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Numerical analysis of a microturbine combustion chamber modified for biomass derived syngas

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ABSTRACT

A CFD analysis was carried out to study the performance of a modified combustion chamber of a micro gas turbine with the objective to change its fuelling from natural gas to biomass pyrolysis gas. The micro gas turbine is a component of a pilot IPRP (Integrated Regenerated Pyrolysis Plant), a distributed energy system, based on a rotary kiln reactor for the pyrolysis of biomass. This paper describes the combustion process occurring inside the combustion chamber of the micro gas turbine. In particular, a new, revised kinetic scheme was implemented in the RANS analysis to better reproduce CO oxidation and flue gases temperature, for both methane and pyrolysis gas combustion; further investigation was undertaken on NO_x formation mechanisms, which are now modeled through a non-adiabatic PPDF approach, also taking into account the effects of turbulence interaction. CFD simulations for natural gas and pyrolysis gas combustion were performed for two different annular rich-quench-lean combustion chamber configurations, one with the original design for natural gas and one with a modified design optimized for syngas, in order to quantify the advantage of using a dedicated design. Furthermore, through the numerical analysis, the hot spots of the combustor have been identified and monitored the to study the possible effects of material corrosion due to high temperatures.

INTRODUCTION

A massive effort towards sustainability is necessary to prevent global warming and energy sources impoverishment: both biomass and waste conversion into energy may represent a key action to reach this goal.

Slow pyrolysis of waste and biomass represents an interesting solution for renewable energy conversion in highly regenerative micro gas turbine based power cycles, also because it is easily scalable. The combined production of a medium LHV gas to fuel the MGT and of a high LHV byproduct (tar and/or char), that may contribute to maintain the pyrolysis process, makes pyrolysis highly competitive when compared to other conversion processes of biomass, like gasification. The ongoing activities on pyrolysis at the

University of Perugia are focused on the IPRP (Integrated Pyrolysis Recuperated Plant) pilot plant [1,2], to address technological barriers on the use of SG derived from slow pyrolysis in a rotary kiln, in commercially available MGT's. Syngas composition is variable and depends on the particular type of biomass used in the pyrolysis reactor, as well as the parameters of the process, such as residence time, temperature and moisture content. In any case, the calorific value is rather low and variable (6000 - 12000 kJ/kg), and it is therefore necessary to adapt the power nozzle useful section in order to ensure the same energy input into the combustion chamber. Moreover hydrogen content fact has a flame speed higher than that of natural gas, which can cause backfire. Hydrogen has also a corrosive effect on the nozzles themselves because of higher combustion temperature. Other critical factors of the use of syngas are related to the presence of particulates and tars, which can cause damage and corrosion as well as alkali metals, together with hydrochloric acid and sulfur.

In previous works by the Authors [3,4], the analysis has concerned validation of a complex chemistry kinetic scheme, through comparison with experimental measurements taken at the Terni IPRP pilot plant, for the main pollutants and the TIT temperature generated during natural gas firing.

OBJECTIVES

This paper focuses on evaluating and quantifying, through CFD analysis, the advantages in using a dedicated combustion chamber design (SG-CC) for biomass pyrolysis syngas firing, in respect to using the standard NG-optimized CC (NG-CC).

A combustion mechanism, already validated in [3] through the comparison of experimental measurements on the MTG for the case of NG fuelling, has been utilized along with a different NO_x formation mechanism, cross checked with experimental data on Natural Gas.

Finally, an analysis on combustion chamber hot spots has been carried out, providing temperature profiles for the most critical area in the CC liner.

MGT AND CC DESCRIPTION

Micro Gas Turbine

The IPRP plant currently uses an ELLIOTT TA-80 R micro gas turbine with radial geometry, generating 80 kW_e at full load when firing NG. It features an annular shaped combustor, designed following an air-staging concept, called RQL (Rich-Burn, Quick Mix, Lean-Burn), as in Figure 1.



Figure 1: RQL Combustion Chamber for MGT ELLIOTT TA-80 R.

ROL combustion chambers, introduced in the early 80's, allow to contain NO_x emissions in burners for gas turbines and are of growing interest in stationary applications for their effectiveness in treating fuels with complex composition [5]. With reference to Figure 1, a rich combustion ($\phi = 2$) in the primary zone (A) improves the stability of the combustion reaction, producing and maintaining a proper concentration of highly reactive species, such as hydrogen and hydrocarbon radical, and secondly, it minimizes the production of nitrogen oxides due to the relatively low temperature and low oxygencontaining intermediates concentration. Effluents from the primary zone are rich in hydrocarbon species, hydrogen, carbon monoxide and partially pyrolyzed compounds which require an additional supply of oxygen. This is done by injecting a large amount of air through the secondary air jets, in the Quick-Mix ($\phi \approx 1$) zone (B). Finally a dilution air, in the Lean-Burn ($\phi = 0.5$) zone (C) lowers the temperature to avoid creep phenomena in turbine blades.

The zones are separated by dam walls (Fig.1) which are placed inside the secondary air holes and the Quick-Mix area. The fuel is injected into the rich combustion zone, with 12 injectors placed inside the mixing tube. The combustion liner and the mixing tubes are made of Alloy-X (UNS N06002) which has a melting point of about 1620 K [6].

The original CC design for NG firing (NG-CC) was modified for firing low LHV gases (SG-CC). The differences are in the dilution holes (Fig.2) and in the injectors geometry (Fig.3). External dilution holes on the outer liner wall have a diameter of 9 mm and the number is respectively 84 for methane and 42 for low LHV gases. The lower dilution is meant to consent an appropriate value of the turbine inlet temperature in case of low LHV gases combustion.



Figure 2: Dilution holes for NG-CC (a) and SG-CC (b).

The nozzle inside the mixing tube was modified to allow higher flows when using low LHV gas (Fig.3). The nozzle for natural gas combustion is radial with three holes, while the low LHV gas nozzle provides the whole available cross section for fuel injection which is axial. This allows, through increasing mass flow of low LHV gas, to provide the same amount of energy with respect to methane with less pressure losses.



Figure 3: Fuel nozzles for NG-CC (a) and SG-CC (b) - computational (left) and real geometry (right).

METHODOLOGY

A commercial, general purpose CFD code, CD-Adapco STAR-CCM+, was used to carry out the numerical activity. Two 3D computational domains, shown in Figure 4, were modeled reproducing the real geometrical and physical properties of the CC, respectively for methane and low LHV gas. Due to the periodical cylindrical symmetry of the volume,

a 30 degree sector of the annular CC, containing one mixing tube, was used. In both cases, the computational domains consist of two regions, fluid and solid. The two geometries differ on the number and diameter of the circular external dilution holes on the outer liner wall respectively: 84 for simulation for SG-CC and 9 mm diameter vs. 48 and a slightly lower diameter for simulation with SG. The number of dilution air holes for SG was changed from 42 to 48 to obtain a number divisible for 12, maintaining constant the total section. The nozzles inside the mixing tube are also different for the two cases according to the real case (Fig. 3).



Figure 4: Computational domains – solid and fluid regions for NG-CC (a) and SG-CC (b).

Physical modeling

Physical modeling involves, for the fluid region, an ideal gas mixture, with non-premixed Hybrid Kinetics/Eddy Break-Up combustion and PPDF equilibrium thermal NO_x models. The RANS turbulence model was switched from Standard *K*- ε [3] to Realizable *K*- ε , as some numerical instability was experienced. For the solid region, thermo physical proprieties for Alloy X were set. All simulation were performed assuming steady state conditions.

Meshing

The volume grids used in numerical analysis are generated within STAR-CCM+. The model used prepares polyhedral meshes with the following numbers of cells:

Table 1: Cell count for the two numerical domains

	NG-CC	SG-CC
Fluid	961477	960703
Solid	49195	278906
Total	1010672	1239609

Through defining volume shapes, the grids are generated customizing the cell dimensions in order to have smaller cells in critical areas such as the injection zone, the mixing zone and the volume where combustion takes place.

Chemical Scheme and Thermal NO_x modeling

A chemistry mechanism, involving a mixture of 7 gaseous compounds (CH₄, CO, CO₂, H₂, H₂O, O₂, N₂) and 9 reactions, has been implemented into an Hybrid Kinetics/Eddy Break-Up non-premixed combustion model. This scheme is based on 2 reduced mechanisms found in the Literature: the 2-step Westbrook and Dryer [7,8] for CH₄ and CO oxidation and the 4-step Jones and Lindstedt mechanism [9] for the dissociation of CH₄ to H₂, for H₂ oxidation and reaction between CO and H₂O. This chemical scheme was first presented and experimentally validated by the Authors on NG in a previous work [3].

A new, non-adiabatic PPDF (Presumed Probability Density Function) equilibrium approach, available through Star-CCM+ libraries, was used in order to better reproduce the mechanism of thermal NO_x formation: in fact, this method allows to account for turbulence/chemistry interaction by calculating an average value for the NO_x production rate. Taking into consideration the Zel'dovich thermal NO_x mechanism [10]:

$$N_{2} + 0 \Leftrightarrow NO + N$$
$$N + O_{2} \Leftrightarrow NO + O$$
$$N + OH \Leftrightarrow NO + H$$

1

since the activation energy for oxidation of N is small, a quasisteady state assumption can be made (d[N]/dt = 0), the average instantaneous rate of thermal NO_x production can be expressed as [17]:

$$\bar{R}_{NO} = \bar{A} - \bar{B}[NO] + \frac{\bar{A}\frac{\bar{C}}{\bar{D}}}{[NO] + \frac{\bar{C}}{\bar{D}}} - [NO]^2 \frac{\bar{B}}{[NO] + \frac{\bar{C}}{\bar{D}}}$$

where [*NO*] is the molar concentration of NO at a given numerical iteration and \overline{A} , \overline{B} , \overline{C} , \overline{D} are functions of *f*, that is the mixture fraction, defined as:

$$f = \frac{m_{fuel}}{m_{fuel} + m_{oxidizer}}$$

The mapping of the mean value of the four scalars to the mean value of the mixture fraction and its variance is accomplished through a pre-computed look-up table, generated by the PPDF model.

This model better accounts for NO_x formation than the one previously used in [3], where the Zel'dovich mechanism was

implemented via an Eddy Break-Up approach, instead of PPDF. Figure 5 shows a comparison of NO_x concentrations resulting from experimental measurements for NG firing and both numerical methods used.



Figure 5: Comparison of experimental and calculated NO_x emissions for NG firing

Boundary Conditions

Table 2 shows the composition of the pyrolysis gas used in this study, along with its main proprieties.

Table 2: Pyrolysis syngas composition and properties.

Composition	Vol. fraction	Mass fraction	Pr	operties
CH_4	21	11.3	AFR_s	2.76
CO	29	27.3	AFT	2069 K
CO_2	38	56.2	k	1.33
H_2	7	0.5	MW	29.74
N_2	5	4.7	LHV	9000 kJ/kg

To simulate the combustion of pyrolysis SG in the CC, the operating conditions were calculated imposing, for both cases, the same values for the fuel thermal load, W_{fuel} , and for the volume-averaged equivalence ratio $\overline{\Phi}$, used in [3] for natural gas combustion. These are defined as follows:

$$W_{fuel} = \dot{m}_{fuel}(NG) * LHV(NG) = \dot{m}_{fuel}(SG) * LHV(SG)$$
(1)

$$\bar{\Phi} = \frac{\frac{m_{fuel}(NG)}{m_{air}(NG)}}{\left(\frac{m_{fuel}(NG)}{m_{air}(NG)}\right)_{s}} = \frac{\frac{m_{fuel}(SG)}{m_{air}(SG)}}{\left(\frac{m_{fuel}(SG)}{m_{air}(SG)}\right)_{s}}$$
(2)

Table 3 shows the values of the resulting boundary conditions. Since the value of the air mass flow rate for SG is similar to

that needed for NG firing, it was also chosen to adopt the same values of temperature and pressure of inlet air. Pressure and temperature for the fuel stream are respectively 5.8 bar and 290 K.

Table 3: Boundary Conditions for SG Simulations at various load conditions.

W _{el} [kW]	W _{fuel} [kW]	$ar{\phi}$	ṁ _{fuel} (SG) [kg/s]	<i>ṁ_{air}(SG</i>) [kg∕s]
80	332	0.129	3.07*10-3	6.66*10 ⁻³
40	295	0.099	$2.73*10^{-3}$	6.34*10 ⁻³
10	260	0.086	$2.41*10^{-3}$	$6.42*10^{-3}$

RESULTS AND DISCUSSION

Combustion Chambers Comparison

The comparison between CFD analysis of 2 different combustion chambers for SG firing was carried out at three load conditions: full load (80 kW), half load (40 kW) and minimum load (10 kW). Tables 4 and 5 show the area-averaged values for flues gas composition and temperature at the CC outlet, for the two different configurations.

 Table 4: SG firing in a SG-optimized CC. Flue gas composition at CC outlet for various load conditions.

		СО	NO _x	O ₂	N ₂	CO_2
W_{el}	T _{flue gas}	[ppm	[ppm	$[\%_{vol}]$	$[\%_{vol}]$	$[\%_{vol}]$
[kW]	[K]	@	@	dry]	dry]	dry]
		15%	15%			
		O ₂]	O ₂]			
10	850.9	21	1	18.96	78.34	2.70
40	960.1	12	1	18.69	78.27	3.03
80	1128.2	5	3	18.02	78.04	3.94

 Table 5: SG firing in a NG-optimized CC. Flue gas composition at CC outlet for various load conditions.

		CO	NO _x	O_2	N_2	CO_2
W_{el}	T _{flue gas}	[ppm	[ppm	$[\%_{vol}]$	$[\%_{vol}]$	$[\%_{vol}]$
[kW]	[K]	@	@	dry]	dry]	dry]
		15%	15%			
		O_2]	O ₂]			
10	833.8	98	0.2	18.77	78.42	2.79
40	936.2	112	0.2	18.83	78.18	2.97
80	1105.2	138	0.5	18.63	77.27	4.07

A decrease in CO concentrations is obtained through an increase of electric load, which allows for higher flame and flue gas temperatures, therefore greater gas turbine cycle efficiency; the parallel increase of CO_2 emissions is a further indicator of the enhancement of radical oxidation mechanisms,

along with higher O_2 concentration at the outlet. A side effect of this is an increase in NO_x emissions with load, which, however, does not appear to be significant. The use of pyrolysis gas allows to obtain very low CO emission figures, compared to those proper of a NG combustion, especially in the case of the SG-CC design. This can be explained taking into account:

- the relatively small concentration of CH₄, source of CO radical precursors;
- the presence of H₂, allowing for significant enhancement in carbon monoxide oxidation [11].

Figure 6 shows temperature fields in a longitudinal plane, intersecting the combustion chamber and the air inlet channel, for three different load conditions. It can be seen that, apart from the expected increase in peak (2220 K at 80 kW_e) and flue gas outlet temperature with increasing loads, the use of a SG-optimized CC leads to an higher average value of temperature, therefore to a presumed higher combustion efficiency and less CO/unburnt hydrocarbons emissions. In the NG-CC, lower temperatures in both the Rich-Burn and the Lean-Burn zones, due to the greater number of dilution air holes, partially inhibit the CO-to-CO₂ oxidation mechanisms and lead to a higher CO content in flue gases, although area-averaged outlet temperature are similar to those experienced with the SG-CC design.

Figure 6: Temperature distribution on a longitudinal plane for both CC configurations

Figure 7 shows temperature fields in a transversal plane, intersecting the mixing tube and the fuel injector. The SG-CC design generates cold flame conditions in the central part of the mixing tube region; however, this does not seem to affect the combustion process, since high temperatures are then reached in the rest of the Rich-Burn zone, along with correct thermal distributions in the longitudinal plane.

The use of NG-CC leads to partial flame flashbacks, as can be seen in further detail in Figure 8, in the case of full load.

This can partially account for the higher concentrations of CO found using this configuration, since it generates lower temperatures in the rich combustion zone and can explain the presence of a CO emission increase with load, instead of the expected decrease, given that the flashback appears to be stronger at 80 kW.

Figure 7: Temperature distribution on a longitudinal plane for both CC configurations

Figure 8: Detail of partial flame flashback using NG-CC at 80 kWe

Since Thermal NO_x generation is mainly temperature-driven, the peak for NO_x concentration is found in the Quick-Mix region, where ϕ values of about 1.05-1.1 lead to the highest temperatures in the CC. The use of SG-CC leads to a more uniform distribution of NO_x production, however, the NG-CC gives slightly lower nitrogen oxide concentrations, due to the temperatures found utilizing this type of design, and an asymmetrical distribution of the NO concentration, with a peak near one the secondary area walls.

Figure 9: Mass fraction of NO_x on a longitudinal plane

Combustion chamber hot spots analysis

Experience [12] indicates that the CC liner material can undergo high-temperature oxidation: it is therefore important

to verify the location of liner hot spots. The combustion liner and the mixing tubes are made of Alloy-X (UNS N06002) which has a melting point of about 1620 K [6]. Table 6 shows the maximum temperatures reached in the CC liner for the two different configurations.

Table 6: CC liner maximum temperatures at the dam walls

	NG-CC	SG-CC
10 kW	1104 K	1355 K
40 kW	1132 K	1404 K
80 kW	1300 K	1437 K

These values are all reached at the dam walls (Figure 5) in the quasi-stoichiometric region, where the highest flame temperatures develop. Another hot spot, where calculated temperatures are near to those at the dam wall region, is the left side of mixing tube wall. Figure 10 shows temperature profiles along the abscissa indicated in Figure 11.

Figure 10: Mixing tube wall temperature profiles

Figure 11: Abscissa for mixing tube temperature profile

Profiles show an increase of the left side wall temperature with the abscissa, as expected given the shape of the flame determined by the inclination of the injector inside the mixing tube. The SG-CC shows the highest values, increasing with the load, and reach a maximum of 1409 K, well below the Alloy-X melting point; however, this could generate high-temperature oxidation phenomena, such as carburization and pitting corrosion, leading to thickness losses in the liner walls [12]. The presence of flame flashbacks in the NG-CC configuration, determines a less developed flame, therefore much lower mixing tube wall temperatures, especially for the 80 kW_e case, where the backfire is more intense and the flame is shorter; this explains the abrupt decrease of temperature at the mixing tube tip and the higher values near the base of the tube, under full load conditions.

CONCLUSIONS

A comparison of the behavior of two different annular micro gas turbine combustion chambers when fuelled with biomass pyrolysis gas was carried out using a commercial CFD software. The investigation has included emissions figures for the main pollutants, flue gas temperature, and CC liner hot spots analysis.

The use of a dedicated CC design (SG-CC) allows to achieve higher flue gas temperature and lower CO emissions, therefore more efficiency for the combustion process and the gas turbine expansion process; also, NO_x emissions are not significantly higher than those found in the lower-temperature NG-CC design, indicating a correct implementation of the RQL strategy.

However, this configuration leads to consistently higher CC liner temperatures, in respect to the NG-CC, needing a careful monitoring for avoiding high-temperature oxidation damage, especially in the mixing tube and dam walls areas.

Further investigation is planned on high temperature creep phenomena affecting the liner walls, in both cases of SG-CC and NG-CC combustion.

NOMENCLATURE

Acronyms	
CC	Combustion Chamber
CFD	Computational Fluid Dynamics
EBU	Eddy Break Up
PPDF	Presumed Probability Density Function
IPRP	Integrated Pyrolysis Regenerated Plant
NG	Natural Gas
MGT	Micro Gas Turbine
RANS	Reynolds-Averaged Navier Stokes
RQL	Rich-Burn, Quick-Mix, Lean-Burn
SG	Synthesis Gas (Syngas)
SG-CC	Syngas-optimized CC design
NG-CC	NG-optimized CC design

Parameters 1		
AFR	air fuel ratio	kg/kg
AFT	adiabatic flame temperature	Κ
LHV	Lower Heating Value	kJ/kg
ṁ	mass flow rate	kg/s
k	specific heat ratio	
MW	molecular weight	kg/kmol
Р	pressure	bar
Т	temperature	K
TIT	turbine inlet temperature	K
W	power	kW
Φ	equivalence ratio	
Subscripts		
е	electrical	
S	stoichiometric	

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