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# Numerical redesign of 100kw MGT combustor for 100% H2 fueling

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**Abstract**

The use of hydrogen as energy carrier in a low emission microturbine could be an interesting option for renewable energy storage, distributed generation and combined heat & power. However the hydrogen using in gas turbine is limited by the NOx emissions and the difficulty to operate safely. CFD simulations represent a powerful and mature tool to perform detailed 3-D investigation for the development of a prototype before carrying out an experimental analysis. This paper describes the CFD supported redesign of the Turbec T100 microturbine combustion chamber natural gas-fired to allow the operation on 100% hydrogen.


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*Keywords:* *Hydrogen, MGT, NOx, CFD*

## 1. Introduction

The development and large-scale use of renewable energy sources has boosted the interest in hydrogen as storage medium of electrical energy [1]. In fact electricity can be stored with high efficiency in hydrogen through water electrolysis and later converted to combined heat and power in electrochemical devices such as fuel cells or in heat engines such as gas turbines producing only water as a by-product.
The gas turbine is a viable alternative to fuel cell technology in terms of reliability, expected life time and cost and also they permit to use hydrogen with a considerable level on impurity as CO; so it is possible to increase in value

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many chemical wastes that could be used to produce a hydrogen rich syngas. Even though gas turbine is a well established technology for natural gas applications, the operation on pure hydrogen is still a challenging frontier for engineering. The combustor is the only component of a gas turbine that requires major redesign effort for operation on 100% hydrogen due to the fuel characteristics. Compared to natural gas, the engine operation with hydrogen produced larger volumes of NO [2,3]. The present paper deals with the CFD redesign for operation on pure hydrogen of the combustor of a 100 kW commercial microturbine actually natural gas-fired. This microturbine, based on a lean premixed staged combustion system, could be the core of a 100 kW class hydrogen energy storage system. There are same experience on the using of Methane-Hydrogen blends as Reale et al. [4] and Delattin et al. [5] with this MGT but in this study the hydrogen level was very low, because the combustor chamber wasn't modified. Lieuwen et al. [6] and Lee et al. [7] report the high sensibility of flame respect the H2 concentration so it suggests a modification on the combustion chamber.

Therkelsen et al. [8,9] show a modification set on a commercial DLN MGT to allow the engine operation with pure hydrogen. These modifications were focused mainly to permit a continuous operating with limited optimizations about the NOx emissions.

The using of CFD approach for the redesign activity is a interesting method to reduce the number of realized prototype for the experimental activity, there are many successful works that justify this way [10–12].

Figure 1 shows a schematic view of the investigated combustion chamber, it is a reverse-flow single-can DLN design. There is a pilot zone on the axis, with a diffusion flame, used for the MGT start-up and for the premixed flame stabilization. The premixing is based on a complex radial swirler used as a premixing duct. More detailed information, in the original configuration and natural gas fuelling, on this unit are in Cadorin et al. [13].

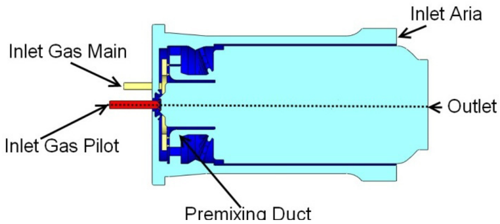


Figure 1:Combustion chamber under investigation

**Nomenclature**

| | | |
|---|---|---|
| T | Temperature | [K] |
| h | Sensitive enthalpy | [J] |
| k | Turbulence kinetic energy | [$m^2/s^2$] |
| κ | Thermal Conductivity | |
| Φ | Equivalence ratio | [-] |
| ϕ | Generic Mean Scalar | |
| ω | Specific dissipation rate | [s-1] |
| ρ | Density | [$kg/m^3$] |
| μ | Viscosity | [Pa·s] |
| $Z_i$ | Elemental Mass Fraction | |
| $S_x$ | Generic Source Term | |
| Sc | Schmidt Number | |
| CHT | Conjugate Heat-Transfer | |
| CTRZ | Central Toroidal Recirculation Zone | |
| DLN | Dry Low NOx | |
| MGT | Micro Gas Turbine | |
| SST | Shear Stress Transport | |
| RANS | Reynolds averaged Navier-Stokes | |

## 2. Numerical Procedure

The numerical procedure uses the commercial code Ansys Fluent [10] ver. 14. The RANS approach used the k-ω SST model [14,15] for the turbulence modelling. The test case under investigation produced a not homogeneous air/fuel mixture in the combustion chamber thus it is necessary a partial premixed. This combustion model is based on the union of a non-premixed model with a pure premixed model, [16]. The non-premixed modeling approach is based on a simplifying assumption: the instantaneous thermo chemical state of the fluid is related to a conserved scalar quantity known as the mixture fraction, *f*:

$$f = \frac{Z_i - Z_{i,ox}}{Z_{i,fuel} - Z_{i,ox}} \tag{1}$$

In the simplified model mixture fraction as the Favre mean (density-averaged) is considered and its transport equation is:

$$\frac{\partial}{\partial t}\left(\rho\bar{f}\right) + \nabla\cdot\left(\rho\vec{v}\bar{f}\right) = \nabla\cdot\left(\frac{\mu_t}{\rho_t}\nabla\bar{f}\right) \tag{2}$$

About the interaction chemistry – turbulence the code applies the β-function shape Probability Density Function (PDF) approach as its closure model. The premixed combustion model [17,18] assumes the laminar flame is thinner thus turbulent flame brush. The model considers the reacting flow field to be divided into two regions: burned and unburned species, separated by the flame sheet. The two regions are described by the progress variable C, where its value varies from 0 to 1, (0 unburned mixture, 1 burned mixture), the evolving zone represents the flame sheet [19]. The transport equation for the progress variable is:

$$\frac{\partial}{\partial t}(\rho\bar{c}) + \nabla\cdot(\rho\vec{v}\bar{c}) = \nabla\cdot\left(\frac{\mu_t}{Sc_t}\nabla\bar{c}\right) + \rho S_c \tag{3}$$

The code uses fitted curves of the laminar flame speed through numerical simulations proposed by Gottgens [20]. The union of two models is performed by the mean scalar, evaluated with this equation:

$$\bar{\phi} = \bar{c}\int_0^1 \phi_b(f)p(f)df + (1-\bar{c})\int_0^1 \phi_u(f)p(f)df \tag{4}$$

Its scope is introducing an element to evaluate the in homogeneity in the flow, typical of partial premixing. The laminar flamelet tables [21], non-equilibrium and non-adiabatic, were generated by using the kinetic proposed by Li [22] for H2 cases and GRi-MECH 3.0 [23] for CH4 cases. The heat transfer between flow and metal wall was introduced to consider the interaction between the flame and the metal wall. The code uses this energy equation in the solid regions:

$$\frac{\partial}{\partial t}(\rho h) + \nabla\cdot(\rho h) = \nabla\cdot(\kappa\nabla T) + S_h \tag{5}$$

The chemical reactions of NO don't influence the macroscopic aspect of the flame [16,24] thus a decoupled post-processor is used to evaluate this emission. This post-processor uses the predicted flow field, temperature and major combustion product concentrations (O and OH) from a converged combustion simulation. The post-processor considers only the thermal mechanism, [24], and uses a simple transport equation [16]. This method was validated in several previous works on hydrogen fueled diffusion flames [10,11]. The boundary conditions were imposed in terms of inlet mass flow rate and outlet static pressure, see Table 1.

Table 1: Reference Operation parameters for the full load

| | | |
|---|---|---|
| *AIR* | | |
| Total Mass Flow | kg/s | 0,7658 |
| Temperature | K | 871 |
| Op. Pressure | Pa | 409025 |
| *FUEL* | | |
| Temperature | K | 333 |
| Total Mass Flow CH4 | kg/s | 0,00696 |
| Total Mass Flow H2 | kg/s | 0,00290 |
| Thermal Input | kW | 348 |

## 3. Solid model and Computational mesh

Figure 2 shows a view of the actual combustion chamber geometric model with details about the air and fuel inlet. The radial swirler and the dilution holes define a 120° rotational periodicity used to reduce the model volume. For the CHT simulations only the more critical zone was modelled, in particular the pilot zone.

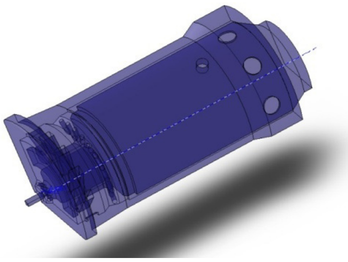

Figure 2: Detail of Solid Model of the fluid

The computational mesh, Figure 3, is hybrid non-structured and it was generated by the commercial code Centaur$^{TM}$ [25]. The grid is composed of 5.5 million of elements with prismatic layers used for near-wall treatment and tetrahedral cells elsewhere. The meshing paid attention to the quality in many critical zones like the injection holes. The mesh quality near the walls was controlled by the analysis of y plus (y+) values [26]. The generation parameters are the same used in previous works Riccio et al. and Brunetti et al. [27,28]. For a specific analysis a CHT simulation was performed thus it needed a mesh for the solid metal, see Figure 3-B .

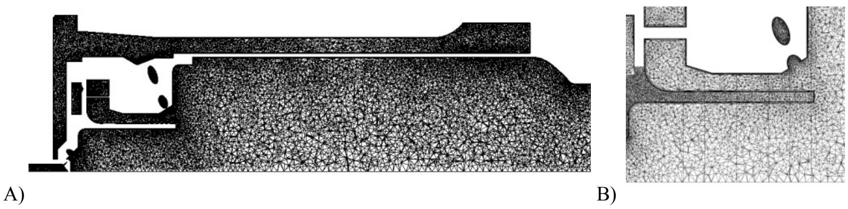


Figure 3: A) Computational Mesh B) Detail of CHT Mesh, Fluid and Metal

## 4. Analysis of original unit

The initial activity was the analysis of original geometry to understand how the 100% H2 fueling influences the operability compared with the CH4 case. The Figure 4 reports the temperature field for the two fuels (CH4 – A; H2 – B) and the main information is the early ignition for the H2 case. The flame develops in the premixing duct where the CH4 case is completely cold. This condition is unacceptable because the premixing duct isn't enough protected by a cooling system.

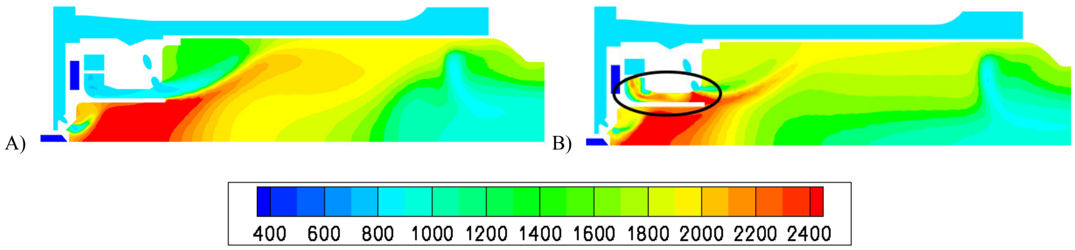


Figure 4: Temperature field on longitudinal plane [K], A)100% CH4 B) 100% H2

The Figure 5 reports the temperature difference fields between the cases on the same longitudinal plane. In CH4 fueling there is a good mixing with ignition delay time sufficiently high so that the mixture doesn't significantly burns in the premixed duct. On the contrary, H2-air mixture burns in the premixed duct, probably because of the lower ignition delay time. In this condition the premixed duct walls show critical temperatures without a cooling system to protect them, because in the original fueling it wasn't necessary.

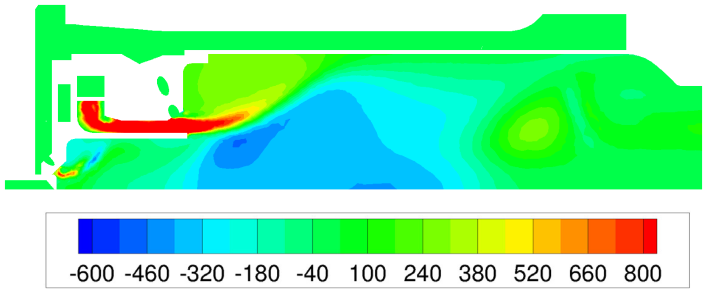


Figure 5: Temperature Difference [100 % H2 - 100% CH4] on longitudinal plane [K]

A useful parameter to evaluate the quality of temperature profile at the outlet of combustion chamber is the Pattern Factor (PF) [29]:

$$PF = \frac{T_{max} - T_4}{T_4 - T_3} \qquad (6)$$

$T_{max}$ = maximum temperature
$T_3$ = mean inlet air temperature
$T_4$ = mean exit temperature

The H2 fueling permit a slight improvement of the PF, see Table 2, but this result is obtained by the H2 early ignition.

Table 2: Pattern Factor

| | |
|---|---|
| **CH4** | *1.18* |
| **H2** | *1.02* |

The preliminary results suggested to investigate the flame's influence on the metal walls in the pilot zone with a Conjugate Heat-Transfer approach. The MGT operates safely in CH4 fueling.

Figure 6 shows the comparison of temperature fields for the analysis with (A) and without (B) CHT. The metal reaches an elevated internal temperature about 1200 °C but the operability is possible because on other side of the wall there is a cold flow that permits an adequate heat exchange. In hydrogen fueling the early ignition in the premixing duct introduce a hot flow so the operability is compromised so a new layout is needed.

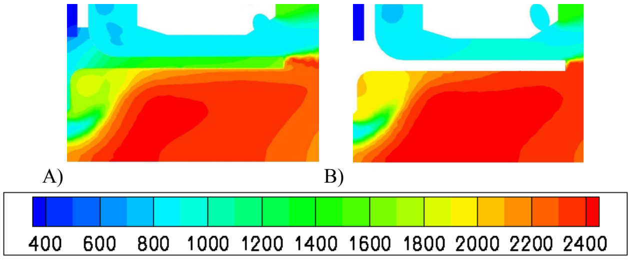


Figure 6:Comparison between analyses with (A) e without (B) CHT [K]

The global NO emission of H2 case is over 30% than the CH4 case (44ppm). In this contest, CFD analysis, is important identify the relative influence of new fuel on the emission and not the value. This increment is justified by the higher production rate in the pilot zone and in the premixing zone where there is the early ignition, see Figure 7.

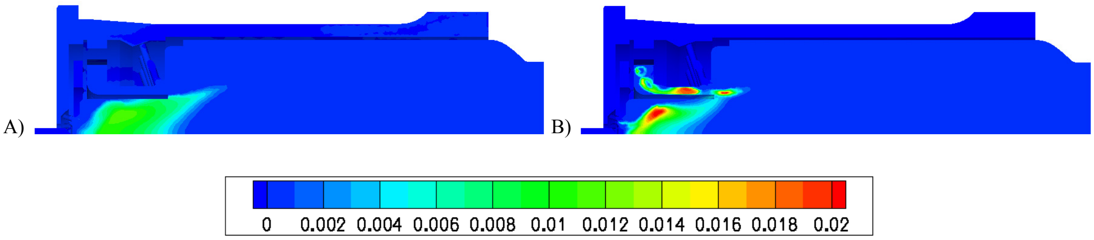


Figure 7: NO rate field on longitudinal plane [kmol/m$^3$s], A) 100 % CH4, B) 100% H2

## 5. Development of a new unit

The target of this study was the design of a unit fueled only 100% H2. A specific H2 fueling design strategy was applied since H2 show a very different operative condition than CH4, as reported in Noblet et al. [30,31].
The causes of NOx emission is the high thermal field thus the design way is the reducing of the local equivalence ratio. The experience from Riccio et Al and Brunetti et Al. [27,28] shows the possibility to operate in hydrogen fueling with very low equivalents ratio, $\Phi < 0.3$, without a pilot. It's possible because the blow off's equivalence ratio is lower than CH4, [32]. Also an increment of air velocity in premixing duct is important to reduce the possibility of flash back; the target was about 120 m/s.
A new air distribution in all combustor chamber is needed to obtain these desiderate conditions, the low local equivalence ratio and the high velocity. The only way is the reducing of dilution air flow and the increasing in the premixing zone. The Table 3 reports the design value of the passage area.

Table 3: Air distribution calculated from Passage Areas

| Zone | Area % |
|---|---|
| Premixing duct | 58.9 |
| Air slot | 6.9 |
| Cooling Holes | 6.6 |
| Dilution | 27.6 |

The pilot duct was modified in a convergent premixing duct and the swirler flows radially in this duct. The swirl number was increased to obtain a stable CTRZ because the flame needs an aerodynamic stabilization, the new layout doesn't use the pilot flame to anchor it in a specific place.
The important aspect was the position of injection holes because the thermal release zone had to be positioned far away from the metal walls. The holes were positioned on the vertical wall in a 1+4+8 disposition skin on different radial distance; see Figure 8 for more details.
To prevent possible thermal damages on some critical walls a cooling system was introduced. The premixing duct was protected by an air slot around it; it is as similar as the original system. In main combustion chamber zone a cooling hole skin was added in the wall where the secondary recirculation zone could transport a hot flow.
The number of dilution holes was increased, from 6 to 8, to improve the pattern factor also the global passage area is changed in according with Table 3; also this modified the axial symmetry condition from 120° to 90°.

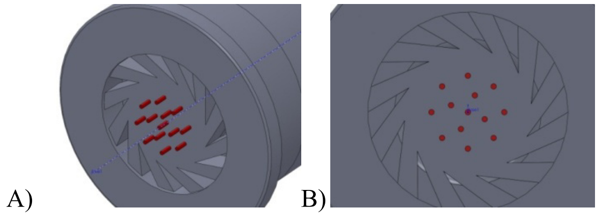


Figure 8: New injection hole skin.

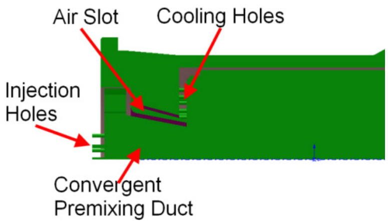


Figure 9: Prototype view on a longitudinal plane

## 6. Analysis of modified unit

The prototype was analyzed by a 3D CFD simulation to verify the design philosophy, in hydrogen fueling. The analysis starts from the velocity magnitude field, see Figure 10. At the outlet of premixing duct there is a big recirculation zone "CTRZ" and the flow makes the typical "V" shape. The outlet velocity is higher than the expected so the density in the premixing duct is lower; this condition suggests the possibility of the flame in the duct. The figure shows a blocked flow in the plenum before the swirler, this effect is highlighted by the deviated flow stream from the inlet. In the premixing duct flows lower air than the expected, see Table 4, thus the local equivalents ratio is higher, about 37%. Probably the wetted surface is too large in the swirler thus the pressure drop is higher than expected as consequence the air flow in the other passages is increased.

Table 4: Air distribution calculated from CFD simulation

| Zone | Air Flow % |
|---|---|
| Premixing duct | 36 |
| Air slot | 15 |
| Cooling Holes | 10 |
| Dilution | 39 |

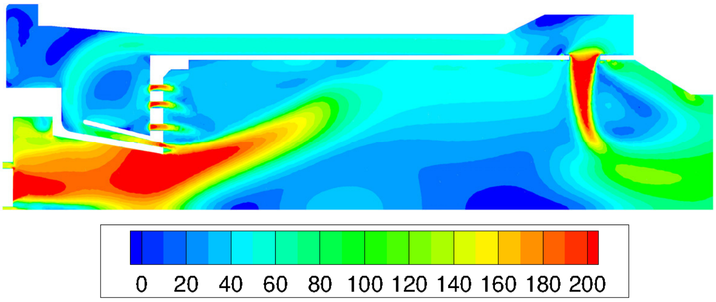


Figure 10: Prototype's velocity magnitude field [m/s]

Figure 11 shows the temperature field and it is possible to individuate the flame position. There is an early ignition in the duct as that was suggested by velocity field. However the flame is placed on the combustor axis and the main metal walls are enough cold. In this condition the flame looks like a stretched diffusion flame. Temperature values are lower than the stoichiometric ones with the maximal value is lower than 2000K. This low temperature field is able to reduce the production of NOx emission.

The new configuration of dilution holes helps to reduce the pattern factor to 0.40; this result permits to increase the safety and operability of the turbine.

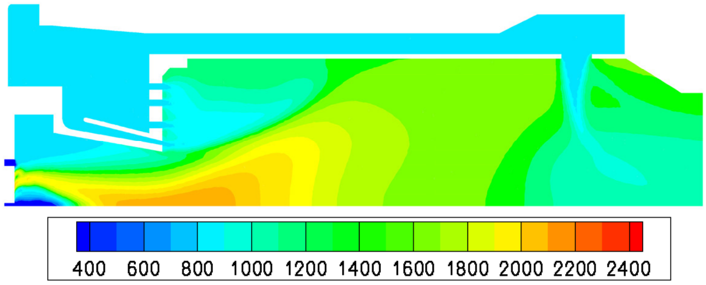


Figure 11: Prototype's temperature field on longitudinal plane [K]

The Figure 12 shows the NO production rate field where the maximal value is lower than the original case. In fact the global emission value is only the 50% of original CH4 case. However the approach used in this paper only considers the thermal NO production. It may be an issue for H2 combustion, since some publications [9,33,34] show the importance of NO production by the NNH mechanism in hydrogen fueling. There isn't any publications that confirms this production way through a CFD simulation on a real combustor.

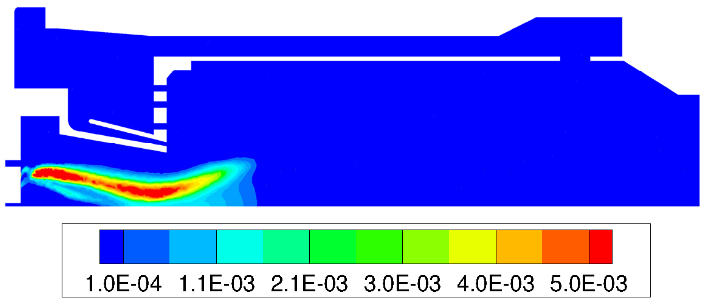


Figure 12: Prototype's NO rate field on longitudinal plane [kmol/m$^3$s]

## 7. Conclusions

The 100% hydrogen fueling of a Micro Gas Turbine could be an interesting opportunity but the original combustion chamber, CH4 fueled, needs to be redesigned.
Preliminary CFD simulation shows how the original unit isn't able to operate in hydrogen fueling safely because the flame ignites in the premixing duct that isn't sufficiently protected from the high temperature.
To resolve this problem the new unit was equipped with a new fuel injection system and a new configuration of main flows. The flame position is moved to the combustor axis and the more important metal walls are protected by new cooling systems.
The new geometry, verified by CFD simulation, isn't able to produce a perfectly premixed flame because there is an early ignition in the premixing duct. However the high velocity and low equivalence ratio permit a very low temperature field. The thermal NO emission of prototype is lower than the CH4 fueled original unit. This is a interesting numerical result because generally the hydrogen fueled combustor produce more NOx than a CH4 fueling, but the hydrogen fueling permits to operate in very lean condition thus with very low temperature field.

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