Can flashback be avoided through humidification in an original micro Gas Turbine combustor? — 0D/1D predeterminations and LES validation

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Abstract - This work presents a feasibility study on the use of combustion air humidification to stabilize hydrogen combustion and to avoid flashback apparition in mGTs without having to redesign the combustor. Using a hybrid model, combining a 0D Chemical Reactor Network and 1D Laminar flame calculations, the laminar flame speed is evaluated at reduced cost to predetermine the necessary minimal water dilution of the combustion air to avoid flashback for several H_2/CH_4 blends. Finally, LES simulation results show stable combustion for these predetermined levels of humidification.

Nomenclature

Acronyms
CRN Chemical Reactor Network
$EINOx$ Emission Index of NO_x
LES Large Eddy Simulation
mGT micro Gas Turbine
$mHAT$ micro Humid Air Turbine
Symbols
$\dot{m}$ Mass flow rate, $\mathrm{kg/s}$
S_L^0 Laminar Flame Speed, $\mathrm{m/s}$
T_{ad} Adiabatic Flame temperature, K
X_k Volume fraction of the species k, $-$
Y_k Mass fraction of the species k, $-$
y^+ Dimensionless wall distance, $-$
Greek symbols
ϕ Equivalence ratio, $-$
Ω Water-to-air ratio, $-$
$\dot{\omega}_T$ Reaction rate, $\mathrm{W/m^3}$

1. Introduction

The absolute necessity to reduce carbon emissions in the next decade has led to a significantly increase in the contribution of renewable energy in the electricity production at the expense of traditional, combustion based thermal power production. Nevertheless, the unpredictable nature of renewable energy sources, like wind and solar, together with the large fluctuations in their production, put some severe constraints on the reliability and stability of the electricity grid. Moreover, large-scale battery storage, still remaining expensive, does not offer a solution for medium- to long-term (seasonal) energy storage. Given these issues, there is nowadays a strong trend towards storing the excess renewable electricity using Power-to-Gas [1], i.e. production of H_2 from excess renewable electricity using electrolysis, so-called green H_2.

The use of green hydrogen, e.g. H_2 produced using electrolysis to store excess renewable electricity, allows for combustion-based technologies to keep playing a key role in the future of power generation. Especially in a decentralised production with cogeneration, micro Gas Turbine (mGT) technologies offer great advantages related to their high adaptability and flexibility, in terms of operation and fuel. Combining the clean hydrogen production from renewable energies using Power-to-Fuel with a carbon-clean combustion in the mGT facilitates the implementation of renewable energies for the energy transition [2]. However, hydrogen (or hydrogen enriched methane/air) combustion is well known to lead to flame and combustion instabilities. While a decrease in CO_2 levels is obviously expected, the high temperatures and reaction rates

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reached in the combustor can potentially lead to flashback, causing thus major and irreversible damages to the facility.

Several approaches have been investigated and can be found in literature to ensure a stable and safe hydrogen combustion. Modifying the geometry and adapting the combustor layout opens the path to stable and controlled combustion, especially with $100\,\%$ H_2 fuelling [3, 4]. Micromix combustors, using rich diffusion flames, have shown their capability to control and stabilize the combustion of hydrogen. Although all the proposed and studied layouts show complete and stable combustion at $100\,\%$ H_2 input, they require a complete combustor redesign. Moreover, these combustors are not always suitable for CH_4 combustion, limiting the fuel flexibility of the mGT. An alternative solution to avoid any redesign of the combustor stands in using diluted conditions to slow down the reaction. Combustion air humidification (steam or water addition) is another route which has proven effective to reduce the combustion temperatures and reaction rates, avoiding thus flashback apparition [5, 6, 7]. Although this solution allow to process with only one combustor, a modification in the global cycle is needed, such as the implementation of a saturation tower or a steam boiler to inject water (or steam) in the cycle. Additionally, knowledge of the hydrogen limit in hydrogen enriched methane combustion in mGTs, still leading to stable and complete combustion without requiring any redesign, is essential and allows future mGT operators to manage safely the combustion of different fuel mixes, without requiring an expensive combustor redesign. Indeed, in the context of increasing the fuel flexibility of small-scale production unit, development must focus on one specific chamber, designed and adapted for various fuels and under specific diluted conditions, while knowing the operating range (conditions and limits) leads to ensure stable combustion. Nevertheless, there is a lack of highly accurate data on real combustor configurations, limiting the technological progress towards more flexible operation and industrial applications.

Aiming at stabilizing hydrogen combustion in mGTs without any redesign of the combustor, this work presents thus a parametric study over a specific range of operating conditions of the T100 mGT combustor to find the optimized humidification level of the combustion air for methane/hydrogen blends (at different hydrogen rate) leading to stable combustion. Using a hybrid model, combining a 0D Chemical Reactor Network (CRN) with 1D laminar flame calculations, the necessary minimal water amount is assessed and optimized to reach the same level of flame speed as reached in classical pure methane combustion. This methodology allows to predict the combustion temperature and emissions at reduced cost. Finally, Large Eddy Simulation (LES) of the actual combustor geometry of the T100 mGT are performed to validate the 0D/1D predetermination, by verifying if the predetermined conditions of humidified oxidizer help to reduce the reaction rate of hydrogen, and thus prevents flashback. In this paper, the combustor layout and operating conditions are first described. Then, the Chemical Reactor Network (CRN) model developed for the 0D/1D simulations of the T100 combustor is presented, as well as the results of the hybrid 0D CRN/1D Flame simulations. Finally, the results of the LES simulations are shown to validate the predetermined operating parameter defined by the 0D CRN/1D Flame simulations to avoid flash back apparition.

2. Combustion chamber of the T100 mGT

In this section, the combustor layout and the operating conditions of the Turbec T100 mGT combustor are first presented. Then, the set-up considered to humidified the mGT cycle, and thus the combustion chamber, is described.

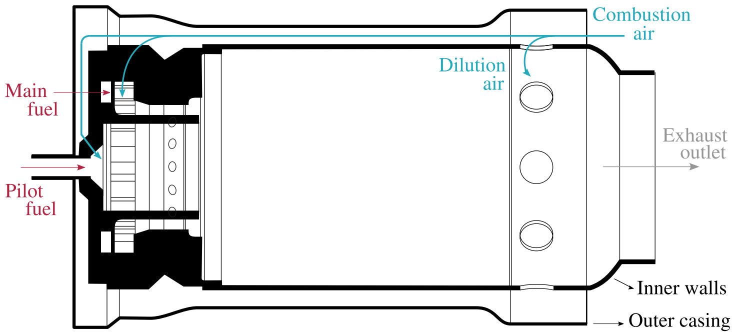

Figure 1: The Turbec T100 combustion chamber is a reverse (or counter-current) flow can burner.

2.1. Combustor layout & Operating conditions

The combustion chamber considered for the simulations is the combustor of the Turbec T100 mGT [8]. At nominal conditions, this mGT produces a net electrical power output of $100\,\mathrm{kW_e}$ while the combustor inlet conditions are a fuel consumption of $333\,\mathrm{kW}$ and an air mass flow rate coming from the compressor of $800\,\mathrm{g\,s^{-1}}$. The T100 combustor features a can swirl burner (counter-current flow) where the combustion air is entering between the outer casing and the inner walls of the combustor. The air reaches then the dilution holes, the pilot, and main injectors by passing on the external surface of the inner walls. The layout characteristics of this combustor are (Figure 1): a pilot flame exploiting a diffusion flame, fed by 12 air injectors and 6 fuel injectors; a premixed combustion as main flame using two rows of swirler (a first one to premix fuel and air, and ending with 30 swirled injectors); and 9 dilution holes to cool down the exhaust gases to avoid any damages at the turbine inlet. Based on numerical investigations, an estimation of this combustion air distribution over the different injectors and dilution holes in the Turbec T100 can be found in literature [9, 10] where: $65\,\%$ of the mass flow rate enters the chamber through the dilution holes, $30\,\%$ via the main premixed injectors, and $5\,\%$ through the pilot injectors. The operating conditions of the Turbec T100 mGT at nominal point for a classical pure methane combustion, considered as reference case (REF case), are presented in Table 1. In case of hydrogen (or hydrogen enriched) combustion, flashback is most likely to appear in the premixing zone of the main injectors. Therefore, the local conditions of the main flame, in terms of fuel and air composition, pressure, temperature and equivalence ratio, are considered to lead the 1D laminar flame simulations.

Table 1: Operating conditions of the Turbec T100 mGT at nominal point for a classical pure methane combustion, considered as reference case (REF case).

Net electrical power output, P_e	$100\,\mathrm{kW_e}$
Fuel consumption, P_{th}	$333\,\mathrm{kW_{th}}$
Air mass flow rate, $\dot{m}_{air}$	$800\,\mathrm{g\,s^{-1}}$
Pressure in the combustor, p	$4\,\mathrm{bar}$
Inlet air temperature, T_{in}	$865\,\mathrm{K}$
Inlet fuel temperature, T_{in}	$300\,\mathrm{K}$
Global equivalence ratio, ϕ_{global}	0.1433
Local equivalence ratio in main flame, ϕ_{main}	0.41

2.2. Combustion air humidification

Combustion air humidification (steam or water addition) has proven effective to reduce the combustion temperatures and reaction rates, avoiding thus flashback apparition. Although this solution allow to operate with only single combustor for different fuel blends, a modification in the global cycle is needed. Literature shows that there are several ways to dilute the combustion air [11, 12]. In the model presented in this study, we consider that the injection in the combustion air is performed, after the recuperator, but before entering the combustor, through direct water (or steam) injection, giving the required most flexible operation. A water-to-air mass ratio is considered to define the level of water dilution:

$$\Omega = \frac{\dot{m}_{water}}{\dot{m}_{air,tot}} \tag{1}$$

3. 0D Chemical Reactor Network - 1D Laminar Flame model

In this section, the Chemical Reactor Network, considered to simulate the T100 combustor, is first described in detail, as well as the numerical set-up of the hybrid 0D CRN/1D Flame simulation. Finally, the results of the 0D/1D benchmarking are presented, showing the predetermined operating condition to avoid flashback for several H_2/CH_4 blends (25/75, 50/50, 75/25 and 100/0).

3.1. Description of the model

The oxidizer and fuel temperatures have a major impact on the flame speed. Therefore, being able to accurately predict the temperature drop when water is added in the system would allow to optimize the water quantity produced by the saturation tower, reducing the operational cost of the mGT (avoiding unnecessary production of hot water). The methodology of this work is based on predicting, when the combustor is fuelled by hydrogen (or hydrogen enriched), the necessary minimal water quantity to add in the oxidizer to reach the same level of flame speed as for classical pure methane combustion. Hence, using a hybrid model, combining 0D Chemical Reactor Network (CRN) with 1D laminar flame calculation, allows to:

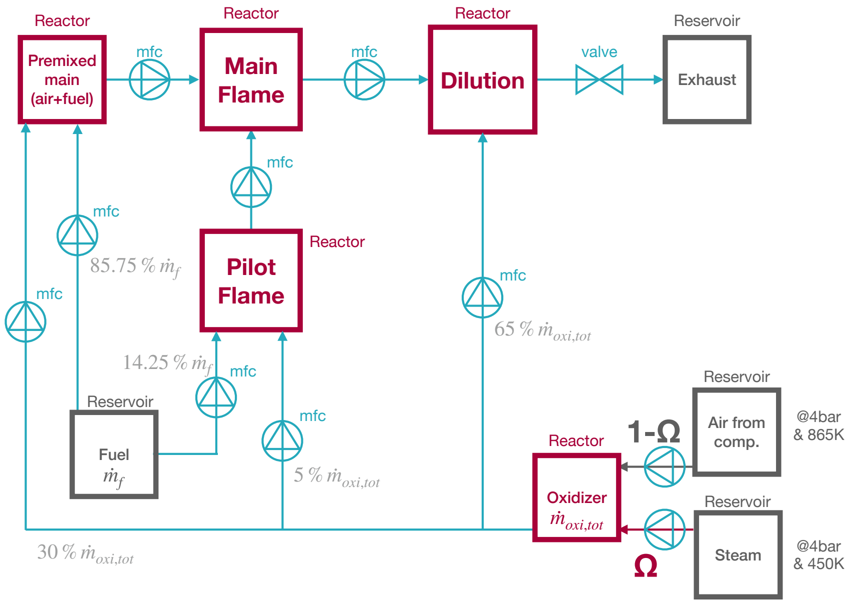

Figure 2: Detailed Chemical Reactor Network model of the T100 combustor.

- to predict the state of the flow at each main section of the combustor
- to take into account the impact of temperature drop on the flame speed, due to the mixing with hot saturated steam at 4 bars and 450K, for the 1D laminar flame speed calculation. The value of 450K for the steam injection corresponds to saturated steam at 10bars. This value was selected to ensure a sufficient high injection pressure to enable injection in the combustion air (at 4 bars) as well as for it sufficiently high temperature to not lead to a drastic combustion air temperature reduction, potentially leading to flameout
- to optimize this quantity of added steam
- to predict the combustor performances and emissions at reduced cost (LES are still necessary to assess the combustion stability)

Computation (both 0D CRN and 1D Flame) are carried out using the CANTERA software [13] with the detailed GRIMech 3.0 (GRI 3.0) [14] mechanisms (53 species and 325 reactions). Cantera allows to simulate Continuously Stirred Reacor (CSR) by solving the mass, species and energy conservation equations. As shown in Figure 2, a network of CSR is build to emulate the behaviour of the T100 combustor. During the 0D CRN simulation, the state of the flow in the premix chamber is calculated, and used to perform the 1D Flame calculation at the operating conditions calculated by the CRN. The one-dimensional unstretched laminar flame velocity S_l^0, defined as the speed at which the flame front was moving with respect to the fresh gases in a one-dimensional geometry, is computed as follows [15]:

$$S_l^0 = \frac{\int_V \dot{\omega}_k dV}{Y_k^{out} - Y_k^{in}}, \tag{2}$$

describing the flame as an interface moving at speed S_L^0 against the local flow, the flame speed is defined from the integral of the reaction rate across the flame front divided by the transport species through this flame front. Finally, the transport model used for the 1D simulation is the mixture averaged model.

3.2. 0D/1D benchmarking

In this part, the colormaps of the dimensionless flame speed, adiabatic temperature and Emission Index of NO_x (EINOx), divided by the values of the reference case, are analysed (Figure 3). First, the colormap of $S_l^0/S_{l,ref}^0$ provides the operating range in which the flame velocity remains lower than the flame speed of the reference case. It allows to determine the level of water dilution to avoid flashback apparition for various H_2/CH_4 blends. The results show that a $\Omega = 10\%$ is sufficient to keep the flame speed at the same level as or lower than the reference case, and thus to avoid any flashback when the combustor is fuelled with 100% of hydrogen. In addition, no flame extinction is observed for the full considered range of Ω. This remaining complete combustion is mainly due to the very low fraction of added water in the oxidizer. At this dilution of 10%, , a flame temperature reduction is observe down to 88% of the adiabatic flame temperature of the reference case, when using pure hydrogen as fuel. This temperature drop has the benefit to reduce the NO_x levels. The NO_x emissions reported in this study are based on the Emission Index of NO_x (EINOx), in $\frac{g}{kWh}$, defined as follow:

$$EINO_x = \frac{X_{NO_x} \cdot \dot{m}_{oxi}}{P_{el}}, \tag{3}$$

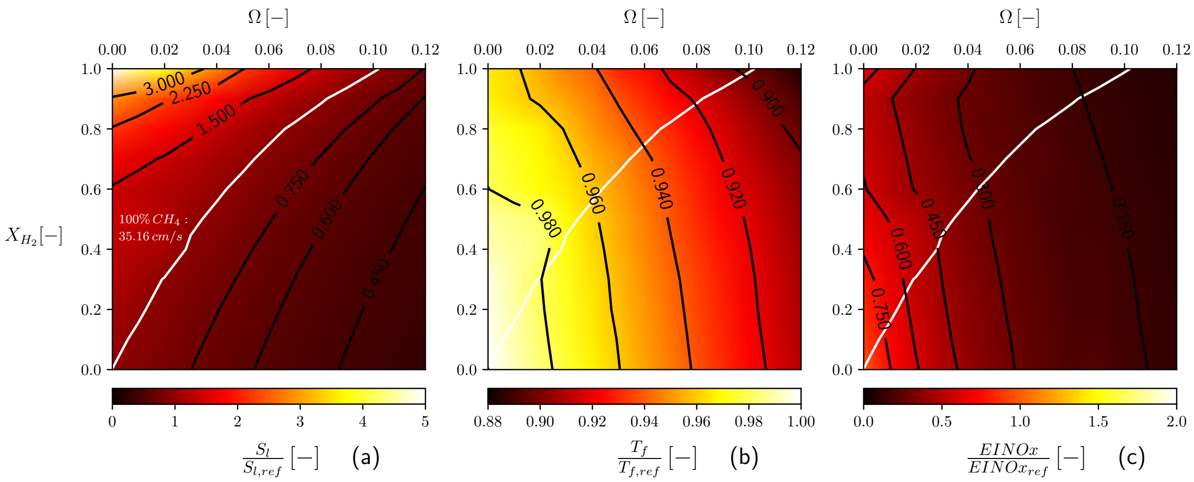

Figure 3: Colormaps of the predicted dimensionless laminar flame speed $S_l^0/S_{l,ref}^0$, adiabatic flame temperature $T_{ad}/T_{ad,ref}$ and NO_x emissions $EINOx/EINOx_{ref}$ for a range of hydrogen blend from 0 to 100% and a range of Ω from 20 to 100%.

where $\dot{m}_{oxi}$ is the total oxidizer mass flow rate and P_{el} is the electric power produced by the mGT at the considered operating conditions. The observed temperature drop when humidification is performed results in a reduction of the EINOx down to 10% of the values obtained for the reference case.

Figure 4 presents a quantitative analysis for a specific range of H_2/CH_4 blends (25/75, 50/50, 75/25 and 100/0), showing that the minimal necessary quantity of water to bring the flame velocity back to the reference level for these blends is respectively a Ω ratio of 1.5, 3.4, 5.9 and 10.25%. These predetermined conditions are validated in next section for the cases $50\%volH_2/\Omega = 3.4\%$ & $100\%volH_2/\Omega = 10.25\%$, using 3D LES on the actual layout of the T100 combustor.

4. Large Eddy Simulation of the T100 combustor

This section present the validation of the 0D/1D predeterminations for the cases $50\%volH_2/\Omega = 3.4\%$ & $100\%volH_2/\Omega = 10.25\%$ using 3D LES of the actual layout of the T100 combustor. First, the numerical set-up is described, and then the LES results are presented.

4.1. Numerical set-up

The LES, presented in this paper, is performed using the massively parallel flow solver YALES2 [16]. The turbulent sub-grid scale stresses are modelled with the local dynamic Smagorinsky model [17]. The stability of the time integration is ensured with an adaptive time step that keeps the CFL number under 0.4. Moreover, the chosen operating conditions lead to a Reynolds Number Re $= 37500$ and a dimensionless wall distance $y^+ = 40$ in the main swirler. Therefore, we use a classical log-law profile as wall model [18] in our simulations. Adiabatic walls condition is considered (no heat losses). The LES of the combustion are performed coupling finite-rate chemistry to a detailed chemical mechanism. The kinetic scheme DRM19 (21 species and 84 reactions) is used in our LES [19]. This reduced kinetic scheme, chosen to reduce the computational cost, have already been compared and validated in the range of the operating conditions of the T100 in a previous work [7] by comparing the results obtained using the well-known detailed kinetic scheme GRI3.0 [14].

A combustion model of artificially thickened flame is used to predict correctly the com-

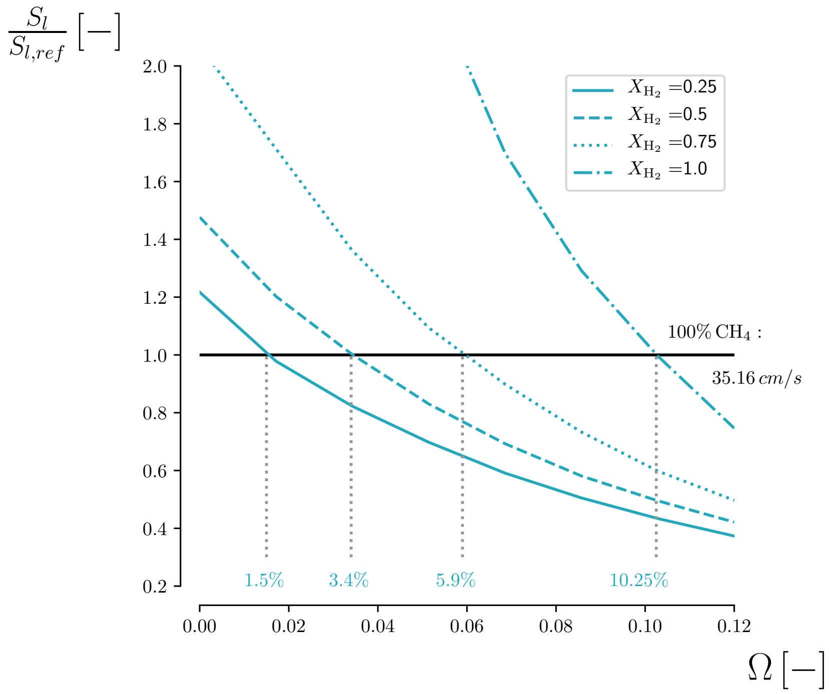

Figure 4: Predicted dimensionless laminar flame speed $S_l^0/S_{l,ref}^0$ compared with the reference case for several H_2/CH_4 blends (25/75, 50/50, 75/25 and 100/0) while the water-to-air ratio Ω is increased. To reach the same level of velocity as the reference case, hydrogen combustion requires respectively a Ω ratio of 1.5, 3.4, 5.9 and 10.25%.

bustion and to model the sub-grid scale turbulence/chemistry interaction on the LES grid. In our LES, the dynamic Thickened Flames model (TFLES) [20] is implemented by modifying the conservation equations with a thickening factor F and the efficiency function E of Charlette et al. [21] (considering a static formulation with β = 0.5), to have the thermal flame thickness $\delta_T = F \cdot \delta_L^0$ and flame speed $S_T^0 = E \cdot S_L^0$ where S_T^0 is the sub-grid scale turbulent flame speed [15]. In addition to this TFLES model, an Adaptive Mesh Refinement (AMR) algorithm is used for the LES simulation. By dynamically refining the mesh in the flame region, based on a combustion criterion using the flame sensor of the TFLES model, the mesh is optimized in terms of cell quantity and distribution. The AMR algorithm dynamically refines the mesh all along the flow simulation to lead to the LES mesh. For the validation and the full details of the AMR methodology, the reader is invited to read [22]. The automatically refined mesh obtained for the LES simulations (Figure 5 (a)) includes almost 53 million of tetrahedral cells where the cells size ranges from $\Delta = 700\,\mu\text{m}$ in the flame front region to $\Delta = 3\,\text{mm}$ in the domain.

4.2. Flame stability

In this part, the LES results for the cases $50\% vol H_2/\Omega = 3.4\%$ & $100\% vol H_2/\Omega = 10.25\%$ of the instantaneous reaction rate $\dot{\omega}_T$, highlighted on the dynamically adapted mesh Figure 5 (a), and the temperature Figure 5 (b) color fields are analysed. First, we can clearly observe that the mesh adaptation follows perfectly the flame in the combustor during the simulation (Figure 5 (a)). Then the instantaneous color field of the reaction rate (Figure 5 (a)), highlighting the flame front, clearly shows that the flame front is not going back in the main swirlers for both cases. In addition, the instantaneous color field of the temperature (Figure 5 (b)) does not show either any temperature increase in the main injectors and swirlers. Therefore, we can conclude that the LES results does not show any flashback apparition for the predetermined condition of dilution ($\Omega = 3.4\%$ for a hydrogen containing fuel of $50\% vol H_2$, and $\Omega = 10.25\%$ for a hydrogen containing fuel of $100\% vol H_2$) obtained using a low cost 0D/1D calculations.

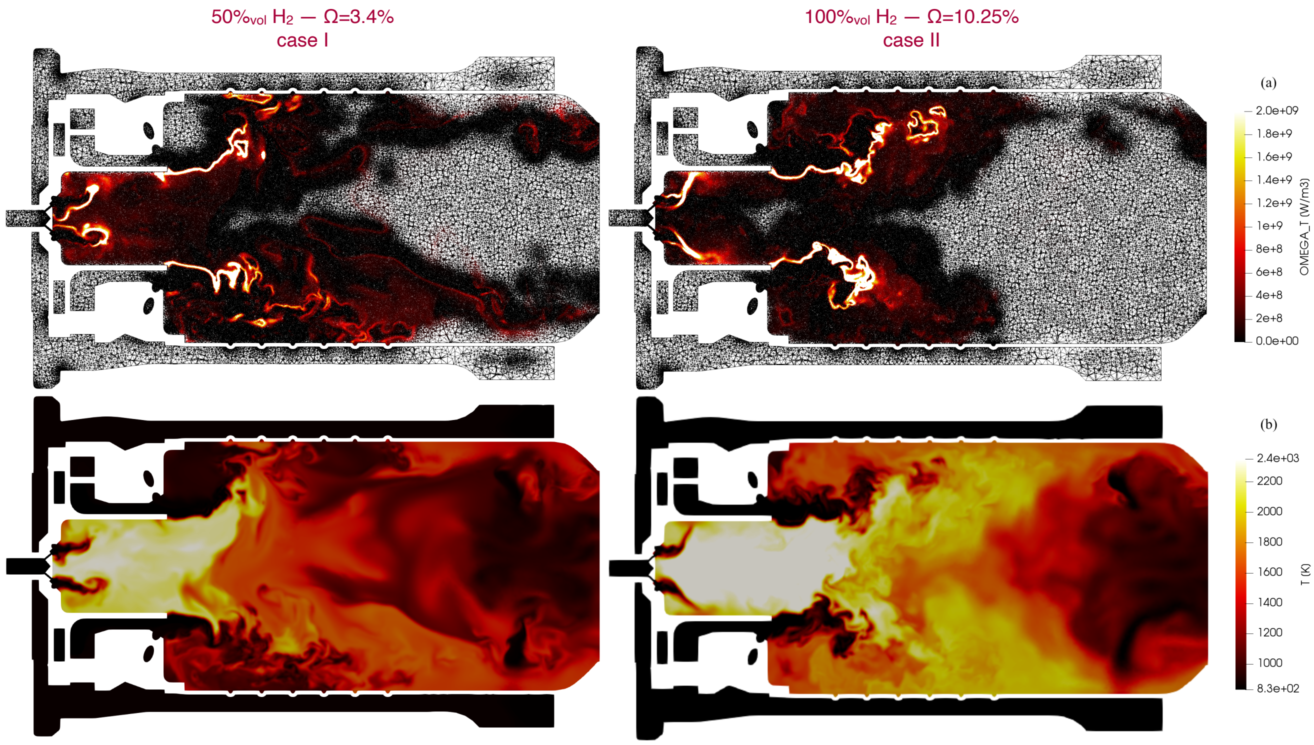

Figure 5: LES results for the cases $50\% vol H_2/\Omega = 3.4\%$ & $100\% vol H_2/\Omega = 10.25\%$ of the instantaneous reaction rate $\dot{\omega}_T$ on the dynamically adapted mesh (a) and the temperature (b) color fields showing no flashback apparition near the main flame swirler for both cases.

5. Conclusion

Aiming at stabilizing hydrogen combustion in mGT without any redesign of the combustor, this work presented the feasibility of water dilution to reduce temperature and flame speed of hydrogen combustion in a typical mGT combustion chamber (Turbec T100) using 0D CRN/1D Flame approach for the predeterminations, and then using 3D LES simulations of the real combustor layout for the validation. The 1D laminar flame calculations results show that the combustion, at nominal operating conditions of the T100 (air mass flow rate of 800g/s, and a fuel consumption of 333kW, fuelled with different H_2/CH_4 blends (25/75, 50/50, 75/25 and 100/0), can indeed reach the same level of flame speed as pure methane combustion by humidifying the combustion air (using a water-to-air ratio of 1.5, 3.4, 5.9 and 10.25% respectively). Finally, the 3D LES simulation results show stable combustion for the predetermined level of humidification when the combustor is fuelled by 50%vol and 100%vol of H_2. No increase of temperature or reaction rate levels are reached in the main injectors of the combustor, ensuring then no occurring flashback. Hence we can conclude that this dilution method allows to stabilize H_2 combustion, and the 0D/1D approach provides accurate and low cost predetermination of the operating parameter to avoid flashback apparition.

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