution.

Two different modified models were developed varying the swirler and the fuel injection scheme.

The impact of modifications on fuel-air mixing, temperature field and NO volumetric formation rate was evaluated using a CFD 3D RANS reactive procedure validated by comparison with the experimental data. The FLUENT commercial code [2] was employed for numerical simulations. Simulations show that the proposed modifications could reduce NO_x emissions up to 30%.

2. DESCRIPTION OF THE COMBUSTOR CHAMBER

The combustor under investigation is installed on a 10 MW class heavy duty gas turbine, suitable for power generation. Figure 1 shows a schematic view of the combustor. The combustion chamber is a reverse-flow single-can design equipped with a diffusion flame burner.

In Table 1, the working parameters at the full-load ISO conditions are given. The burner contains an axial swirler. The fuel injection holes are located in the swirler between two adjacent blade vanes, in an alternating pattern.

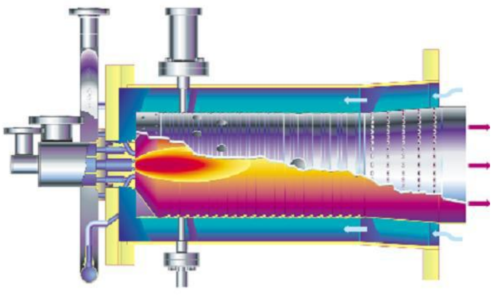


Figure 1: Combustion chamber under investigation

p	[bar]	15,6
T air	[K]	687
m air	[kg/s]	36,5
m H_2	[kg/s]	0,292

Table 1: Combustor working parameters at full-load ISO conditions

3. VALIDATION OF THE NUMERICAL PROCEDURE

Modeling a typical gas turbine combustion process requires a turbulent combustion model to reproduce the interaction between chemistry and turbulence, a turbulent model and a chemical model for the definition of the chemical species and their reactions.

Barlow and Carter [3] have shown that a non-premixed hydrogen turbulent flame with steady state boundary conditions is characterized by very complex structure and chemical kinetics. So, the choice of the combustion model must be made carefully. The commercial code used in this work for numerical simulations contains different combustion models, some specific for non-premixed flames (like the mixture fraction-equilibrium model, the laminar flamelet model, and the Monte Carlo PDF model), and some specific for partially premixed flames and other models for generic reactions like EDC.

The Monte Carlo PDF model treats reaction exactly and evaluates PDF considering physics and chemistry of the system [4]. However, such model has two main disadvantages: 1) it's very computationally expensive (it's currently affordable only for reduced chemistry [5,6]) and 2) it requires the modelling of the molecular transport.

Also the EDC model is rather computationally expensive because it solves so much transport equations as the chemical species included in the kinetic mechanism. Besides that, the EDC model can produce mean temperature's spurious peaks in the reaction zone [4].

Some studies on hydrogen combustion [3], [7] lead to assume that partially premixing in hydrogen non-premixed turbulent attached flames is not a relevant phenomenon; for this reason, the use of a partially premixed combustion model was discarded.

For all the above mentioned reasons, the Mixture Fraction-equilibrium and the Laminar Flamelet models seem to be the more appropriate, among the available combustion models, for the industrial combustor analysis. They allow the simulation of complex chemistry in complex geometries using pre-processing tables for the evaluation of temperature and chemical variables. The assumed PDF method used by the Laminar Flamelet model (the mixture fraction model is very similar) works reasonably well for non-premixed combustion [8]. In the mixture fraction approach, chemistry is modelled in a less accurate way than in the laminar flamelet one (only the equilibrium is considered) but this model results less computationally expensive and above all some CFD commercial codes don't require the user to implement the equilibrium kinetic mechanism.

The numerical analysis developed by Riccio et al. [1] showed that for the combustion chamber under investigation, the Laminar Flamelet model gives a better agreement than the Mixture Fraction model with the available experimental data.

For the modelling of the turbulence chemistry interaction β PDFs were employed [2].

The choice of the Laminar Flamelet model requires to verify that the characteristic turbulence and chemistry time and length scales of the combustor under investigation are consistent with the Flamelet combustion regime. Basing on the diagram proposed by Veynante and Vervish [9] for turbulent diffusion flames, the Flamelet model seems to be appropriate for the simulation of the investigated combustor.

In order to take radiation into account, non adiabatic pre-processing tables were used; the combustor's solid walls were considered to be adiabatic.

A RANS approach with a k-ε realizable model was selected for turbulence modelling. In addition, numerical simulations were employed using the kinetic mechanism "Hydrogen37" proposed by Peters and Rogg [10]. This mechanism contains 13 species and 37 reactions.

NO_x chemistry is too slow to be accurately represented by the Laminar Flamelet model: the use of a specific modelling tool is required for the accurate evaluation of NO_x. In hydrogen combustion, only NO_x generation from the intermediate N_2O [11] and from the Zeldovich mechanism must be considered. The tool used in this work solves a transport equation for nitric oxide (NO). NO_x was calculated by the post processing of the reactive simulations. NO_x chemistry and turbulence interaction was modelled using assumed shape PDF distributions of temperature.

The working pressure, the inlet temperature and mass flow rate of fuel and air, and the air split were imposed to the numerical simulations as boundary conditions from the experiments. The experimental data available for the validation of the numerical analyses are NO_x and H_2 concentrations, which were measured at the transition piece exit section. The transition piece was not included in the solid domain in order to reduce the computational costs and to speed up the numerical simulations. It can be noted that in all cases, CFD underestimates NO (Table 2). The CFD and experimental data about NO_x emissions are not relative to the same combustor positions in the CFD calculations NO_x concentrations were evaluated at the liner outlet. In addition, the CFD simulations show that at the combustor outlet (where NO_x concentration is calculated) there are hot spots with temperature close to 2000 K. Therefore, it can be expected that a small but not negligible amount of NO_x is generated within the transition piece. Besides that, H_2 concentration at the combustion chamber exit section results to be zero in all the numerical simulations, as in the experiments.

Thus, the agreement between the CFD and experimental data can be considered satisfactory.

The previously described numerical procedure was used to investigate modifications of the original gas turbine combustor for NO_x reduction.

			NO_x ppm@15%O_2		
LOAD	**1/AFR**	**T air [K]**	**EXP**	**CFD**	**% (EXP-CFD)/EXP**
90%	0,0076	692	693	656	5
90%	0,0081	649	672	563	16
90%	0,0083	624	579	495	14

Table 2: Experimental vs numerical NO_x concentrations at the combustor discharge

4. INVESTIGATION OF MODIFICATIONS OF THE ORIGINAL COMBUSTOR

Scientific literature reports two main different technologies for NO_x reduction in gas turbine combustion: dry and wet. With regard to dry approach, some general criteria are: producing a more homogeneous fuel-air mixture in the combustor primary zone [12], minimizing the simultaneous residence time of N_2 and O_2 in the region with the highest temperature [13], and reducing temperature in the combustor's primary zone. These approaches can be applied to the original gas turbine combustion chamber. The numerical simulations performed by Riccio et al. [1] underlined that the fuel air mixing is not homogeneous: H_2 distribution remains strongly localized near the mean diameter of the swirler; the air from the liner primary holes poorly interacts with the H_2 rich flow from the swirler. In addition, the original combustor has a relative low air flow rate from the swirler (3.9 % of the total); on the contrary, the air flow rate from the liner final part is relatively high.

Based on general guidelines suggested by scientific literature, dry modifications to the numerically analyzed combustor are proposed and investigated.

4.1. The solid models and the computational Grids

Figure 2 shows a view of the combustor's base version solid model. The actual geometry is rotationally periodic with respect to the combustor axis with an angle of 180°. This periodicity was reproduced in the solid model.

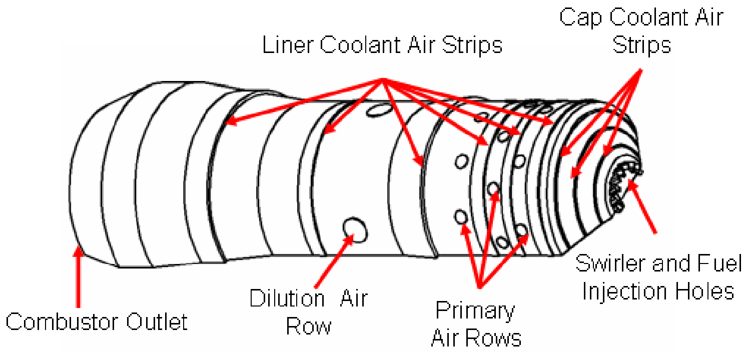


Figure 2: Base version solid model

The swirler and the fuel injection holes are identical to the real geometry.

The actual liner is characterized by a large number of slots and louvers for cooling; a coolant air flows modelling close to the real geometry implies highest computational costs. Besides that, NO production is supposed to be controlled mainly by the fuel-air mixing and to be scarcely influenced by the mixing between the hot gases and the coolant air, which is confined close to the liner. Finally, considering that the thermal exchange through the liner wall is beyond the scope of this work, a simplification of the coolant air geometry appears reasonable.

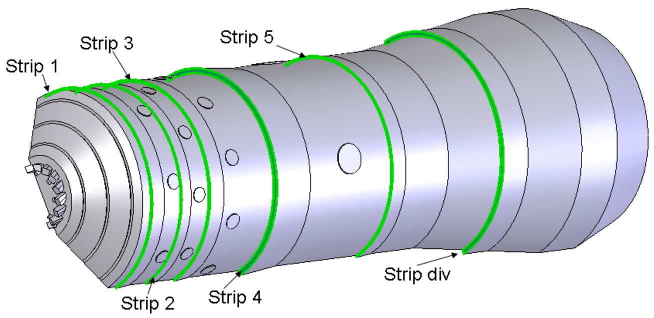
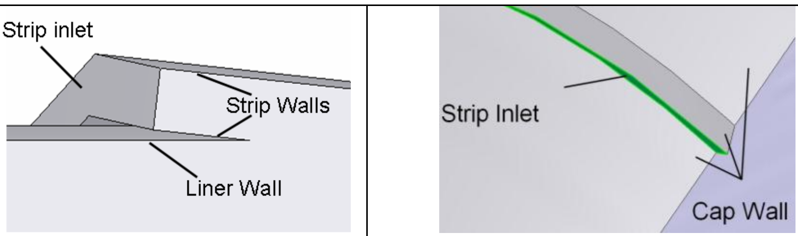


Figure 3: Views of the coolant strips

Both the louvers on the dome and the slots on the liner were collected in apposite strips (see Figure 2 and Figure 3). Three strips were defined on the cap, five on the cylindrical liner and one on the divergent liner. The strips both on the cap and on the divergent liner have the same total passage area of the correspondent louvers in the actual geometry.

For the strips definition, the cylindrical liner can be ideally divided into five portions, delimitated by its extreme positions and by the primary air and the dilution air rows. A single strip was associated to each of these parts (Figure 3): every strip has the same total passage area of the slots located in the correspondent part of the actual liner. Figure 4 shows detailed views of the coolant strips. For the liner strip, the walls were defined to be parallel to the slot walls in order to assign to the flow the same direction of the actual geometry. By this way, forcing each strip to have the same mass flow rate of the flows that are aggregated in it, the penetration of the cooling flows is similar to that of the real combustor.



(a) Solid Model Liner Strip (b) Solid Model Cap Strip

Figure 4: Views of a liner strip (a) and a cap strip (b)

In the following, the base and the modified versions of the combustor are referred to with the abbreviations BASE, MOD-B and MOD-C respectively.

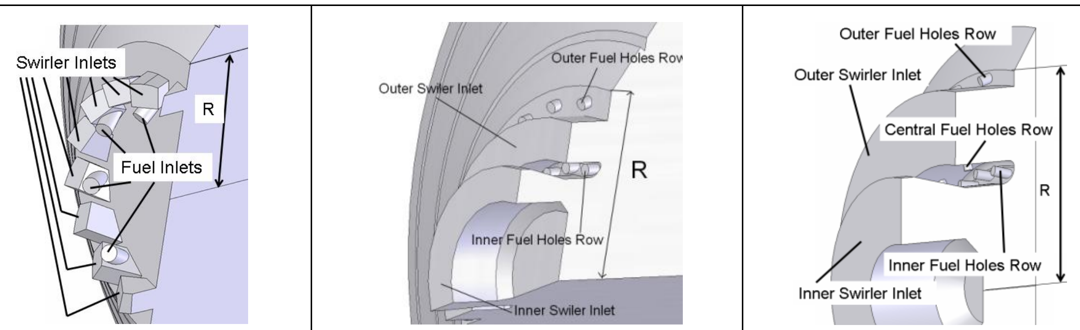
Also the modified versions of the solid model have a rotational periodicity of 180° with respect to the combustor axis. In the modified versions the primary and dilution air rows were not changed and the liner was modelled identically to the BASE configuration. The combustor re-design was performed at full load ISO conditions: air and fuel working conditions (pressure, inlet temperature, and global mass flow rate) were unchanged. Figure 5 shows the burner’s models for the BASE and the modified cases. The burner maximum radial dimension *R* was maintained identical. In the modified version, an axial double swirler with a larger overall effective area than the original was adopted to increase the airflow rate in the combustor primary zone. In particular, the air flow rate trough the double swirler is about 9%, 12% and 3,9 % of the total for the MOD-B, the MOD-C and the BASE version respectively. The inner and the outer swirlers are co-rotating and contain straight vanes that were not included in the solid model. The effect of the swirler vanes on the flow was accounted for imposing the actual flow velocity direction as boundary condition at the solid domain inlets of the two swirlers.

In all cases the air split is the same except for the swirler and the *Strip* 4 (see Figure 3). All the configurations are supposed to work with the same pressure loss in the combustor annulus and so with the same characteristic air inlet velocity. Therefore, in the MOD-x version the passage area of the *Strip 4* was decreased compensating the increase of the swirler area, in order to make the total air flow rate to be the same in all cases, maintaining the same $\Delta p/p$.

Double swirler characteristic parameters are given in Table 3.

		Stagger Angle [°]	air flow rate %	v [m/s]
MOD-B	**Inner Swirler**	45	6%	60
	Outer Swirler	45	3%	60
MOD-C	**Inner Swirler**	45	9%	60
	Outer Swirler	30	3%	60

Table 3: Double swirler characteristic parameters



(a) BASE (b) MOD-B (c) MOD-C

Figure 5: Swirler and fuel injection holes schemes views

To achieve a better local fuel-air mixing the number of the fuel injection rows and fuel holes in each row was increased.

Two and three rows were defined (Figure 5) in the MOD-B and the MOD-C respectively; in each row the fuel holes were equally spaced (Figure 6).

Fuel injection scheme characteristic parameters are reported on Table 4, where n is the number of fuel holes for row.

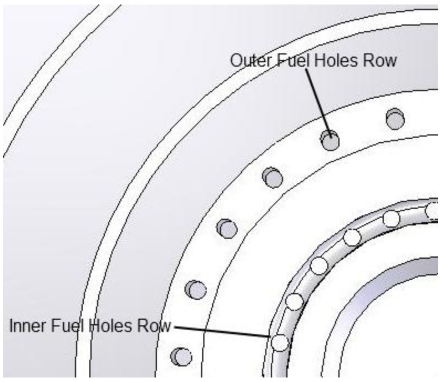


Figure 6: Frontal view of the modified burners

In the MOD-C, yaw and pitch angles to the fuel injection holes were adopted too. The fuel holes on the inner and the outer row give hydrogen a tangential velocity component that is counter-rotating with respect to the air swirler to promote an improvement of the fuel-air mixing. Besides that, the inner and the outer rows have respectively a positive (hydrogen is inward directed) and a negative pitch angle (hydrogen is outward directed), to extend as much as possible the mixing zone in the radial direction. For the outer row, the pitch angle must be defined carefully in order to avoid hydrogen to react too close to the cap walls, inducing excessive local metal temperatures. The central row is located at an axial position internal to the blade vanes, to promote fuel air partial premixing.

		Φ [mm]	pitch [°]	yaw [°]	n	v [m/s]
MOD-B	**Inner fuel holes**	5	0	0	24	239
	Outer fuel holes	5	0	0	24	239
MOD-C	**Inner fuel holes**	3,2	15	15	24	475
	Central fuel holes	2,7	90	0	16	490
	Outer fuel holes	3,2	-15	10	24	470

Table 4: Fuel injection scheme characteristic

The hybrid non-structured grids were generated by the commercial code *Centaur*™ (see Figure 7). The meshes are composed of prismatic layers near the solid wall delimiting the flow field and of tetrahedral elements within the flow volume.

Riccio et al. [1] developed a sensitivity analysis varying grids, using the same numerical procedure described for this work. They showed that a grid of about 2 million elements, opportunely refined in the primary zone and near the flow inlets, gives the most reasonable results. In this work, the same mesh was used for the base version and similar ones were built for the modified versions of the combustor.

Mesh quality near the wall can be characterized by y+ distribution on the wall surfaces. Standard wall functions require y+ values between 30 and 300 [2]. About 95% of the wall surfaces area has y+ values in the mentioned above range for the generated grids.

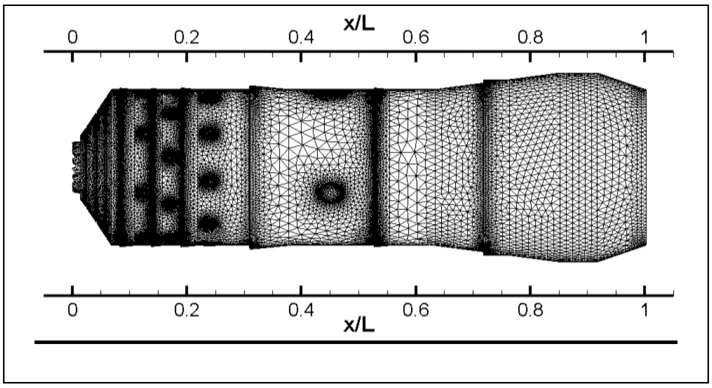


Figure 7: Views of the superficial grids

5. RESULTS AND DISCUSSION

The modified versions of the combustor described in the previous paragraph were numerically investigated and compared with the original one. Particular attention was paid to the differences in mixing field, temperature distribution and NO_x production.

5.1. Base Vs modified versions of the combustor

The planes used for the post-processing of the data are shown in Figure 8 and described in Table 5, with reference to the MOD-C combustor. In all the combustor's versions, thermo-chemical variables fields are not axial-symmetric. However a qualitative analysis of the spatial distributions on the periodic plane can be helpful for the understanding of the reactive phenomena.

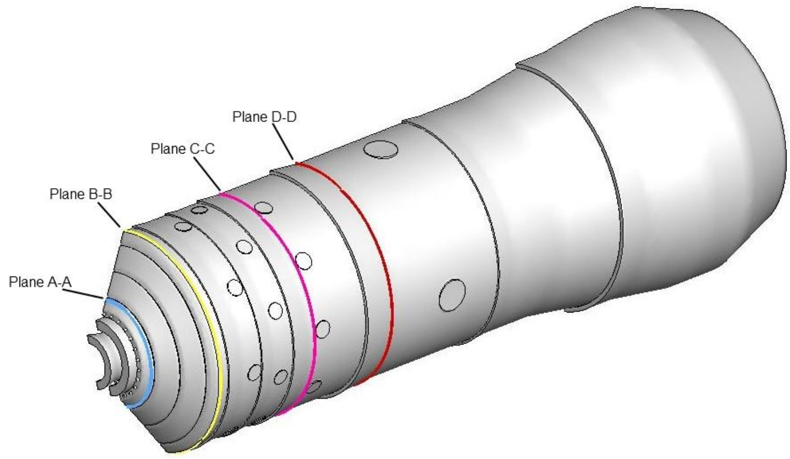


Figure 8: Planes visualization

For all models, the origin of the axial coordinate (*x*) coincides with the swirler outlet section.

Plane	Description	x/L
A-A	Passing near the swirler outlet	0,02
B-B	Passing upstream of the Strip 1	0,07
C-C	Passing downstream of the Strip 3	0,22
D-D	Passing upstream of the Strip 4	0,35

Table 5: Planes description

The analysis of NO_x emissions (see Table 6) shows that modified versions are characterized by a production of NO_x substantially lower than the original one (-30%) and that they have comparable emissions. Table 7 underlines that the different NO_x production between the Mod-C and the BASE can be explained by a better fuel air mixing for the MOD-C: the values of the f_{mean}/f_{stoic} standard deviation result lower at all the investigated transverse plane for the MOD-C.

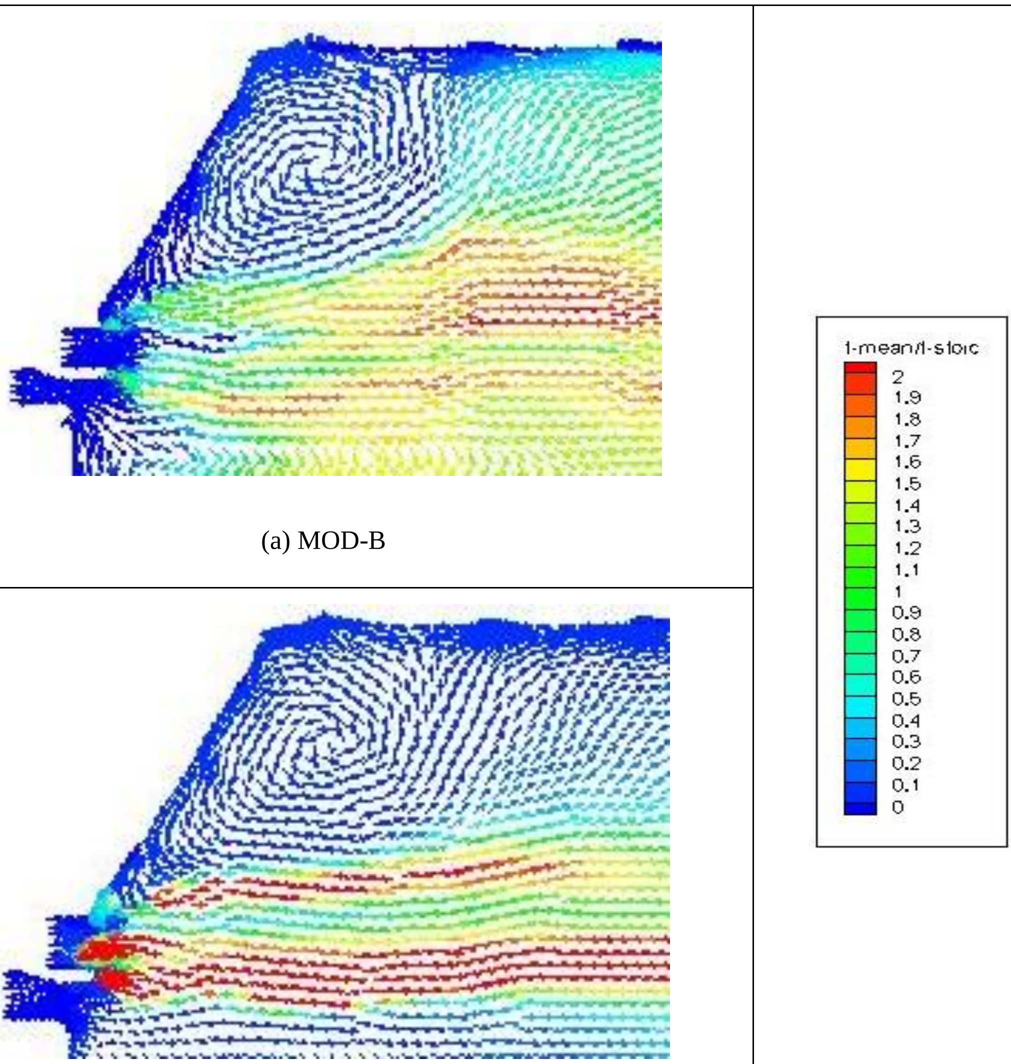
NO_x (ppm@15% O_2)		
Version	**CFD**	**Δ %**
BASE	753	
MOD-B	541	-30%
MOD-C	543	-30%

Table 6: NO_x concentration at the combustor discharge

Plane	BASE	MOD-B	MOD-C
	$\sigma(f_{mean}/f_{stoic})$	$\sigma(f_{mean}/f_{stoic})$	$\sigma(f_{mean}/f_{stoic})$
A-A	0,145	0,332	0,076
B-B	0,070	0,068	0,050
C-C	0,062	0,060	0,053
D-D	0,056	0,059	0,055

Table 7: f_{mean}/f_{stoic} standard deviation on transverse planes

However the description of the fuel-air mixing by a global parameter like $\sigma(f_{mean}/f_{stoic})$ is not able to justify the comparable NO_x formation in the modified versions. The examination of the local concentration of the reactive mixture is needed, especially in the region near the swirler exit, whose mixing field strongly influences NO_x production. The Figure 9 highlights that the MOD-B is characterized by a recirculation zone around the combustor axis larger than the MOD-C version mainly because of the higher value of the hub diameter of the swirler. As consequence of it, in the MOD-B only the fuel is attracted by the recirculation zone where it burns with relatively low temperature (about 1550 K) and a negligible NO_x formation. Conversely, in the MOD-B, the fuel from the external row burns near the swirler's outlet with lower temperature than the MOD-C.



(a) MOD-B

(b) MOD-C

Figure 9: f_{mean}/f_{stoic} distributions on the periodic plane

The different velocity and mixing fields nearby the swirler exit section entails different local distribution of NO_x production not only in the more upstream part of combustor but also in the more downstream regions, see Figure 10. The MOD-B version presents a larger volume where NO_x is generated, but the peak values of the NO formation rate are lower. The graphic of the Figure 11 highlights that the modified versions have a similar trend for the average NO production at transverse plane although the local differences in NO_x production are rather relevant.

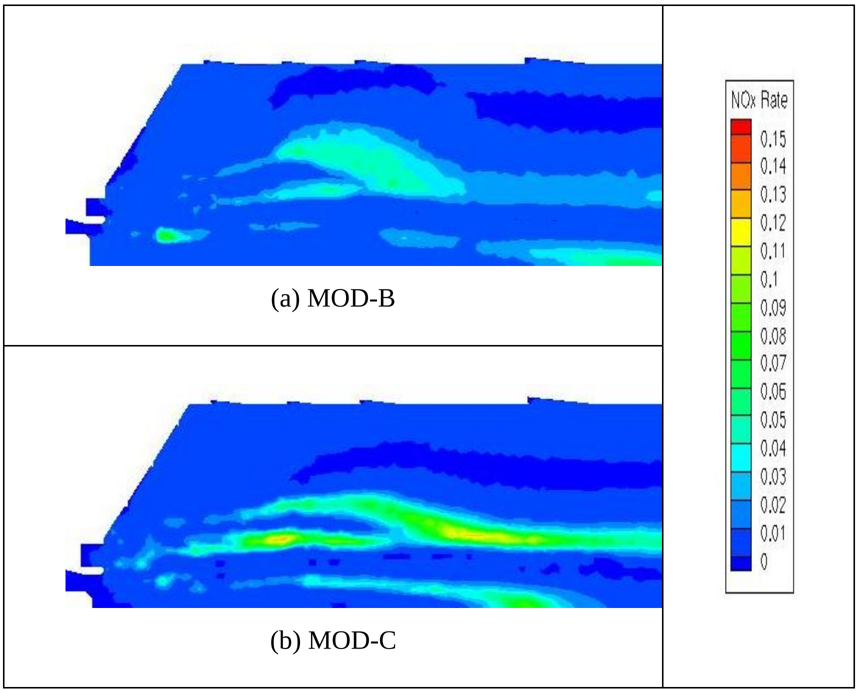


Figure 10: NO production [kmol/m^3s^{-1}] on the periodic plane

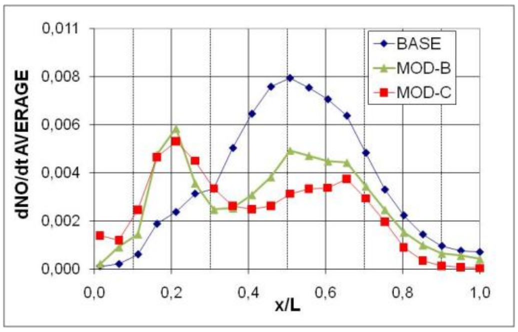


Figure 11: dNO/dt [kmol/m^3s^{-1}] average values in transverse planes

5.2. MOD-B version of the combustor: the effect of varying diameter of the injection hole

Relating to MOD-B, the effect of fuel velocity on NO formation was investigated. The version analyzed in the previous paragraph was compared with the configuration MOD-B-D3 which differs from the MOD-B for the diameter of the fuel injection holes only (3mm versus 5 mm). The Figure 12 underlines the different fuel air mixing close to the swirler outlet. In the MOD-B-D3, the fuel velocity is high enough that hydrogen scarcely spread in the recirculation zone produced by the inner swirler, differently from the MOD-B. The comparison between the thermal fields (see Figure 13) shows that temperature is not strongly affected by the fuel velocity, excepting the above mentioned region. However, for the MOD-B NO_x production in this zone is negligible respect to the total because temperature is lower than 1550 K. In conclusion, NO_x emissions results poorly influenced by the investigated variation of the fuel velocity (see Figure 14, Table 8).

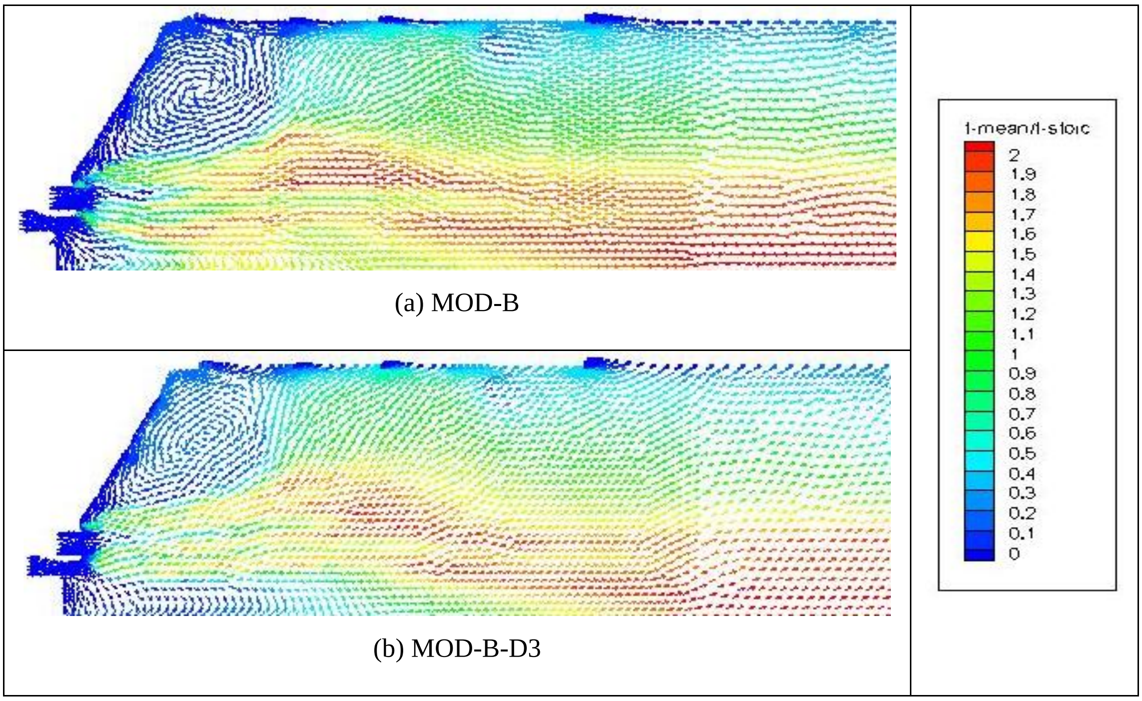


Figure 12: MOD-B-D3 version, f_{mean}/ f_{stoic} coloured velocity vectors on the periodic plane

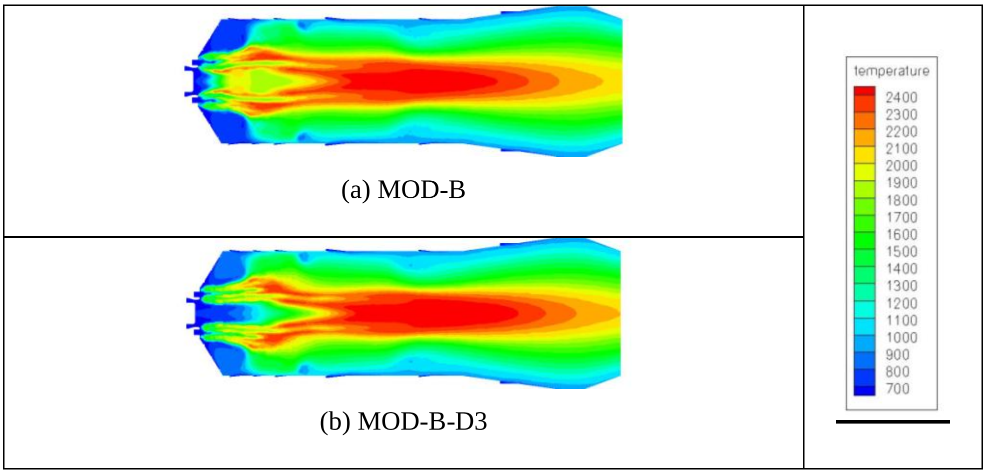


Figure 13: Temperature distribution on the periodic surface

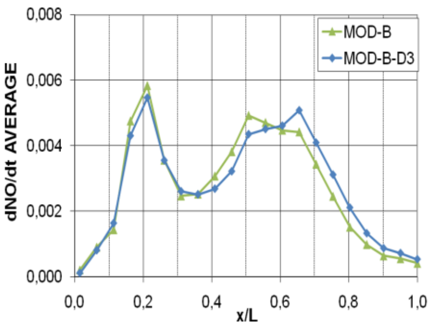


Figure 14: dNO/dt [$kmol/m^3s^{-1}$] average values in transverse planes

NO_x (ppm@15% O_2)	
Version	**CFD**
MOD-B	541
MOD-B-D3	546

Table 8: NO_x concentration at the combustor discharge

6. CONCLUSIONS

A RANS methodology for the accurate prediction of NO_x emissions in non-premixed gas turbine combustors fired with 100% H_2 was defined. It was validated through the comparison with full scale experimental tests, with a satisfactory agreement. The selected numerical procedure was employed for the analysis of modifications of a gas turbine combustion chamber 100% H_2 fired. The study of the combustor's base version mixing field and air flow rate distribution showed that NO_x formation may be reduced by 1) increasing the air flow rate in the primary zone of the combustor, 2) trying to promote an improvement of the fuel air mixing. First, applying these criteria to the original configuration, the modified version MOD-B was defined. As further step, another modified version called MOD-C was built starting from the MOD-B following the above mentioned criteria. In both modified configurations the flame was maintained purely diffusive, the burner and the fuel injection schemes were redesigned but the burner maximum radial dimension was unchanged respect to the original one. The modified versions adopt two different double co-rotating axial swirler: the air flow rate through the swirler is 9 % and 12 % of the total in the MOD-B and in the MOD-C respectively. For better radial fuel-air mixing the number of fuel holes rows was increased: the MOD-B and the MOD-C present two and three rows respectively, while the original combustor has one row of fuel holes. Besides that, pitch and yaw angles were assigned to fuel in the MOD-C.

The numerical simulations performed at full load ISO conditions showed that NO_x production was lower for the modified combustors (about 30%). However the MOD-B and the MOD-C configurations present the same NO_x emissions, differently from how it could be expected in the design phase.

This study highlights that, for hydrogen, the a priori evaluation of the effect of modifications of the combustor's geometry on NO_x emissions is not intuitive. The production of NO_x is strongly influenced by the local distributions of several parameters (mixing, residence time, radical concentrations, etc.) which can be difficultly linked with the geometric parameters of the combustor. The two modified version present the same NO_x emissions although the swirler and the fuel injection schemes produces different velocity, mixing and consequently NO_x rate local fields.

In the numerical comparison between the MOD-B and the MOD-C cases, the determination of the effects of the single design variables (i.e. pitch and yaw angle of the fuel holes, air flow from the swirler, etc) on NO_x emission is very hard because of the complexity of the fields of the thermo-fluid dynamic variables. Relating to the MOD-B, the result of the fuel velocity only on NO_x production was investigated, considering fuel holes diameter of 5mm and 3mm. In this case, NO_x emissions are not affected by the fuel velocity.

Besides, the developed analysis showed that referring to dry operation NO_x reduction based on "Minor Modification" applied to pure diffusive 100% hydrogen flame combustion chamber is limited to around 30%. For a further relevant reduction of NO_x formation, different approaches must be taken into account: wet operation if water recovery is allowed by the plant cycle or premixed combustion, which may be an important research area for hydrogen's employment in gas turbine.

7. ACKNOWLEDGMENTS

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NOMENCLATURE

f_{mean}	Mixture fraction mean value	[-]
f_{stoic}	Stoichiometric mixture fraction	[-]
k	Turbulence kinetic energy	[m^2/s^2]
L	Liner length	[m]
m	Mass flow rate	[kg/s]
p	Pressure	[Pa]
T	Temperature	[K]
v	Velocity magnitude	[m/s]
x	Axial coordinate	[m]
y+	y plus	[-]

Greek

χ	Scalar dissipation rate	[s^{-1}]
ε	Turbulenț dissipation rate	[m^2/s^3]
Φ	Hole diameter	[mm]
ρ	Density	[kg/m^3]
σ	Standard deviation	[-]
τ	Characteristic time scale	[s]

Abbreviation

AFR	Mass air fuel ratio
BASE	Combustor base version
CFD	Computational fluid dynamics
DNS	Direct numerical simulation
EDC	Eddy dissipation concept
EXP	Experimental
LES	Large eddy simulation
MOD-B	First combustor modified version
MOD-C	Second combustor modified version
PAH	Polycyclic aromatic hydrocarbon
PDF	Probability density function
RANS	Reynolds averaged navier stokes
STD	Standard
UHC	Unburned hydro-carbons
WF	Wall functions

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