Ammonia blends for gas-turbines: preliminary test and CFD-CRN modelling

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Abstract

Ammonia, with its high hydrogen density, cost effectiveness and ease of storage, is emerging as a potential fuel to meet decarbonisation targets in various sectors. However, the combustion of pure ammonia poses challenges due to its low calorific value and reactivity. Existing gas turbine combustion systems, refined over decades with conventional fuels, struggle to maintain comparable flue gas emission concentrations when burning ammonia.
Overcoming this challenge requires a paradigm shift in gas turbine combustion, with implications for chemistry and combustor design methodology. Research into the chemical kinetic mechanism for ammonia combustion worldwide reveals differences in flame radical pools compared to methane combustion. The dominant NOx formation mechanism shifts to a "fuel-bound nitrogen" type, which differs from the "thermal" mechanism in hydrocarbon and hydrogen combustion.
The integration of chemical reaction rates into Computational Fluid Dynamics (CFD) models with transport equations results in impractical computational times for industrial applications. Therefore, streamlined approaches such as chemical reaction reduction methods are being developed. This involves the construction of lumped parameter models (Chemical Reactor Network - CRN) to identify key parameters that affect species production. A reliable CRN implementation involves the identification of critical volumes using a preliminary CFD approach (CFD-CRN).
This paper analyses preliminary experimental tests by Baker Hughes on an industrial burner using different ammonia, hydrogen, and methane fuel mixtures. The NOx results show a different behavior between methane and hydrogen. While the detailed mechanisms behind these results remain open questions, the CFD-CRN modelling approach is adopted. A proposed CRN is investigated for methane, hydrogen, and ammonia blends, providing insight into key parameters and a reasonable physical explanation for the different NOx results. A single calibration parameter (ϕ_{pilot}/ϕ_{ref}) is used to predict accurately NOx emissions using experimental data available from experimental campaign.

Keywords: ammonia; gas turbine; emissions; experimental; chemical reactor network

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1. Introduction

Governments and scientific community recognize that combustion is currently the main process for energy generation in both transport (road and maritime) and power generation (e.g., power plants or stationary power generation) thanks to its numerous technological advantages and capability to improve process efficiency and sustainability of energy sources [1]. Within the decarbonization objectives that run through industrial and civil world, combustion plays a key role to get the "most" and the "best" energy from smart and clean fuels; and the playing field is not only the energy transfer step from chemical to thermal but spreads across different processes regarding fuel and materials preparation [2]. Ammonia as fuel emerges as a potential decarbonization enabler thanks to the high hydrogen density, reasonable costs and easy of storage and transportation [3]. Nonetheless, the combustion of pure ammonia is quite challenging due to the extremely low heating value and burning velocity; current gas-turbine combustion systems are not able to sustain ammonia combustion keeping the same exhaust emission concentrations [4, 5, 6, 7]. Based on the most recent experiences very well reviewed and summarized by Elbaz [8], the most promising enablers for ammonia combustion in gas turbines relies on staged combustion [9] and fuel blending, the latter being very interesting in this transitioning period where gas turbine customers would like to keep still the hydrocarbon fuel application.

Many studies on ammonia blending strategies can be found in the literature. Only a few of them are mentioned here. Detailed tests on a premix swirl stabilized flame have been conducted in KAUST center [10]. Flame stability limits have been measured for different blends with hydrogen, hydrogen-nitrogen, and methane at various levels of pressures up to 5 bars; furthermore, NO exhaust emission was measured showing the beneficial effect of hydrogen addition to ammonia for the blow-out limit and then for the capability to reach lower NO by making the premix flame leaner.

Cardiff University is very active in the ammonia combustion studies taking the opportunity to obtain very interesting data from the low-pressure test bench (< 10 bar) equipped with a swirl burner capable to run in non-premixed and premixed modes [11, 12, 13]. Important contributions have also been found in the studies of humidified cycles where the water addition to the fuel could significantly decrease the NO emission [14] and in combustion modelling with particular attention to new methodologies in CFD to consider the ammonia chemistry [15].

Baker Hughes is an energy technology company, committed to making energy safer, cleaner, and more efficient for people and the planet; for this reason, several collaborations and partnerships have been put in place to develop gas turbine combustion for hydrogen and ammonia fuels. For example, a partnership within the H2020-FLEXnCONFU European project allowed to familiarize with ammonia combustion in terms of testing and modelling [16] through the collaboration with Cardiff University and together with University of Genova to investigate any potential benefits by integrating the GT cycle with ammonia cracking process.

General review of the current literature on ammonia combustion for gas turbines leads to the persuasion that residence time and thermal boundaries conditions around the flame are the most important parameters affecting the chemical evolution of NOx inside the combustor (this is well summarized by Elbaz [8]).

Given such context, in Baker Hughes Florence test bench it has been tested an industrial burner typically applied on the 12-17 MW GT class (NovaLT™16 and NovaLT™12) with various mixtures of ammonia-hydrogen and ammonia-methane. Test's goal was to explore preliminary behavior of NOx versus fuel composition with no modifications applied on the burner; thanks to the collaboration with Universities of Pisa and Rome (La Sapienza), this allowed to start building the right scientific background necessary to conduct the next developments of GT ammonia combustor.

Following this, the goal of this work aims to validate a simplified model consisting in the interaction between a CFD simulation and a Chemical Reactor Network (CRN), to predict NOx emissions downstream of the combustion process, using data derived from the experimental campaign and employing a *single* calibration parameter.

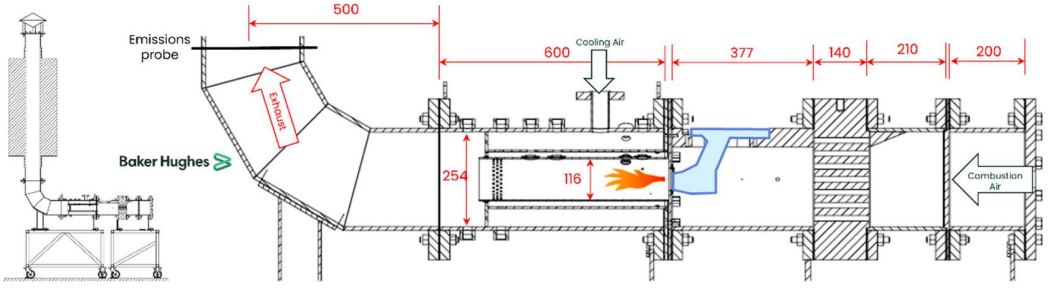

Figure 1: Test-article cross-section and general dimensions.

2. Experimental Facility

BlueRig test bench in Baker Hughes Nuovo Pignone Florence plant is a single-cup atmospheric combustion rig where Baker Hughes executes explorative and preliminary test on fuel burners for its GT products.

The validation process adopted during the development of a gas turbine combustor runs through a series of test with increasing complexity from a first single-phenomena characterization up to the final validation on the engine.

Correlating the phenomena to be investigated and the needed measurements for various test benches along a scale of complexity indicated in terms of pressure and size level (so reflecting a different test cost per day), BlueRig appears nearly at the base of scale, being useful to explore innovative combustion features in a fast and cheap way.

The core of the test-bench (the test-article) is made by an internal cylindrical flame-tube in Hast-X surrounded by a flow-sleeve and an outer vessel in AISI 310S; at the inlet section (right side of the Figure 1) fuel burner is engaged and the outlet section discharges exhaust gases towards the stack. In Figure 1, together with the test-article cross-section, some capability data are reported. A conceptual schematic of the test bench is made of air from plant network split into two mainstream, one typically used for combustion and the other for test-article cooling. Fuel system is organized in such a way that each line to the fuel burner is equipped with a mixing pipe where different species can be fed; hydrogen and ammonia

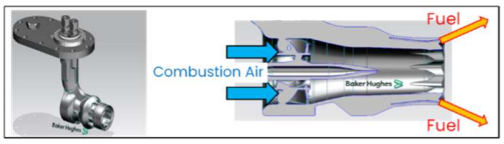

Figure 2: Baker-Hughes fuel burner.

have their own skid for staged expansion, heating, flow controlling and safety. Ammonia skid is a recent investment installed and commissioned in the first half of 2023. The skid is made by a vaporization and pressure control module, a mass flow control system split into two lines and an isolation module; special attention is dedicated to the safety functions avoiding any leakages to the environment. The fuel burner (Figure 2) is the standard component of NovaLT™16 and NovaLT™12 described in previous paper [17]; it is a swirled stabilized type integrally printed in Additive Manufacturing with the fuel injection in diffusive mode oriented outward from the tip of the burner.

The Flame Tube is equipped with a provision for a secondary fuel / air injection downstream the primary flame zone; this allows to test eventually in the future a staged combustion. Ignition of the test article is realized through an electric spark-plug (Champion) typically used on GT combustors. After such phase, the test bench is brought to test point conditions targeting the burner pressure drop and flame temperature according to the test-matrix indications; variations are realized through control of the air and fuel mass flows.

Fuel burner is fed through one fuel line with variable fuel composition in terms of methane, hydrogen, and ammonia. Emission measurement probe is located at 1000 mm along the flow path from the Primary burner; the probe sucks a uniform exhaust gas mixture from the cross section of the stack. Gas mixture is first dried and then analyzed by the devices listed in the Table 2 with the related physical principle of measurement and expected accuracies in the measurement ranges. Fuel mass flows are measured and regulated through Bronkhorst mass-flow-controllers while combustion and cooling air flows are measured by Coriolis devices and regulated through control valves; devices are listed in Table 1.

The test rig is equipped with other sensors like thermocouples, static pressures, pressure pulsation probes and flame detector, all necessary for the safety and control of the test bench.

Table 1: Mass flow meters for all the fluids entering the test-article.

Fluid	Mass flow device	Accuracy
Comb. Air	Emerson CMFS075	0.5% of reading
Cooling Air	Yokogawa RCUS38S	0.3% of reading
CH_4	Bronkhorst F-202AI-M20	3% Full Scale
H_2	Bronkhorst F113AI-1M0	3% Full Scale
NH_3	Bronkhorst F-113AI-M50	3% Full Scale

Methane fuel has a purity of about 98.7% in volume, the rest being high-hydrocarbons and 0.5% CO_2 (analysis provided from the natural gas plant network and verified through microGC PGC490 gas

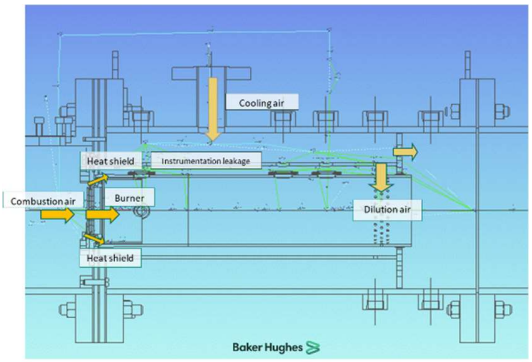

Figure 3: Schematic of the air flow network within the test-article.

chromatography).

The test rig has been characterized in terms of air splits along with the internal flow path: some.

Table 2: Exhaust emission measurement devices characteristics.

Chemical species	Analyzer / Principle	Range of measurement	Expected accuracy
NOx	CAI Noxmat 600 / Chemiluminescence	0–3000 ppmvd	30 ppmvd
O_2	Siemens Oxymat 6E / Paramagnetic	0 – 25 %vol	0.4 %vol
CO_2	Siemens Ultramat 6E / Infrared	0 – 5%	0.1 %vol

dedicated flow test allowed to implement a flow network in Altair Flow simulator to retrieve the flow split along the test rig. As depicted in Figure 3, the combustion air is divided between the air flowing into the burner and the air used for the heat shield cooling. The cooling air is instead partitioned between the leakage at the instrumentations interface and the cooling rows placed at the end of the liner. The model is run imposing the combustion and cooling air mass flow inlets and a pressure at the outlet of the test rig. All the geometric features are simplified in a series of orifices, considering the actual test rig geometry. The effective area of some of the orifices composing the flame tube were tuned to match the experimental pressure drop along the combustion chamber. The chamber flow split is then retrieved form the adjusted flow network. For all test points air split to the primary flame zone is around 85% of the total combustion air flow while dilution air split is around 40% of the cooling air flow.

3. CFD-CRN methodology and setup

The integration of CFD with Chemical Reactor Networks (CRNs) is a combined approach that allows for the correct setup of the CRN itself, as it permits the precise discretization of volumes, thus obtaining the residence times for each section of the geometry. This approach, also employed in the literature [18, 19], features the combustion process in complex systems such as gas turbines. It has been utilized to achieve favorable performance results in terms of emissions at a relatively low computational cost and, consequently, within short timeframes. This enables a thorough study of sensitive parameters.

In this study, a synergic CFD-CRN approach is utilized to simulate and analyse the combustion of ammonia-hydrogen and ammonia-methane mixtures within the complex and dynamic environment of a gas turbine. The approach is schematically summarized in Figure 4.

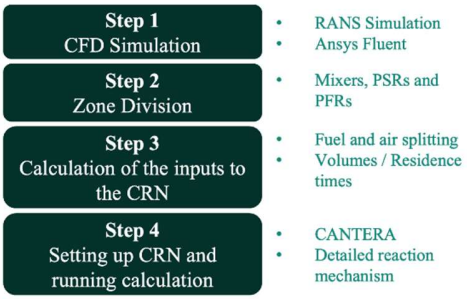

Figure 4: CFD-CRN methodology steps.

3.1 CFD Setup

Initially, a test case is identified for the numerical simulation using computational fluid dynamics based on the solution of Reynolds-Averaged Navier-Stokes (RANS) equations using the finite volume code ANSYS Fluent 22R2 (*Step 1* in Figure 4). The chosen test case refers to one experimental point with a blend of 70%NH_3/30%H_2 (%wt) and dry air. The geometry of the combustion system is modelled using a three-dimensional (3D) computational domain, with a total of 7M polyhedral cells. Reynolds stresses are closed through the Realizable k-ε model with an enhanced wall function, while Partially Premixed Combustion Model with FGM (Flamelet Generated Manifold) approach [20] is employed to solve the chemical source terms. The 1D diffusion non-adiabatic flamelets are computed by using the KAUST [21] chemical kinetics, with 31 species and 203 reactions for the oxidation of NH_3/H_2 blends. The turbulence–chemistry interaction is handled by pre-integrating the look-up tables with a β - PDF. The Turbulent Flame Speed Closure (TFSC) by Zimont [22] is used to

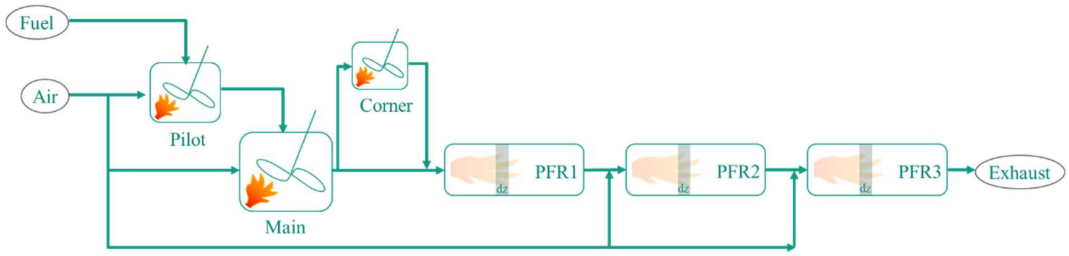

Figure 5: Chemical Rector Network (CRN) sketch.

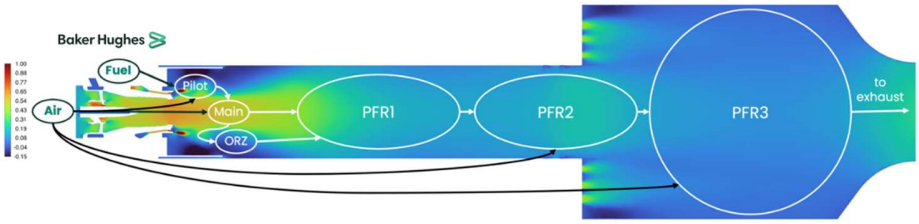

Figure 6: Normalized axial velocity field predicted by the CFD simulation. Volumes discretization and zones division for CRN analysis.

model the source term for the progress variable which is defined as $c = Y_c/Y_{eq}$ where $Y_c = Y_{NO}+Y_{N_2}+Y_{H_2O}-Y_{H_2}$ and Y_{eq} is its equilibrium value. In a previous study [15] we have shown that such a CFD surrogate model can well predict NOx emissions, temperature and velocity fields for similar configurations and conditions.

3.2 Chemical Reactor Network (CRN) Setup

The Chemical Reactor Network (CRN) is developed as shown in Figure 5, by using the open-source kinetic processor Cantera [23]. The reactor zones are defined (*Step 2* in Figure 4) and interconnected (*Step 3* in Figure 4) from the CFD outcomes by analysing the axial velocity field reported in Figure 6. We observe three Perfectly Stirred Reactors (PSRs) representing the Flame zone, and three Plug Flow Reactors (PFRs) mimicking the unidirectional flow zones corresponding to the primary zone of the combustion chamber and the second part where the cooling air also converges. The CRN is characterized using reservoirs upstream of the reactors to maintain pressure and volume constant. The volumes, mass flow rates and residence times are extrapolated from the CFD simulation using temperature, velocity and radical species and maintained constant for all simulations carried out and shown in the following results section. The ignition point of CRN is selected in the Pilot reactor for both NH_3/CH_4 and NH_3/H_2 mixtures.

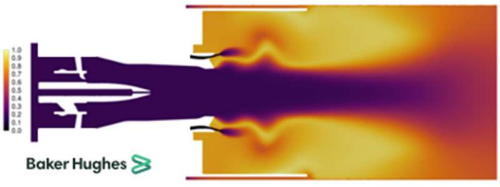

Figure 7: Contour of the normalized temperature field predicted by the CFD simulation in the burner primary zone.

Figure 7 shows the temperature field from the CFD simulation, that help us to validate the temperature trends within the PSRs and PFRs within the CRN. As we can observe from the CRN in Figure 5, the distribution of air flows should be identified properly.

Finally, CRN calculations are carried out also for different kinetic mechanisms (Okafor et al. [24] with 59 species and 256 reactions, POLIMI [25] with 31 species and 203 reactions, GRI 3.0 [26] with 53 species and 329 reactions and Tian et al. [27] with 84 species and 703 reactions), to investigate sensitivity to the chemical model, and fuel blends (*Step 4* in Figure 4). Following studies will include more comprehensive CFD investigations for the other test points, as well as the possible introduction of secondary combustion to further reduce NOx emissions.

4. Results and discussion

4.1 Test results

During test execution, it is useful to check the consistency of major species at the exhaust like O_2 and CO_2 with numerical equilibrium calculation for

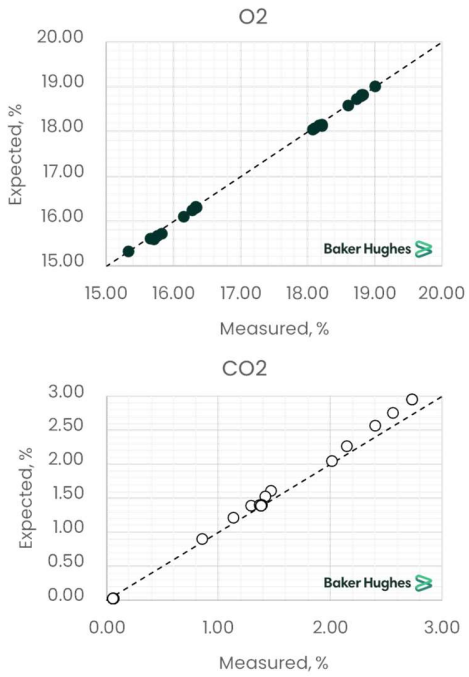

Figure 8: Measured vs expected exhaust emission of oxygen and carbon dioxide.

each test point. Figure 8 shows expected O_2 and CO_2 calculated from equilibrium conversion and compared with measured values, considering all the air and fuel introduced in the volume down to the emission probe location. Relative deviations of measured values from expected ones are below 1% for O_2 and below 10% for CO_2; this higher value most probably due to the assumption of equilibrium.

All the test point with variable NH_3 fuel content have been done at equivalence ratio and thermal power constant in the primary zone; the only exception regards the NH_3/H_2 blend with NH_3 90% wt where primary thermal load has been slightly reduced keeping the same primary equivalence ratio (the reason was due the minimum upstream pressure reached by the Bronkhorst regulator).

Raw NOx measurements (dry basis) are reported in Figure 9 and a comparison with different blends can be discussed.

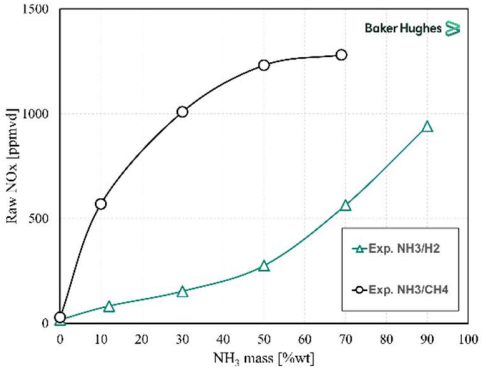

Figure 9: NOx raw exhaust emission measurements for NH_3/CH_4 blends (circles) and NH_3/H_2 blends (triangles).

NOx emissions are higher for NH_3/CH_4 blends respect to NH_3/H_2 ones. This trend is investigated by the CRN in the Section 4.3. It was not possible to reach 90%wt of NH_3 with CH_4 because of maximum NH_3 flow reached by Bronkhorst device at 70%; the curve seems to flatten at high NH_3 content but then it is plausible to figure out an inflexion point towards higher NOx.

Some additional study should be done to understand the different concavities between CH_4 and H_2 blends; to adopt the best combustion strategy, it could be worth to identify if behind the behavior the prominent mechanism is purely chemical kinetics or influenced by the kind of specific burner aerodynamic.

4.2 CRN results

The Chemical Reactor Network is applied to test cases of the experimental campaigns for both NH_3/CH_4 and NH_3/H_2 mixtures. The sensitivity analysis to investigate the effect of the kinetic mechanism for the NH_3/H_2 and NH_3/CH_4 mixture is shown in Figure 10 where we compare the schemes from KAUST, POLIMI and Okafor et al. for NH_3/H_2 (Fig. 10a) and GRI 3.0, Tian et al. and Okafor et al. for NH_3/CH_4 (Fig.10b).

The selection of these mechanisms from the literature is based on our preliminary study for NH_3/H_2 blends [15]. The analysis is carried out using the equivalence ratio in the pilot zone equal to 3.42 for all blends. This value is obtained by preliminary CFD analysis for the test point at X_{NH3} = 0.3 (%wt). The NOx emissions results are shown in Figure 10,

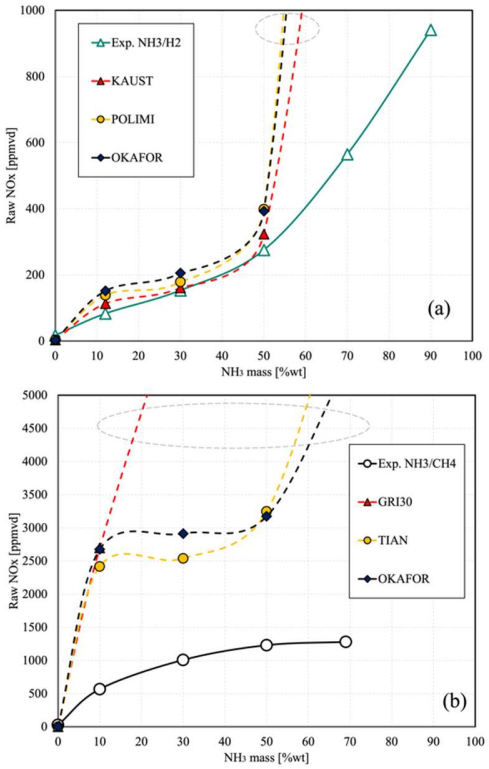

Figure 10: Measured and predicted NOx emissions as a function of ammonia content in the fuel for NH_3/H_2 (a) and NH_3/CH_4 (b) blends. Sensitivity to kinetic mechanisms and ignition zone. ratio in Pilot zone constant at ϕ=3.42.

compared with experimental data, varying the NH_3 content within the mixture. The NOx emissions estimated with the CRN are evaluated at the exit of the PFR3, i.e. at the end of the combustion process (see Figure 5) in agreement with the experimental data probe.

Figure 10a shows the NOx emissions estimated through the CRN (without calibration) compared to the experimental data for the NH_3/H_2 blends. The experimental trend is captured by all kinetic mechanisms chosen with greater accuracy for that of KAUST up to the 50% NH_3 mixture (by weight).

Above this value of NH_3 content, there is a significant overestimation of emissions which

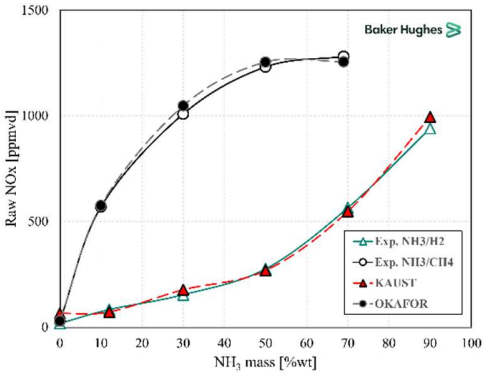

Figure 11: Measured and predicted NOx emissions as a function of ammonia content in the fuel. Results for both NH_3/CH_4 and NH_3/H_2 blends.

requires calibration of the CRN by the model parameters. Figure 10b shows the effect of the kinetic mechanism on NOx emissions for NH_3/CH_4 mixtures, using different kinetic schemes (except Okafor et al) for the need for C-based species.

It is noted that, also in this case, up to 50% NH_3 (by weight) the qualitative trend is captured by the schemes of Tian et al and Okafor et al, while for the GRI 3.0 there is a significant overestimation in agreement also with the literature [15].

Considering these results, the calibration of the CRN by maintaining the volumes of individual reactors and the air split constant is conducted.

The only free parameter is the equivalence ratio in the pilot zone. In this context, a calibration campaign is conducted to achieve a match between NOx emissions estimated by CRN and experimental data. The results are shown in Figure 11; except for the first point in pure H_2, the other points are fitted with and average accuracy below 10%.

Figure 12 shows the equivalence ratio in the pilot zone normalized to the global equivalence ratio as a function of the ammonia content in the methane and hydrogen mixtures. There are two distinct regimes with varying ammonia content. The trend in the equivalence ratio is increasing up to 10%wt of ammonia in the mixture, but after that, the trend exhibits two different behaviors depending on the mixture. In particular, the equivalence ratio for NH_3/H_2 decreases as the ammonia content increases, whereas the ratio for NH_3/CH_4 does not change significantly as the ammonia content increases. A correlation is developed between the pilot zone equivalence ratio and the amount of ammonia in the mixture resulting in a CRN that can be used as the mixture changes. Table 3 displays these correlations for both examined mixtures, namely L_1, L_2 for NH_3/CH_4 and L_3, L_4 for NH_3/H_2.

As shown in Figure 12, the decreasing equivalence ratio to obtain more accurate NOx emissions trend from NH_3-H_2 blends could be aligned with the work done by Khateeb et al. [28] where it can be seen (Fig. 9 in Ref. 28) that moving from 90% wt to 80% wt NH_3 in the rich zone it is necessary to increase the equivalence ratio to have higher NOx.

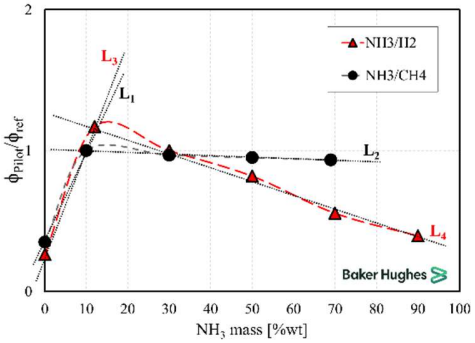

Figure 12: Calibrated equivalence ratio as a function of the ammonia mass fraction in the fuel and correlations (i.e., L_1, L_2 for NH_3/CH_4, L_3 L_4 for NH_3/H_2).

Table 3: Correlations between normalized equivalence ratio of pilot zone and ammonia mass fraction in the fuel.

$$L_1=\frac{\phi_{PL}}{\phi_{ref}}=0.065X_{NH_3}+0.35$$

$$L_2=\frac{\phi_{PL}}{\phi_{ref}}=-0.0011X_{NH_3}+1$$

$$L_3=\frac{\phi_{PL}}{\phi_{ref}}=0.075X_{NH_3}+0.26$$

$$L_4=\frac{\phi_{PL}}{\phi_{ref}}=-0.01X_{NH_3}+1.3$$

Additional studies should be done to understand any possible prevalence of flow dynamics/mixing phenomena (like for example strain rate effects acting in different ways between CH_4 and H_2 blends) or any possible change of chemical regime linked to the Fuel Bound NOx mechanism [29]. Furthermore, additional tests should be done to investigate the mixtures with NH_3 content below 10%wt and to confirm the linear dependence of equivalence ratio.

4.3 [NO] Rates Of Production analysis

Figure 13 shows the NO net Rate Of Production (ROP) estimated by the CRN in the pilot reactor for each test case of NH_3/CH_4 and NH_3/H_2 mixtures. The trend of the net ROP is compared with the experimental NOx emission (solid lines). We can note that, the ROP behaviors of the NO agree with the trend of the experimental emissions. In particular, in Figure 14 the most significant reactions are compared for two blends both with 30%NH_3 wt and 50%NH_3 wt respectively. The production of the NO by reactions R1-R2-R4 is greater for NH_3/CH_4 than NH_3/H_2 in

agreement with the gap between the experimental NOx values.

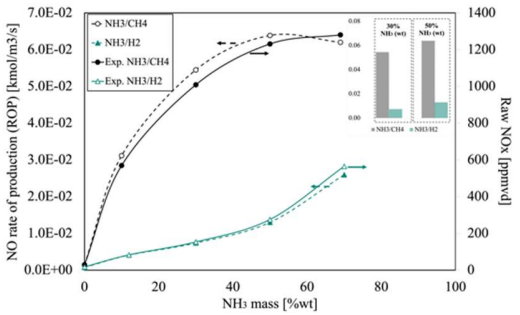

Figure 13: Net rate of production of NO from CRN (Pilot) for NH_3/CH_4 (black line) and NH_3/H_2 (green line).

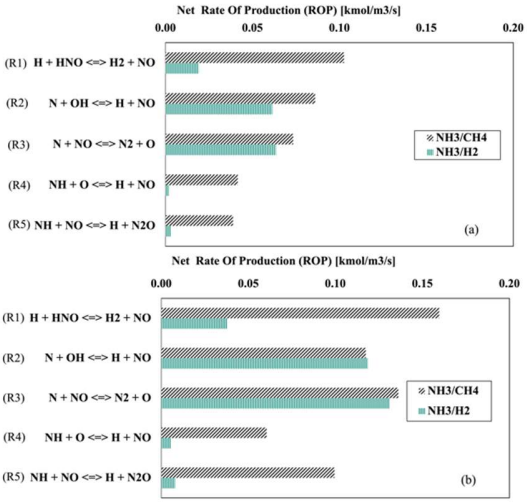

Figure 14: Net rate of production of NO from CRN (Pilot) for 30%NH_3 (a) and 50%NH_3 blended with CH_4 and H_2.

5. Conclusion

First explorative tests with NH_3/H_2 and NH_3/CH_4 blends on an industrial burner for the Baker-Hughes gas-turbine NovaLT™ in atmospheric conditions have been carried out, introducing in detail *for the first time* the experimental setup, showing valuable experimental data, with the goal to analyze the influence of ammonia on NOx emissions. Exhaust NOx emissions are measured at different blend compositions. A Chemical Reactor Network of the entire system, developed and calibrated using a CFD simulation of a reference test point, is applied to provide a first basic tool to explore the use of ammonia blend and eventually guide the system design improvement. The key conclusions are:

- The NOx emissions for NH_3/CH_4 blends are higher than H_2 ones for all ammonia contents (at least up to 90%wt) due to the higher rate of production of NO.
- A CRN model, composed of 3 PSRs in the flame zone and 3 consecutive PFRs in the dilution zone is developed.
- An analysis of the effect of the kinetic mechanism on the estimation of NOx emissions is carried out. Using the pre-calibration CRN, it is shown that for NH_3/H_2 mixtures, all selected mechanisms predict the quantitative and qualitative trend for NH_3 contents up to 50%. The KAUST kinetic scheme is the one that predicts results in better agreement with the experimental data. For NH_3/CH_4 mixtures, the mechanisms of Tian et al. and Okafor et al. can qualitatively capture the experimental trend of NOx emissions up to 50% NH_3 (by weight). While GRI 3.0 appears to be the least suitable for the treatment of mixtures containing ammonia.
- A single calibration parameter (ϕ_{pilot}/ϕ_{ref}) is used to predict accurately NOx emissions using experimental data available from experimental campaign.
- The trend of the NO production rate derived from CRN justifies the experimental NOx trends. In particular, the higher values of NOx in the CH_4/NH_3 mixtures compared to those of the NH_3/H_2 mixtures are due to the reduction and production mechanisms by the H and O species, which have a greater contribution for the NH_3/CH_4 mixtures.

The test bench and the numerical model suggest a potential introduction of staged combustion in future. The interesting linear correlation between pilot equivalence ratio and ammonia content in the fuel asks for further comprehension of the physical/chemical phenomena and their implementation on the CRN. As concerning the CFD-CRN approach, the current work has shown the validation of the model for a single equivalence ratio for different mixtures; the calibration of the model to different equivalence ratios will be extended in the future. It is still appreciable the significant support to model new challenging combustion systems, and we expect to proceed with the development of surrogate models through the introduction of adequate reduced mechanisms.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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