Numerical Investigation in a Gas Turbine Burner Operating with Hydrogen-Ammonia Blend using Large Eddy Simulation and LES-CRN Methodology

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Abstract

A non-premixed burner fed with a blend of ammonia-hydrogen is investigated numerically with the goal to validate the NO_x emission against the corresponding experimental measures, retrieved at atmospheric condition. Although the prediction of the CFD model is satisfactory in line with the experimental data, also a CRN is derived leveraging the time-averaged solution: such model provides a fast and reliable tool to deeply investigate the most significant NO_x formation pathways at the investigated operating conditions.

Introduction

The interest in ammonia as fuel for Gas Turbine (GT) combustors has triggered the development of fundamental research in the last decade [1]. In this context, combustion models embedded into CFD software are yet not fully able to predict several aspects associated with ammonia combustion. NO_x emission quantification is probably the main area where the numerical methodologies need to be improved [2]. It must be also admitted that even the understanding of the most fundamental NO_x formation paths are not always fully clear: the majority of the chemical mechanisms nowadays present in literature struggle on being fully predictive against the corresponding experimental data and very often a good agreement is achieved only on narrow operating windows. Since ammonia is always mixed with other fuels to overcome its chemical drawbacks from a combustion perspective [3] (i.e., natural gas or hydrogen), the challenge is also related to the global proprieties of the blend: depending on the specific operating conditions of the combustor, some NO_x formation paths could be favoured, compromising the generality of a given chemical mechanism. From an industrial perspective, the validation of the numerical approaches is also very often limited to simplified hardware working significantly far from the operating conditions of a modern GT combustor. This is another gap that OEMs should fill in the next future to make ammonia fired GT competitive. In this context, a CFD model as well as a CRN of an industrial burner operated at atmospheric pressure are investigated to develop a procedure able to better

understand the dominant NO_x formation pathways at a specific condition. The details of the test rig and the numerical approaches will be provided in the next sections.

Experimental facility and Campaign

The tests are executed in a single cup BH "*BlueRig*" facility with two independent air lines, one dedicated to the combustion air (Figure 1-a), the second, cooling the flame tube by external convection. The two streams meet at the dilution section placed at the end of the flame tube. Pollutant emissions are sampled downstream the dilution section with the sampled gas sent to a HORIBA PG250 gas analyser.

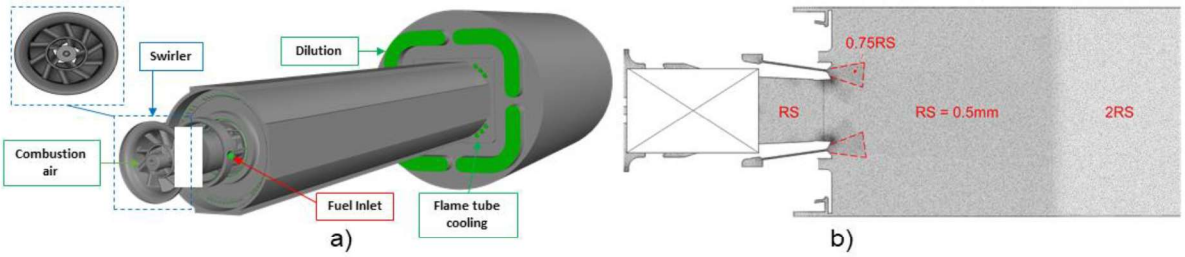

Figure 1: Computational domain (a) and details of the mesh with local refinements in function of the Reference Size (RS) (b).

The burner is a double counter-rotating swirler with two independent fuel lines: a premix and a pilot one [4]. Only the latter is used for the test with ammonia-hydrogen here discussed. Such configuration leads to a non-premixed flame that is dominantly diffusive. The temperature of the air and the global equivalence ratio are set to reach a flame temperature that is fully compatible with the ISO base load of the NOVA^{TM} LT16 engine. A sweep of ammonia content ranging from 0% up to 70% by weight is experimentally investigated [5] and the corresponding NO_x measurements are shown in Figure 2: the latter is selected among all the test points for the numerical investigation.

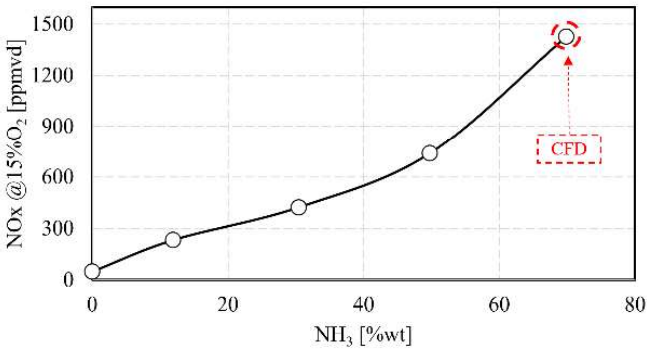

Figure 2: NO_x emissions measurements from the experimental campaign.

Numerical modelling

The commercial code Ansys Fluent is used to obtain the numerical CFD results shown in this work using Large Eddy Simulations (LES). The adopted computational domain is represented in Fig. 1a, while Fig. 1b shows some details of the

computational mesh used for the current investigation, having a total of 27×10^6 polyhedral elements. A Reference Size (RS) equal to 0.5 mm is used as reference to describe the discretization of the domain. The Smagorinsky – Lilly model with dynamic stress closure is employed at the turbulence subgrid scale. The chemistry of the hydrogen/ammonia mixture is modeled using the Flamelet Generated Manifold (FGM) approach [6]. The Stagni et al.'s [7] chemical kinetic scheme, which includes 31 species and 203 reactions, is selected as chemistry set. Additional scalar transport equations for NO and NH_3 are used to better capture nitrogen oxides and unburned ammonia emissions from the LES. Finite Rate closure is used to model the source term for the progress variable. Both spatial and implicit temporal discretization are solved with a second-order upwind scheme along the SIMPLEC scheme for pressure-velocity coupling. The constant time step size is defined in order to maintain the Courant-Friedrichs-Lewy number below unity across the domain, particularly in the flame zone region. After a preliminary wash-out phase, 5 FTT of the burner are simulated to collect statistics. A combined CFD and Chemical Reactor Network (CRN) technique is used to investigate the NO_x formation in the GT system. This approach allows the correct estimation of the number of reactors and their respective volumes, thus obtaining the residence times for each region of the domain. Moreover, the CFD-CRN technique allows to obtain reliable results in terms of NO_x emissions with a relatively low computational cost and, therefore, in a short time, allowing a broad study of the different parameters involved. The CRN to emulate the combustion of NH_3-H_2 mixtures in the complex and dynamic environment of a GT is developed based on the identification of the average zones of the temperature, flow, and radical species, obtained from the LES simulation. The individual reactors with their respective volumes are defined using the open-source software Cantera [8], based on two different types of reactors: the Perfectly Stirred Reactors (PSR), which represent the reactive zone, and the Plug Flow Reactors (PFR), which mimics the unidirectional flow zones of the combustion chamber and the dilution zones due to the injection of cooling air. The CRN is made up of three PSRs, which emulate the Diffusive (DIFF), Flame Zone (FZ) and CORNER regions, and two PFRs, which characterise the post-combustion and cooling zone. This configuration is previously validated in [5] and analysed to establish analytical correlations between the percentage of NH_3 by mass and the network calibration parameter, based on the equivalence ratio of the DIFF reactor. In this work, by exploiting the results obtained from the LES and applying them to the CRN structure, accompanied by the analytical correlations, it is possible to study the evolution of NO_x emissions and compare them with the LES and experimental results.

Results and Discussion

The main instantaneous and time-averaged fields derived from the LES analysis are shown in Figure 3. The axial velocity contour is useful in quantifying the volume associated with the recirculation zones and consequently the regions where fuel is trapped, creating high-temperature zones. As a consequence, the regions with the highest temperature are highlighted in the external recirculation zones where the

temperature is above 1800 K. NO emission is concentrated where the temperature is highest due to the thermal NO_x and fuel-bound mechanisms, the latter due to the significant amount of nitrogen in the fuel mixture. Figure 3 also shows the NO density difference between the flame zone and the post-flame zone where a decrease in temperature leads to a decrease in emissions.

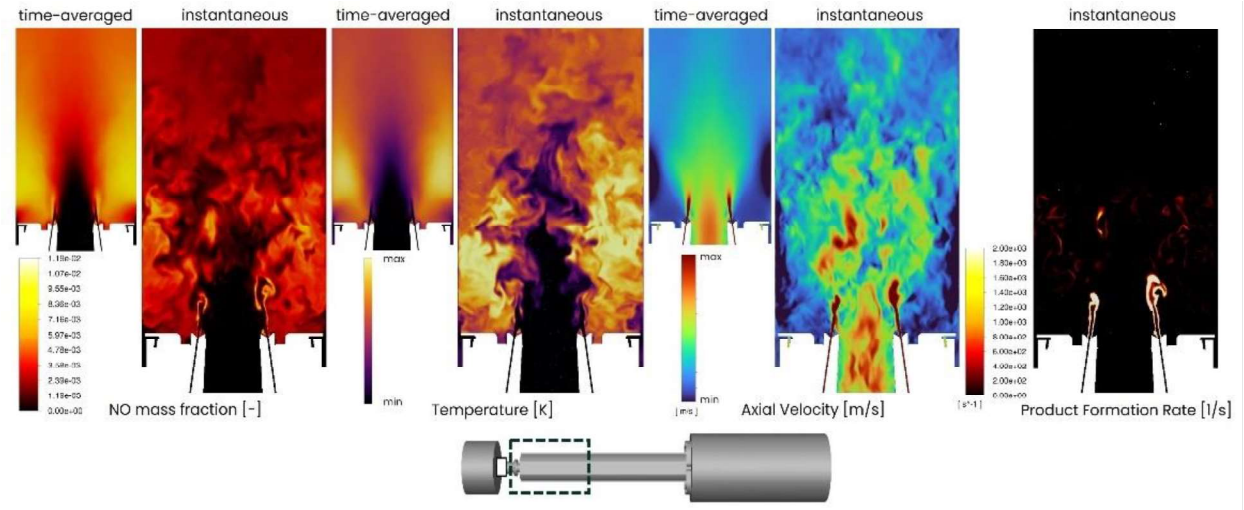

Figure 3: Instantaneous and time-averaged NO mass fraction, temperature, axial velocity and Product Formation Rate fields derived from LES in a longitudinal cross section.

The relationship between the temperature and the NO emissions can be demonstrated looking at the rate of production in the DIFF, in the FZ reactors and the formation pathways shown in Figure 4. In the diffusion zone (see Fig. 4a), the thermal NO_x mechanism derived by Zeldovich's reactions is dominant due to the high temperature present in the flame front. Most of the NO is produced by the reaction $N + OH \leftrightarrow H_2 + NO$.

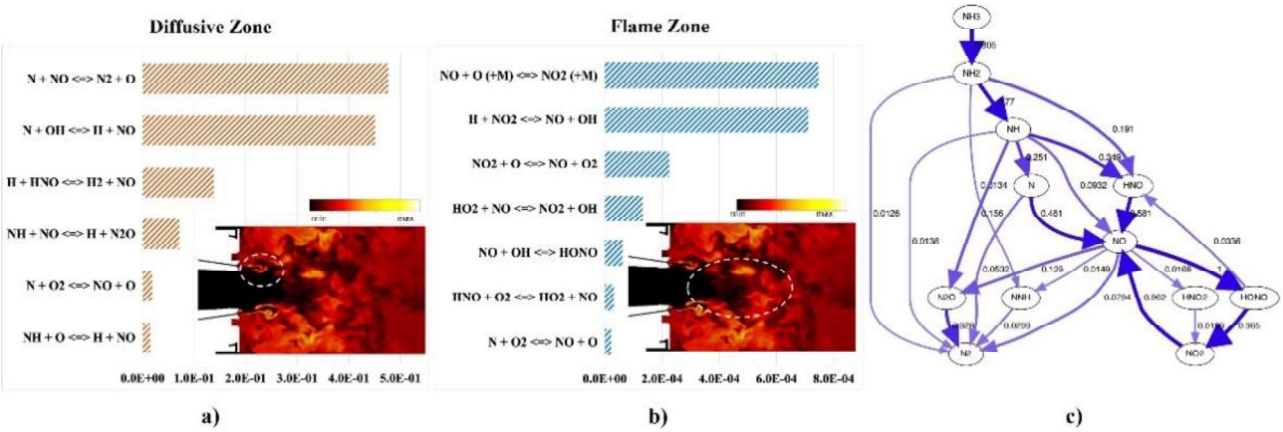

Figure 4: Net Rate of Production (ROP) [Unit: kmol/m^{3}s, Scale: $6x10^{-5}$] of NO in the Diffusive (a) and Flame Zone (b) reactors. Formation pathways following nitrogen species (c). The instantaneous contour plots are retrieved from the LES.

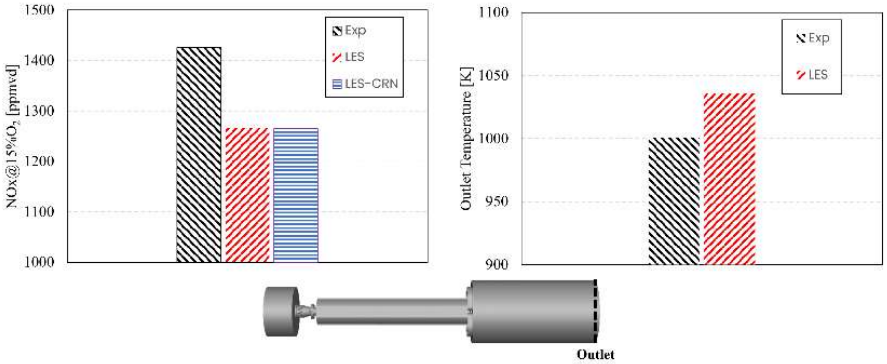

Figure 5: NO_x emission and outlet temperature derived from experimental campaign and numerical simulations.

Regarding the Flame Zone, an increase in the production of NO_2 from the reaction with the third body (NO + O (+M) ⟷ NO_2 (+M)) is observed (see Fig. 4b); with regard to the production of NO, the most important reactions are those linked to the dissociation of NO_2 (H + NO_2 ⟷ NO + OH and NO_2 + O ⟷ NO + O_2). Figure 4c shows a diagram of the most relevant sources of nitrogen oxides in the combustion process due to the dissociation of N-species like NH, NH_2 and HNO. Figure 5 shows the results of the experimental test point and CFD and CFD-CRN simulations in terms of NO_x and exhaust temperature. In terms of emissions, both the LES and CFD-CRN approaches successfully capture NO_x emissions with an error of less than 10% although underestimating it. Opposite to this, there is an overestimation of outlet temperature with an error for LES of less than 3% which corresponds to 30 K.

Conclusion

A LES simulation of a non-premixed burner fed with ammonia-hydrogen mixture under atmospheric conditions is developed and showed good validity compared to experimental data, especially for NO_x emissions. This indicates that the CFD model used is reliable in predicting emissions under specific atmospheric conditions. Furthermore, a CRN based on the time-averaged solution of the LES is implemented. This CRN provides an efficient and reliable approach to analyze in detail the NO_x formation mechanisms under the investigated operating conditions, while allowing a wide sensitivity to the main parameters of interest. The use of this CFD-CRN model can enable a more in-depth investigation of the reaction pathways responsible for NO_x formation, thus providing a better understanding of the chemical processes involved in ammonia-hydrogen combustion. This work focuses on combining advanced numerical modelling approaches with experimental data for a better understanding and prediction of emissions in unconventional combustion systems such as the one studied. The validity of the CFD model and the effectiveness of the proposed CRN provide a solid basis for optimizing the performance of burners fired with ammonia-hydrogen mixtures while reducing NO_x emissions.

Nomenclature

BH	Baker Hughes	*FZ*	Flame Zone
CFD	Computational Fluid Dynamics	*LES*	Large Eddy Simulation
CRN	Chemical Reactor Network	*OEM*	Original Equipment Manufacturing
GT	Gas Turbine	*FGM*	Flamelet Generated Manifold
FTT	Flow Through Time	*PSR*	Perfect Stirred Reactor
PFR	Plug Flow Reactor	*DIFF*	Diffusive Zone

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