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CFD study case of ammonia-hydrogen mixture powered methane gas microturbine combustor in the context of the temperature repartition modifications

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Actually, much research has been conducted on the ability of hydrogen-ammonia mixture fuel to replace classical fuel such as methane for gas (micro)turbine use. These studies concern the combustion stability and NO_x formation. Temperature repartition in gas (micro)turbine combustor is very important from a thermomechanical point of view. This issue is often omitted in research. If modifications occur in temperature repartition, an overheating zone can appear and lead to mechanical damage to the combustor liner. Numerical studies, CFD method based with the use of Ansys Fluent tools, were conducted on a self-designed gas microturbine combustor for methane application, using various ammonia-hydrogen mixtures and methane fuelling. Then, the obtained temperature maps were compared between methane and ammonia-hydrogen mixtures with various compositions to find an ammonia-hydrogen mixture composition that permits to reproduce a similar temperature repartition as for methane fuelling; this mixture contains maximally 10% mass hydrogen (or 48% vol). This ammonia-hydrogen mixture composition was compared to other research where the ammonia-hydrogen composition was optimized for combustion stability and NO_x reduction (hydrogen content of 30% vol). According to performed studies, the proposed ammonia-hydrogen composition in other research is confirmed to be safe for gas microturbine applications from a thermomechanical point of view.

Key words: *ammonia, hydrogen, methane, CFD, gas microturbine*

1. Introduction

1.1. The emerging potential of hydrogen-ammonia fuel application

Nowadays, renewable sources of energy production, such as hydropower, wind power, solar panel power, geothermal power, etc., are strongly linked with meteorological conditions. However, the energy demand does not always match the momentaneous energy production, which may be a source of power plant overrun, limitation of energy consumption, expensive power deals, etc. An issue that could solve this energy management issue would be storing electrical energy when possible and using it when energy deficiency appears in the power grid.

Today, there are direct or indirect ways to store electrical energy: batteries, flywheels, supercapacitors, compressed air, hydroelectric pumping, and "fuel production" such as for example, hydrogen, methane, ammonia, and their mixtures. All these electrical storage methods are actually studied to be more efficient and more accessible around the world. In this paper, the use of renewable fuels, especially hydrogen and ammonia mixtures, was discussed.

The electrical energy excess can be stored under the fuel aspect [26]. Firstly, using the excess electrical power, it is easily possible to produce hydrogen using the hydrolysis process (efficiency of about 70%). This hydrogen can be considered as renewable fuel and it can be stored in order to be converted into electrical energy using combustion engines. Hydrogen is a very simple fuel (only two hydrogen atoms), but few issues appear in the context of its storage and transport (safety issues) and in terms of its use in power plants (safety issues and different combustion properties from those fuels often used, such as for example methane). Hydrogen is characterised by a lower heating value of 120 MJ/kg, a laminar burning velocity of 291 cm/s and an adiabatic combustion temperature of 2383 K, while for methane these parameters are, respectively, 50 MJ/kg, 37 cm/s and 2223 K (parameters near to stoichiometric conditions) [23]. The obtained hydrogen fuel can be converted into methane through the methanation process (efficiency of about 60%). It permits the production of renewable methane fuel but with reduced efficiency as a result of the complete conversion of the hydrogen fuel into methane. There is also the possibility of converting just a part of the hydrogen into methane and then it is possible to mix hydrogen and methane to obtain a mixture supported by classical storage, transport and power plants. This solution is just partially interesting because the reference fuel properties (as for example, methane) are overpassed when adding hydrogen to the reference (methane) fuel. This issue reduces the lifetime of storage, transport, and energy conversion devices. Finally, there is a third possibility to store energy in the fuel form; a portion of the obtained hydrogen can be converted into ammonia (by the Haber process – efficiency of about 50%), and a mixture of hydrogen – ammonia can be used as a renewable fuel. As hydrogen has combustion parameters higher than those of methane, while ammonia has combustion parameters much lower than those of methane, the adequate mixture of hydrogen with ammonia could permit one to obtain an average combustion parameter fuel, corresponding approximatively to the combustion properties of methane. Ammonia is characterised by a lower heating value of 18.6 MJ/kg, a flame speed of 7 cm/s and an adiabatic combustion temperature of 2073 K [23]. The second and third solutions involve participation in the decarbonisation of the energy and transport industries. This last solution was discussed in this paper.

1.2. Hydrogen-ammonia mixture fuel research

Actually, much research was conducted on the ability of hydrogen-ammonia mixture fuel to replace classical fuels such as methane [1, 4, 12, 15, 28].

In the paper [1] studied a code permitting the control of a gas turbine once fuelled by an ammonia-hydrogen mixture (70% vol. of ammonia and 30% vol. of hydrogen) and once fuelled by methane. The studies were conducted using a virtual control system and gas turbine (LabView). The results of this study demonstrated that it is possible to fuel a methane-powered gas turbine by an ammonia-hydrogen mixture. Despite the success, the control code dedicated to steer the gas turbine during ammonia-hydrogen fuelling was different and more complex than that used for pure methane fuelling.

In the next paper [28], the applicability of ammonia fuel was analyzed in various energy conversion devices (for example, gas turbines, piston engines, fuel cells, etc.), and its combustion properties were largely discussed and compared to other traditional fuels. The authors underlined that the use of ammonia fuel would help and support the decarbonisation process. The discussion in the paper ended with the remarks that ammonia fuel is and will be a challenge, but it is a promising technology in the context of decarbonisation.

In paper [12], numerical, analytical and experimental studies on fuelling a gas turbine were conducted with a mixture of ammonia and hydrogen fuel (70% vol. of ammonia and 30% vol. of hydrogen). The aim was to analyse the combustion stability and NO_x production in a humidified environment (combustor), in order to reduce the NO_x production when ammonia was applied. The results between the numerical studies (CHEMKIN-PRO) and experimental studies were concordant and allowed to demonstrate that the humidification of the combustion zone in the gas turbine combustion chamber while fuelling with ammonia-hydrogen mixture, permits stable combustion and reduced NO_x emissions, comparable to the DLE gas turbine methods. This technology proposal seems to have an important potential for application.

In the next article [15], the authors performed a numerical study of the ammonia-hydrogen mixture applied to a gas turbine engine used in marine. The aim of this study was to check the operation parameters and NO_x creation using three ammonia-hydrogen fuels (50/65/90% vol. of ammonia completed with hydrogen). The results have shown that the use of ammonia-hydrogen fuelling is possible, but stability of the combustion is stronger as more hydrogen is in the fuel, but it provokes an increase in temperature peak. The results also showed that NO_x production is reduced in rich combustion conditions. The pressure increase also permits to reduce the NO_x creation.

Finally, cooperations between various institutes and industry were, are and will be created to conduct common works linked with the use of ammonia-hydrogen fuel. As an example, the cooperation of the Electric Power Research Institute and the Low-Carbon Initiative can be cited [4]. Their goals are to check whether the use of ammonia can contribute to the decarbonisation, to develop new tools for the analysis of ammonia-hydrogen fuel combustion and to perform experimental studies to validate the created calculation models.

According to the previous research/analysis papers, the ammonia-hydrogen fuel is a potential fuel participating in the energy sector green transformation but few challenges need to be achieved in order to use it fully; the combustion properties are studied, especially the combustion stability and NO_x creation. The ammonia-hydrogen mixture fuel that offers correct combustion stability and lowest NO_x production is composed of 70% vol. of ammonia and 30% vol. of hydrogen [27]. Another aspect that is often omitted in the paper is the temperature field repartition in the combustor liner when replacing the classical fuel with an ammonia-hydrogen mixture fuel. The studies presented in this paper aimed to assess the temperature field changes in the combustion chamber liner for various compositions of ammonia-hydrogen mixtures. The temperature field repartition is very important from a mechanical resistance point of view. If modifications occur in temperature repartition, an overheating zone can appear and lead to mechanical damage to the combustor liner and then to the gas microturbine.

1.3. The gas microturbine drive units

Gas microturbines are interesting energy conversion devices nowadays. Gas microturbines may be used in the energy sector (generation of electrical and head power), in the automotive industry to increase the range of car (Pininfarina H600 or Jaguar CX75) and in aviation, to power drones, jetpacks or even ultralight aeroplanes. Gas microturbine engines present many advantages; low noise level, cheap operation, limited number of moving parts, low emissions, high efficiency, etc. [7]

Gas microturbine engines can be equipped with a premixed or diffusion combustor. The premixed combustor burns a premixed air-fuel mixture, allowing it to lower the peak temperature and the temperature gradient, resulting in low NO_x emissions. These combustion chambers are used in modern devices. The diffusion combustors burn fuel from a very rich air-fuel mixture to a very lean air-fuel mixture. The diffusion flame is much more stable than the premixed flame. Despite the higher NO_x emissions than for the premixed combustors, the diffusion combustion chambers are still wildly used in gas microturbines due to their manufacturing simplicity and stable combustion process (permitting the mixing or change of fuel) [5].

As diffusion type gas microturbine engines can be used in various sectors, this kind of engine was discussed in this paper in the context of hydrogen-ammonia mixture application.

1.4. Novelty of the study

According to the information provided previously, the ammonia-hydrogen mixture combustion was studied in the context of a study case combustion chamber of a gas microturbine. The used combustor was previously designed for methane fuelling (reference fuel), 3D modelled and a flow-combustion model of this combustor was created for CFD (Ansys Fluent) studies [5–7]. This combustor model was used in the past for other researchers [5–7]. This is a typical diffusion combustor design. The aim and novelty of this paper is to analyse the temperature field repartition while replacing the reference fuel (methane) with an ammonia-hydrogen mixture. Temperature repartition is very important from a mechanical resistance point of view. If modifications occur while changing the fuelling mode, in temperature repartition, a local overheating can appear, leading to mechanical damage of the combustion chamber liner and then of the gas microturbine device.

Numerical studies (CFD – Ansys Fluent) were performed on a self-designed gas microturbine diffusion type combustor liner, using various ammonia-hydrogen mixtures (from pure ammonia to pure hydrogen, with a step of 10% mass). The studies were repeated for traditional fuelling (methane). The obtained temperature maps were compared between methane and ammonia-hydrogen mixtures with various compositions. The comparative studies permitted us to find an ammonia-hydrogen mixture composition that permits us to reproduce similar temperature repartition in the liner for the suitable fuelling case – methane fuelling. Finally, the ammonia-hydrogen composition that offers the best combustion behaviour (taking into account temperature repartition) was compared to the mixture composition previously exposed in the literature review – 70% vol. of ammonia and 30% vol. of hydrogen.

2. Study case combustion chamber

In order to obtain a gas microturbine combustion chamber with defined operation parameters, a gas microturbine combustor was designed and 3D model was created. This reference device was designed to operate with methane fuel and is assumed to generate about 40 kW of mechanical energy. The combustor main operating parameters (total pressure (p_{total}), static pressure (p), total temperature (T_{total}) and static temperature (T) at the combustor inlet and outlet) were listed in Table 1. The design and general description of this combustor are available in Fig. 1. This combustor model was applied to the next CFD studies. Previous studies also used this combustor model [5–7].

Table 1. The gas microturbine combustor work parameters

Parameters	Combustor inlet	Combustor outlet
p_{total} [Pa]	324,992	311,992
p [Pa]	306,584	301,133
T_{total} [K]	433	1185
T [K]	426	1175
c [m/s]	120	155
$\dot{m} = 0.251 \frac{kg}{s}$; c_s = [see Table 4] $\frac{kg}{s}$		

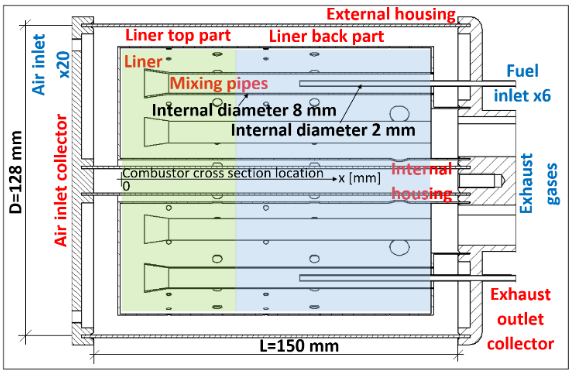

Fig. 1. Description of the combustor model for CFD studies

3. Numerical methods

3.1. Computational domain

The tridimensional model of combustors was created using Solid Edge [33] and Ansys DesignModeler softwares [30]. The combustor model was then exported to Ansys Meshing software to generate the mesh. The generation of the combustor mesh was one of the most important steps. Tetrahedral elements are often applied to generate meshes of gas microturbines [3, 10, 11, 24, 29]. This element is capable of filling complex geometry while keeping acceptable values of quality parameters (skewness, orthogonality and aspect ratio). Indeed, many numerical studies demonstrated the advantage of applying polyhedral elements. The main advantages of polyhedral elements are good accuracy and the ability to fill complex geometry with better values of quality parameters than tetrahedral elements [14, 17, 20]. This is the reason why the polyhedral elements were chosen to generate the combustion chamber mesh. A cell length of 0.8 mm was selected. Five layers of mesh in the near-war region were added to avoid Y+ overtaking the value of 300. The mesh of the combustion chamber generated as described above was applied to the CFD software to perform suitable combustion-flow simulations. The number of generated cells is 5.8 million, the maximum aspect ratio is 38.3, the maximum skewness is 0.898, and the minimum orthogonal quality is 0.435. According to the literature review [10, 24], the obtained mesh is sufficient for accurate simulations. The view of the calculation domain and the cross-section of the combustor mesh are shown in Fig. 2.

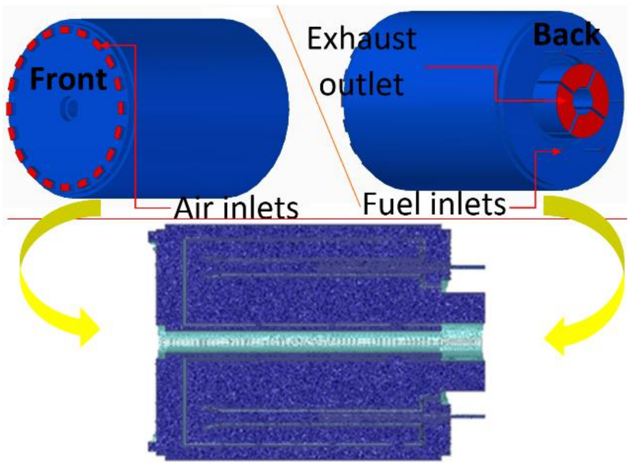

Fig. 2. View of the computational domain and mesh

3.2. Flow and combustion mathematical models

To perform suitable numerical studies, the flow and combustion were modelled with the use of Ansys Fluent software. The following phenomena needed to be taken into consideration: turbulent flow, non-premixed combustion and radiative heat exchange.

The inner-combustor flow turbulence phenomena were modelled applying the Reynolds Averaged Navier-Stokes model (RANS) with turbulence Realisable k-ε model [9, 25]. Due to its low computational cost and acceptable results, this turbulence model is commonly used for industrial and even scientific issues. The enhanced wall treatment was enabled to improve the near-wall flow calculations. Using this option permits the resolution of the flow in the vicinity of the wall when Y+ is less than or equal to unity or applying an enhanced wall function otherwise. This model is a reasonable compromise between computational cost and accuracy when the near-wall phenomena are not primordial, as in this study case.

In gas microturbines or generally in gas turbine devices, in the combustion chamber liner, the heat exchanges are achieved mainly by the radiation phenomena. This makes it necessary to use the radiation model to perform accurate simulations. The Discrete Ordinate (DO) [9, 24] model was applied in this study. This radiation model considers the combustion environment as a grey body. The additional use of the Weighted Sum of Grey Gases Model (WSGGM) [9] permitted us to take into account the radiation absorption in the combustion zone. The WSGGM model is based on experimental data [18]. The wall was treated as a black body, according to common practice when modelling radiation in the combustion chamber of gas turbines [8].

To model combustion phenomena, the non-premixed steady diffusion model [16] was applied. This model supposes that a set of small laminar flames creates the combustion zone called "flamelets". This model permits to take into consideration kinetic and turbulence effects. A look-up table is generated to start the calculation. This table permits the determination of the mean mass fraction of species, density, and temperature in the combustion zone as a function of the mean mixture fraction, as well as its variance, enthalpy, and strain rate. These four last parameters are obtained by solving their transport equations during the calculation process. The use of a lookup table permits reducing the computational cost compared to the full chemistry models. This combustion model permits one to reach accurate results while maintaining acceptable computational cost.

The look-up table generation described for the combustion model requires a combustion kinetic mechanism. In the study case, two kinetic mechanisms were applied: the GRI-MECH 3.0 (for methane calculations) [13, 32] and the NH3 mechanism [19, 21, 22, 31] (for ammonia-hydrogen calculations). The GRI-MECH 3.0 considers 53 species and 325 chemical reactions, while the NH_3 mechanism considers 31 species and 203 reactions. Depending on the fuel composition, an adequate set of flamelets was generated. Using these flamelets and the probability density function (PDF), the look-up tables were created for each combustion case.

After enabling the mathematical models described above, the boundary conditions were set. The inlets (fuel and air) were set as "mass flow", while the outlet (exhaust gases) was set as "pressure outlet". The parameter values for the inlet and outlet boundary conditions were taken from Table 1. The no-slip condition was chosen for the domain's walls. In Table 2, the parameter values and setups of the boundary conditions are described.

In terms of fuel inlet boundary conditions, the mass flow of the fuel was determined according to the principle of constant fuel enthalpy introduced inside the combustion chamber. As the combustion chamber used in this study was designed for methane fuel, this fuel enthalpy was selected as the reference. According to the design process of the combustor, the needed mass flow of methane is 0.004874 kg/s. The lower heat values (described in the introduction) and eq. (1) allowed the mass flow of the ammonia-hydrogen mixture to be determined, taking into account its composition. The calculated mass flows for ammonia-hydrogen mixtures were listed in the Table 3.

Then, for the calculations, the pressure-based solver was enabled with second-order discretization with pressure-velocity coupled methods [2, 24]. Finally, the simulations were run.

The methods and models presented in the literature review [3, 9–11, 13, 14, 16–18, 20–22, 24, 25, 29], applied in the current research, were validated.

Table 2. Implemented general boundary conditions

Boundary condition	Type	Parameters
Air inlet	Mass flow inlet	Mass flow = 0.251 kg/s Turbulent intensity = 15% Turbulent viscosity ratio = 10 Total temperature = 433 K Mean mixture fraction = 0 Mixture fraction variance = 0
Fuel inlet	Mass flow inlet	Mass flow = 0.004874 kg/s Turbulent intensity = 15% Turbulent viscosity ratio = 10 Total temperature = 300 K Mean mixture fraction = 1 Mixture fraction variance = 0
Exhaust	Pressure outlet	Static pressure = 0 Pa Turbulent intensity = 15% Turbulent viscosity ratio = 10 Backflow total temperature = 300 K Mean mixture fraction = 0 Mixture fraction variance = 0
Wall	Wall	Stationary wall No slip No heat exchange Internal emissivity = 1 Opaque wall Diffuse fraction of radiation = 1
Operating conditions	-	Operating pressure = 301133 Pa Gravity off

$$c_s^{i\%H_{2mf}} = \frac{LHV_{CH_4} \cdot c_s^{CH_4}}{LHV_{H_2} \cdot H_{2mf} + LHV_{NH_3} \cdot (1 - H_{2mf})} \quad (1)$$

where $c_s^{i\%H_{2mf}}$ is the fuel mass flow for hydrogen mass fraction i in ammonia-hydrogen fuel [kg/s], $c_s^{CH_4}$ is the fuel mass flow for methane fuelling mode [kg/s], H_{2mf} is the hydrogen mass fraction in ammonia-hydrogen fuel [–], LHV_{CH_4}, LHV_{H_2} and LHV_{NH_3} are respectively the lower heat value of methane, hydrogen and ammonia fuel [kJ/kg].

Table 3. Fuel mass flow as a function of hydrogen mass percentage in ammonia-hydrogen fuel

H_2 mass percentage [%]	Fuel mass flow [kg/s]
0	0.013102
10	0.008479
20	0.006268
30	0.004971
40	0.004119
50	0.003517
60	0.003068
70	0.002720
80	0.002444
90	0.002218
100	0.002031

4. Results and discussion

In this part of the paper, the results were presented and discussed. First, the exhaust total temperature and the total pressure drop occurring in the combustor were assessed when an ammonia-hydrogen mixture replaced methane fuel. These two parameters are crucial for the work performance of gas turbines and it is suitable to assess these two parameters when modifying the fuelling mode of the gas microturbine device. Then, the maximum combustion temperatures were exposed and analysed in selected combustor cross-sections. Finally, the homogeneity of the combustion temperature in the cross sections was presented and analysed.

4.1. The total pressure drop

The total pressure drop is a very important parameter when dealing with the combustor of gas turbine devices. The main objective when designing a combustion chamber is to obtain the lowest total pressure drop. In this study case, the aim was not to obtain the lowest possible total pressure drop but to check if the replacement of the methane fuel by the ammonia-hydrogen fuel would have impacted this combustor parameter. The total pressure drop was calculated according to the eq. (2), while the obtained values for this parameter were listed in Table 4.

$$\Delta p_{total} = \frac{p_{2.total} - p_{3.total}}{p_{2.total}} \cdot 100 \tag{2}$$

where Δp_{total} is the total pressure drop in combustor [%], $p_{2.total}$ is the total pressure at combustor's inlet [Pa] and $p_{3.total}$ is the total pressure at combustor's outlet [Pa].

Table 4. Total pressure drop in the combustor in function of the fuelling mode

Case	$p_{2.total}$ [Pa]	$p_{3.total}$ [Pa]	Δp_{total} [%]
00H2	350,336	315,014	10.1
10H2	350,361	315,003	10.1
20H2	350,229	314,812	10.1
30H2	350,331	314,807	10.1
40H2	350,297	314,763	10.1
50H2	350,165	314,751	10.1
60H2	350,018	314,584	10.1
70H2	350,120	314,716	10.1
80H2	349,862	314,639	10.1
90H2	349,874	314,544	10.1
100H2	350,023	314,694	10.1
CH4	349,849	314,604	10.1

According to the results presented in Table 4, the total pressure drop in the combustion chamber, while modifying the fuelling mode, is stable (10.1%) and does not differ from the methane fuelling. The replacement of methane reference fuel in this study case seems not to have an impact on the total pressure drop in the combustor, which is a suitable phenomenon.

Replacement of the reference fuel by an ammonia-hydrogen mixture does not impact the total pressure drop in the gas microturbine's combustion chamber.

4.2. The exhaust total temperature

Another crucial parameter that describes the performance of a gas turbine device is the total temperature of the exhaust gases (at the outlet of the combustor). In this part, it was checked if modification of the fuelling mode, replacing the reference fuel (methane) with an ammonia-hydrogen mixture, would have impacted this parameter. In order to assess this parameter, the deviation from the reference (methane fuel) of the total temperature was calculated and expressed in percentage using the eq. (3). The obtained values of these deviations were listed in Table 5.

$$\Delta T_{total} = \frac{T_{total} - T_{CH4.total}}{T_{CH4.total}} \cdot 100 \tag{3}$$

where, ΔT_{total} is the total temperature deviation between actual and methane fuelling mode [%], T_{total} is the total temperature of exhaust gases [K] and $T_{CH4.total}$ is the total temperature of exhaust gases for methane fuelling [K].

Table 5. The exhaust gases total temperature deviation for ammonia-hydrogen fuelling relatively to the methane fuelling

Case	$T_{3.total}$ [K]	ΔT_{total} [%]
00H2	1179	4.96
10H2	1199	3.37
20H2	1207	2.69
30H2	1214	2.11
40H2	1221	1.57
50H2	1229	0.97
60H2	1220	1.67
70H2	1234	0.53
80H2	1220	1.64
90H2	1224	1.31
100H2	1235	0.42
CH4	1241	X

According to the data presented in Table 5, the total temperature deviation of the exhaust gases for ammonia-methane fuel relative to the methane fuel (reference) is in the range from 0.42% to 4.96%. The values obtained from this parameter are acceptable, and it can be considered that the replacement of the reference fuel by an ammonia-hydrogen mixture in gas turbine devices does not seem to impact the exhaust gases' total temperature, which is a suitable observation.

When hydrogen participation in the ammonia-hydrogen mixture increases, the total temperature deviation of the exhaust gases relative to the methane fuel is reduced. This observation may be related to the fact that the combustion reactivity of the ammonia fuel is much lower than that of the methane and hydrogen fuels. So when ammonia-hydrogen fuel is richer in ammonia, the combustion reactivity drops and may lead to not complete and not total combustion, resulting in lower heat release and then lower exhaust gases total temperature. When hydrogen is added to the ammonia-hydrogen mixture, the reactivity of the combustion increases and the heat release tends to be more complete; the temperature deviation reduces.

To resume this part, it can be considered that the replacement of the reference fuel by an ammonia-hydrogen mixture in gas turbine devices does not seem to affect the exhaust gases total temperature, which is a suitable observation.

4.3. The maximum combustion temperature

The aim of these studies was to assess whether the replacement of the reference fuel, here methane, by an ammonia-hydrogen mixture would have modified the temperature map in the combustion chamber liner. From a mechanical point of view, as previously exposed, no suitable modification consists of a local combustion temperature increase. An increased combustion temperature indicates that the thermal load of the liner would also increase, and it may lead to liner and then combustor damage or to lifetime reduction of these components. This is the reason why, in this study case, the maximum temperature of combustion was studied in a few cross-sections of the combustor. Figure 3 permits to visualise the cross-section positions. The locations of these sections are expressed in millimetres according to the coordinate system presented in Fig. 1. The maximum combustion temperature obtained on these sections allowed us to create a graph presented in Fig. 4.

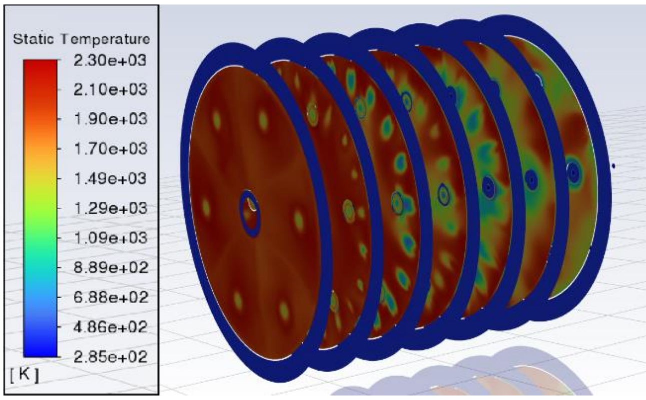

Fig. 3. Visualisation of the cross sections studied of the combustor

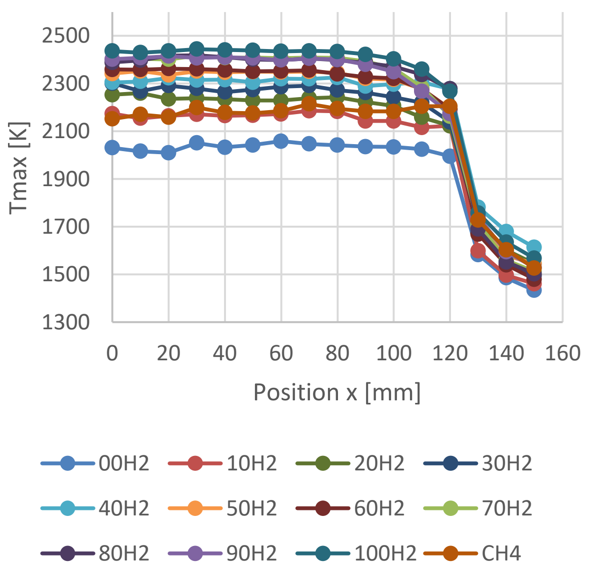

Fig. 4. Maximum combustion temperature in studied cross sections of the combustor

Firstly, the maximum temperature evolution as a function of hydrogen content in ammonia-hydrogen fuel was analysed. As can be read in Fig. 4, the maximum combustion temperature evolves from 2436 K for pure hydrogen supply to 2030 K for pure ammonia supply. Maximum temperatures of ammonia-hydrogen mixtures range between these two extremes. It must also be noticed that the maximum combustion temperature increases with increasing participation of hydrogen in ammonia-hydrogen fuel. The increase in hydrogen leads to an increase in combustion reactivity. An increased combustion reactivity may lead to faster heat release and to the formation of local hot spots. As the adiabatic combustion temperature of hydrogen is higher than for ammonia (respectively 2383 K and 2073 K – in the introduction), the increase in hydrogen content leads to an increase in the temperature of created hot spots. The formation of hot spots is generally not suitable from a thermomechanical and NO_x formation point of view. These phenomena are difficult to eliminate in diffusion-type combustors due to the combustion mode. In this study, it was shown that the increase in the hydrogen content of the ammonia-hydrogen mixture leads to a maximum temperature increase, which is not a suitable phenomenon. The behaviour of the maximum combustion temperature in the liner may be justified and is comprehensible.

Then, the evolution of the combustion maximum temperature across the liner length was discussed. As can be noticed in Fig. 4, the maximum combustion temperature is quasi-stable along the combustor and stays in the same relative position (compared to other fuelling modes). This phenomenon is observed until 110/120 mm. Then, the maximum temperature rapidly decreases to a range of 1434 K to 1613 K. This quick decrease in temperature is designed, and it is linked to the inlet of mixing and cooling air-flow into the liner. From the beginning of the liner to the 110/120 mm, the maximum combustion temperature is linked to fuel combustion properties and moderately turbulent flow. After the main combustion zone, at the mixing and cooling zone of the liner, the temperature decreases quickly, and the new relative positions of the maximum temperature are mostly linked to the turbulent mixing process rather than to the combustion fuel properties. The most important thing to notice is the fact that the range of maximum temperatures after the cooling process is lower than the temperature range at the beginning of the liner. It means that the replacement of the reference fuel by an ammonia-hydrogen mixture affects mainly the top part of the liner. The maximum combustion temperature in the top part of the liner is crucial to establishing the suitable ammonia-hydrogen mixture composition from a thermomechanical point of view. The behaviour of the maximum combustion temperature along the liner may be justified and is comprehensible.

Finally, the last step was to establish the suitable ammonia mixture composition in order not to overload the liner from a thermal point of view. According to the above analysis, it is crucial to select an ammonia-hydrogen mixture for which the maximum combustion temperature matches the maximum combustion temperature for the reference fuel (here it is methane). According to Fig. 4, in the location range from 0 to 110/120 mm, the curve that matches better with the methane curve is that for ammonia-hydrogen mixture with hydrogen content of 10% (massic participation).

To resume this section, the maximum combustion temperature behaviour in the liner for various fuelling modes is justified and comprehensible. Taking into account the maximum combustion temperature criterion, from a thermomechanical point of view, the most suitable composition in massic participation for an ammonia-hydrogen mixture is 10% mass of hydrogen and 90% mass of ammonia.

4.4. The combustion zone temperature homogeneity

In this section, the homogeneity of the temperature of the combustion zone was assessed. The homogeneity of the combustion temperature is important not only in the reduction of NO_x creation but also in the thermal load of the liner. If the combustion temperature is not homogeneous, the thermal load in the liner structure is not uniform, and this may cause mechanical failure in the liner. The temperature homogeneity was studied in the selected combustor cross section, as done above, applying the function of uniformity index (described by eq. (4)). The calculated uniformity indexes are shown in Fig. 5. An uniformity index near unity indicates good temperature homogeneity, while a uniformity index near zero indicates poor temperature homogeneity.

$$UI_{area}^{plane} = 1 - \frac{\sum_{i=1}^{N}\left[\left(\left|T_{face_i} - T_{average}\right|\right) \cdot A_i\right]}{2 \cdot T_{average} \cdot \sum_{i=1}^{N}[A_i]} \quad (4)$$

where UI_{area}^{plane} is the area averaged uniformity index [–], T_{face_i} is the static temperature on i-th facet defining analysed surface [K], $T_{average}$ is the average static temperature in analysed cross-section [K] and A_i is the area of facet defining analysed surface [m^2].

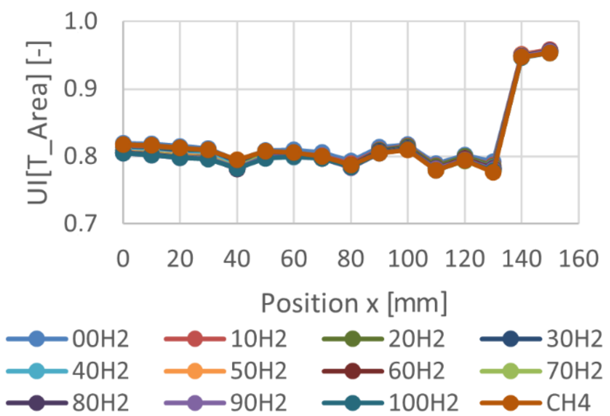

Fig. 5. The temperature uniformity index in combustor while modifying fuelling mode

On the one hand, it must be noticed that the uniformity index evolves from 0.804 (for pure hydrogen fuelling) to 0.819 (for pure ammonia fuelling). The ammonia-hydrogen mixtures temperature uniformity indexes are ranged between these two extremes. It must also be noticed that the temperature uniformity indexes decrease when hydrogen participation increases in ammonia-hydrogen fuel. This observation is correct and in accordance with the fact that the addition of hydrogen increases the reactivity of the combustion, resulting in higher peak temperatures and then in reduced temperature homogeneity. This trend is conserved throughout the combustion liner up to 130 mm. After the position of 130 mm, the temperature homogeneity increases and tends to a common value of 0.95 for all the fuelling modes. In the first part of the liner, the combustion is driven by chemical kinetics and turbulence; this is the reason for keeping the relative position between the curves – the fuel properties are taken into consideration. In the second part of the liner, the mixing and cooling air is supplied to the liner, and it provokes the combustion inhibition and homogenisation of the gas temperature. Here, the turbulence is primordial, which is why the temperature uniformity indexes tend to have a common value. The behaviour of the temperature uniformity indexes is justifiable and comprehensible.

On the other hand, the temperature uniformity indexes for methane fuelling need to be compared to the ammonia-hydrogen mixture fuelling. According to the Fig. 5, the temperature uniformity indexes of the methane fuelling mode match most of the temperature uniformity indexes of the ammonia-hydrogen mixture, with hydrogen massic content ranging between 0% and 10%. This correspondence is available all along the combustor liner.

To resume this section, the temperature uniformity indexes decrease as the hydrogen participation in ammonia-hydrogen fuel increases and the most comparable ammonia-hydrogen mixture to methane, from a temperature uniformity index point of view, is that with a hydrogen massic content ranging from 0% to 10%.

5. Conclusions

According to the presented studies, the following remarks need to be listed:

- the replacement of reference fuel (here methane) by ammonia-hydrogen mixture does not impact the total pressure drop occurring in the combustion chamber of gas microturbine; it is a suitable observation
- the replacement of the reference fuel by ammonia-hydrogen mixture in gas turbine devices does not impact the exhaust gases total temperature; it is a suitable observation
- the increase in hydrogen content in the ammonia-hydrogen mixture leads to a maximum temperature increase; it is not a suitable phenomena
- the maximum combustion temperature in the top part of the liner is crucial to establishing the suitable ammonia-hydrogen mixture composition from a thermomechanical point of view
- taking into account the maximum combustion temperature criterion, from a thermomechanical point of view, the most comparable (to methane fuel) composition in massic participation for ammonia-hydrogen mixture is 10% mass of hydrogen and 90% mass of ammonia
- the temperature homogeneity decreases when increasing the hydrogen participation in ammonia-hydrogen fuel; it is a not suitable observation
- in the second part of the liner, the mixing and cooling air is supplied to the liner and it provokes the combus-

tion inhibition and homogenisation of the gases temperature
- the most comparable ammonia-hydrogen mixture to methane, from a temperature homogeneity point of view, is that with a hydrogen massic content ranging from 0% to 10%.

This study allowed to demonstrate that the replacement of the reference fuel (here methane) by an ammonia-hydrogen mixture does not impact the combustion chamber work parameters (exhaust gases total temperature and total pressure drop). The most suitable massic composition of the ammonia-hydrogen fuel, from a thermal load point of view, comparable to the reference methane fuel, is 10% hydrogen and 90% ammonia. This massic composition corresponds to a volumic composition of 48.4% of hydrogen and 51.6% of ammonia. According to the research review exposed in the introduction, the most suitable ammonia-hydrogen volumic composition for stable combustion and reduced NO_x creation is 70% of ammonia and 30% of hydrogen. As 30% is less than the established 48.4% for hydrogen-safe content, it means that the commonly applied volumic composition of 70% of ammonia and 30% of hydrogen is safe for combustor structure from a thermal load point of view.

This study allowed to demonstrate that the commonly applied volumic composition of 70% ammonia and 30% hydrogen, for ammonia-hydrogen fuelling, is safe for gas microturbine combustors from a thermal load point of view.

The next step would be to validate the presented results in order to confirm their full accuracy, as the performed studies were conducted using CFD methods.

Nomenclature

CFD	computational fluid dynamics
CH_4	methane
DO	discrete ordinate model
H_2	hydrogen
NH_3	ammonia
NO_x	nitrogen oxides
PDF	probability density function
RANS	Reynolds Averaged Navier-Stokes model
WSGGM	weighted sum of grey gases model
% mass	percentage of the mass
% vol.	percentage of the volume

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