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NO_x EMISSION MEASUREMENT AND NUMERICAL VALIDATION FOR CRACKED AMMONIA

COMBUSTION IN A SEMI INDUSTRIAL BURNER DESIGN

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ABSTRACT

Ammonia cracking is a promising solution for the abatement of the NO_x emissions since it allows to partially avoid the fuel bound formation pathway. Rising with the cracking percentage, the benefit of the emission reduction is partially mitigated by a higher complexity of the auxiliary system, especially when such strategy means to be coupled with an existing gas turbine plant. With regard to the numerical models, the growing interest in ammonia combustion highlights the need for methods that are able to predict the intricate NO_x emissions production. In the present paper, the experimental measurements of a semi-industrial burner operated in non-premixed mode and fed with a mixture corresponding to 99% of cracked ammonia will be presented. The experimental measures aim to characterize both the flame morphology, and the pollutant emissions. Different operating pressures will be explored with the thermal power of the rig remaining constant. From the numerical point of view, three test conditions will be simulated by Large-Eddy Simulation (LES) relying on a pre-tabulated approach for turbulence-chemistry interaction. The main goal of the numerical campaign is the prediction of the flame shape at the different operating conditions. Conversely, LES won't be used for the assessment of the pollutant

emissions, but they will support a Chemical Reactor Network (CRN) built at this scope. The time averaged fields coming from the Computational Fluid Dynamic model will be leveraged to set up the network and retrieve the trend of the main pollutant emissions. The flexibility of this methodology allows for detailed sensitivity to the chemical mechanism, with a focus on Rate of Production (ROP) analysis of the main NO_x-forming reactions. This will allow for in-depth investigation of the dominant pathways of NO_x formation.

Keywords: NH₃, Cracking, Hydrogen, CFD, CRN, LES

NOMENCLATURE

Symbols

c	Progress variable	[-]
h	Enthalpy	[J/kg]
δ_l^0	Laminar Flame Thickness	[m]
S_c^0	Laminar Flame Speed	[m/s]
Z	Mixture fraction	[-]

Greek

Φ	Equivalence ratio	[-]
Δ	Cell size	[m]
ρ	Density	[kg/m ³]
$\dot{\omega}$	Source Term	[1/s]

Subscripts / Superscript

ad	Referred to adiabatic conditions
0	Laminar

Acronyms

CFD	Computational Fluid Dynamics
CRN	Chemical Reactor Network
FGM	Flamelet Generated Manifold
FR	Finite Rate

FTT	Flow Through Time
FZ	Flame Zone
GT	Gas Turbine
GTRC	Gas Turbine Research Center
HRR	Heat Release Rate
I/ERZ	Internal / External Recirculation Zone
LES	Large-Eddy Simulation
LHV	Low Heating Value
PDF	Probability Density Function
UDF	User Defined Function
WALE	Wall Adaptive Local Eddy

1. INTRODUCTION

Ammonia has emerged as a viable and sustainable energy carrier due to the high hydrogen content, allowing the reduction of the carbon footprint in the energy sector. However, the direct use of ammonia in conventional combustion systems poses several challenges: low flame speed as well as narrow flammability limits and high ignition energy compromise the flame stability [1]. Additionally, ammonia is a corrosive gas and its handling and combustion present significant health and safety risks [2]. In addition, ammonia leaks in a conventional gas turbine require stringent containment measures and ventilation systems [3]. When burning ammonia mixtures, the formation of harmful byproducts, such as nitrogen oxides (NO_x), represents one of the biggest challenges related to the employment of ammonia as fuel [2].

A promising workaround is represented by the usage of cracked ammonia. Ammonia cracking is the process of thermally decomposing ammonia (NH₃) into hydrogen (H₂) and nitrogen (N₂). This reaction typically occurs at high temperatures, often with the aid of catalysts, to ensure efficient conversion [4]. Such process can lead to several benefits, such as an improved flame stability due to the higher hydrogen content, and also a potential NO_x emission reduction. Regarding the later aspect, ammonia cracking is surely the most effective way to abate NO_x since the fuel-bound pathway is partially inhibited [5]. Obviously, higher and higher cracking percentages lead to a significant drop of this formation mechanism even if there could be technical issues in reaching decomposition fractions close to the full cracking. As a matter of fact, such process is performed leveraging the flue gas stream coming out from the GT unit. Depending on the thermodynamic cycle, the temperature of the exhaust gas may enable a certain degree of ammonia cracking, though this could be significantly lower than the complete decomposition of ammonia. The thermodynamic conditions influence the

extent of cracking that can be achieved, making partial cracking a more common outcome rather than full decomposition. Furthermore, the layout constraints of the power plant must be carefully considered, as the integration of the cracking unit with the existing heat recovery system can be complex. This integration may involve trade-offs, potentially affecting the final ammonia cracking efficiency. These factors highlight the need for a balanced approach in designing the system to optimize both the thermal recovery and ammonia cracking processes. From the combustor design point of view, the use of a fuel coming from partially cracked ammonia can complicate the management of the fuel system especially when the ammonia decomposition is not constant over time since the fuel properties variation (Wobbe index, LHV, etc.) can have consequences on the auxiliary systems. Also, major modifications could be necessary in the combustor architecture, like the implementation of fuel staging strategy when very high hydrogen fractions are reached [6].

Dealing with cracked ammonia, the verification of the design modifications and their impact onto NO_x emission is not a trivial task. Even the most complex and accurate Computational Fluid Dynamics (CFD) methodologies currently employed during the design phase of GT combustor struggle in capturing the trend when it comes to fuel-bound NO_x prediction [7]. There could be several reasons behind such issue. One of the most important one is that the numerical models suffer in reproducing adequately the inner structure of the flame front especially dealing with non-premixed regime, requiring extremely fine grid resolutions able to capture the species concentration profiles inside the flame front thickness. Secondly, the chemical scheme employed to describe the ammonia oxidation is far from being clearly understood in the scientific community [8-10]: many uncertainties about the influence of the different NO_x formation pathways depending also on the operating conditions of the combustor are still to be clarified. At this regard, it is also worth mentioning that most of the literature concerning the application of ammonia as fuel in GT combustor is retrieved at conditions quite far from the full scale of modern GT unit, especially in terms of operating pressure. This is for sure another point of uncertainty about NO_x emission.

From an industrial perspective, the employment of CFD methods for the prediction of NO_x emission along relevant hardware can result in very expensive simulations, far from being accurate and able to drive the design. At this stage, another possible strategy is the coupling of the numerical simulations with low order models: CRNs represent an efficient way to exploit the data coming from the CFD and provide precious information about the NO_x formation pathways [11-12]. In this context, the numerical simulations are performed to provide a reliable and as much accurate as possible characterization of both the heat release region (i.e., flame topology) and the flow field. With these features being captured, the CFD solution can support the design of a network along which the NO_x emission can be subjected to a huge screening of different parameters. One of these is surely represented by the chemistry set which can be changed to detect the differences in the several NO_x formation pathways and, having experimental data as benchmark, shed some light on the most important driving factors.

This is the approach adopted also in the present paper. Considering a semi-industrial swirler operating with a 99% of cracked ammonia fuel gas, three CFD simulations are executed at different operating pressures to feed a CRN from which the experimental data regarding pollutant emissions are validated. The next paragraphs will provide more information about the combustion model employed during the CFD stage as well as the experimental setup from which the data are recorded. The Results and Discussion Section will be focused on the validation of the numerical simulations in terms of flame shape, comparing the corresponding numerical maps with the available chemiluminescence. Lastly, the procedure coupling these results with the CRN will be introduced with a deep dive into the pollutant emission predictions against the measured value of NO_x emission.

2. NUMERICAL MODELLING

2.1. Combustion Model

The combustion model used to perform the numerical simulation is a customized version of the original Flamelet Generated Manifold (FGM) [13] through which the turbulent flame is described as an ensemble of laminar flames, known as flamelets. Such approach allows to tabulate in a pre-processing phase all the thermodynamic quantities (i.e., species concentration, temperature, etc.) as a function of two primitive variables: the mixture fraction Z and the progress variable c . In the present paper the chemical mechanism proposed by Stagni et al. [14] is employed to calculate the flamelets database, assuming the un-normalized progress variable equal to the H_2O mass fraction. The turbulence-chemistry interaction is considered integrating the flamelet database through a β -shape Probability Density Function (PDF) of both mixture fraction and progress variable variances ($\tilde{P}(Z, c)$). In this way, it is possible to store the thermodynamic state in an additional look-up table, avoiding the integration of the chemical solution during the simulation. Both the primitive variables and their variances needed to query the PDF table are calculated solving dedicated transport equations. In this way, the source term of the progress variable transport equation can be expressed as:

$$\overline{\dot{\omega}_c} = \bar{\rho} \iint \frac{\dot{\omega}_c(Z, c)}{\rho(Z, c)} \tilde{P}(Z, c) dZ dc \quad (1)$$

Mimicking what originally proposed by Klarmann et al. [15] and further developed in [16,17], this standard Finite-Rate (FR) closure is modified in the context of Large-Eddy Simulation (LES) to account for the effects of strain (a) and heat loss (Ψ) on the progress variable source term. At his regard, a corrective function $\Gamma(Z, a, \Psi)$ is derived leveraging laminar flames computed in Cantera [18] where parametric 1D laminar simulations are performed sweeping both the strain and the heat loss values in counterflow flames. Here, the strain is imposed changing the velocity of the opposite jets while the heat loss fixing the temperature of the products to values progressively lower than the equilibrium temperature. Γ is then defined as follows:

$$\Gamma(Z, a, \Psi) = \frac{\max(\dot{\omega}_c(Z, a, \Psi))}{\max(\dot{\omega}_c^0(Z))} \quad (2)$$

with $\dot{\omega}_c^0$ the progress variable rate along a freely propagating flame (zero strain at adiabatic conditions). So, an external look-up table containing both numerator and denominator of Eq. (2) is created allowing for the eventual calculation of Γ during the CFD simulation. Figure 1 shows, as an example, the contour plots of $\max(\dot{\omega}_c(Z, a, \Psi))$ for the three investigated conditions at different pressure levels whose details will be provided in the next paragraph. Eventually, combining Eq. 1 and Eq. 2, the source terms of c is calculated as:

$$\overline{\dot{\omega}_c} = \Gamma(Z, a, \Psi) \bar{\rho} \iint \frac{\dot{\omega}_c(Z, c)}{\rho(Z, c)} \tilde{P}(Z, c) dZ dc \quad (3)$$

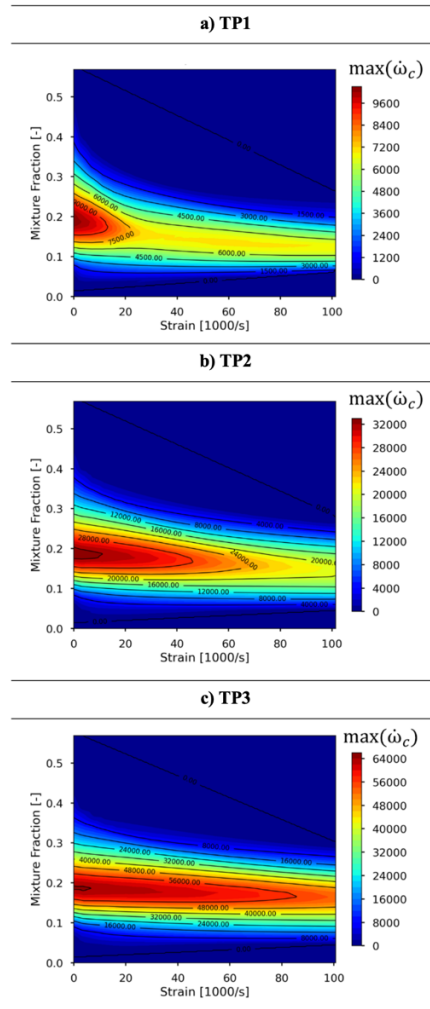


Figure 1. Maximum value of $\dot{\omega}_c$ as a function of strain and mixture fraction at the different pressure levels simulated. Maps refer to adiabatic conditions ($\Psi = 1$).

As stated above, during the CFD simulation, both the strain and the heat loss need to be calculated to query the table containing the elements for the assessment of $\Gamma(Z, a, \Psi)$. As for the strain, neglecting the contribution of the flame curvature, its calculation is based on Eq. 4:

$$\kappa = (\delta_{ij} - n_i n_j) \frac{\partial u_i}{\partial x_j} \quad (4)$$

with n the normal vector to the flame front surface, whose components are retrieved from the gradient of the progress variable field. In the LES context, Eq. 4 has both the resolved and the sub-grid scale contribution:

$$\tilde{\kappa} = (\delta_{ij} - \tilde{n}_i \tilde{n}_j) \frac{\partial \tilde{u}_i}{\partial x_j} + \left[(\delta_{ij} - \widetilde{n_i n_j}) \frac{\partial u_i}{\partial x_j} \right] \quad (5)$$

The latter is calculated leveraging the work from [19]:

$$\tilde{a}_{sgs} = \Gamma_k \cdot \frac{\sqrt{k_{sgs}}}{\Delta} \quad (6)$$

where Δ is the cell size acting as filter, k_{sgs} the sub-grid scale turbulent kinetic energy and Γ_k the efficiency function, assessed as:

$$\log_{10} \Gamma_k = -\frac{1}{s+0.4} e^{-(s+0.4)} + (1 - e^{-(s+0.4)})(s\sigma - 0.11) \quad (7)$$

with:

$$s = \log_{10} \left(\frac{\Delta}{\delta_l^0} \right) \quad (8)$$

$$\sigma = \frac{2}{3} \left(1 - \frac{1}{2} \exp \left[- \left(\frac{u'_\Delta}{S_c^0} \right)^{1/3} \right] \right) \quad (9)$$

u'_Δ representing the sub-grid scale velocity fluctuations.

The heat loss is assessed during the CFD stage as the ratio between the actual temperature of the cell and the adiabatic temperature at the same conditions, the latter retrieved from the PDF table knowing the required quantities, such as Z , its variance Z''^2 , the corresponding adiabatic enthalpy h and imposing $c = c''^2=1$ to mimic the equilibrium:

$$\psi = \frac{T(Z, Z''^2, c, c''^2, h)}{T_{ad}(Z, Z''^2, c, c''^2, h_{ad})} \quad (10)$$

The above reported procedure for the extension of the FGM-FR combustion model is performed through a UDF compiled in the solver of the commercial code Ansys Fluent.

2.2. Computational Domain and Mesh Strategy

The computational domain is made of four components, namely the duct through which the combustion air is delivered toward the combustor, the radial swirler, the quartz flame tube and the discharge volume including the emission sampling probe. Figure 2 shows the first three with a detailed view of the radial swirler characterized by a swirl number of 0.8. Leveraging the trends of several thermocouples installed all around the test rig, the temperature is imposed on the burner tip and the dome plate. A temperature profile is retrieved and imposed also for the quartz, being the temperature measured on this component at different distances from the burner tip. The figure highlights also the position of the air and the fuel mass flow rate inlet boundaries adopted in the simulations. For the outlet, a pressure outlet is used instead. Regarding the computational grid, Figure 2 provides the main information about the different mesh sizes adopted. While the mesh for the upstream duct is left coarser with respect to the remaining regions, a resolution of $700 \mu m$ is applied inside the swirler and around the fuel line characterized by a 5 mm injecting orifice. Additionally, a further mesh refinement is applied inside the combustor: this region has a conical shape and covers the entire flame tube length. Inside this volume the mesh resolution is equal to $500 \mu m$. The choice behind the adoption of such discretization strategy is based on what reported by Ansari et al. [20] where the same rig configuration is investigated.

Depending on the specific operating conditions of each simulated test point, the residence time inside the flame tube is subjected to change. To ensure consistency among the simulations, the same number of Flow Through Times (FTT) is calculated in each case.

All the transport equations as well as the temporal discretization are solved at the second order scheme. The WALE model is chosen as sub-grid turbulence closure for the LES.

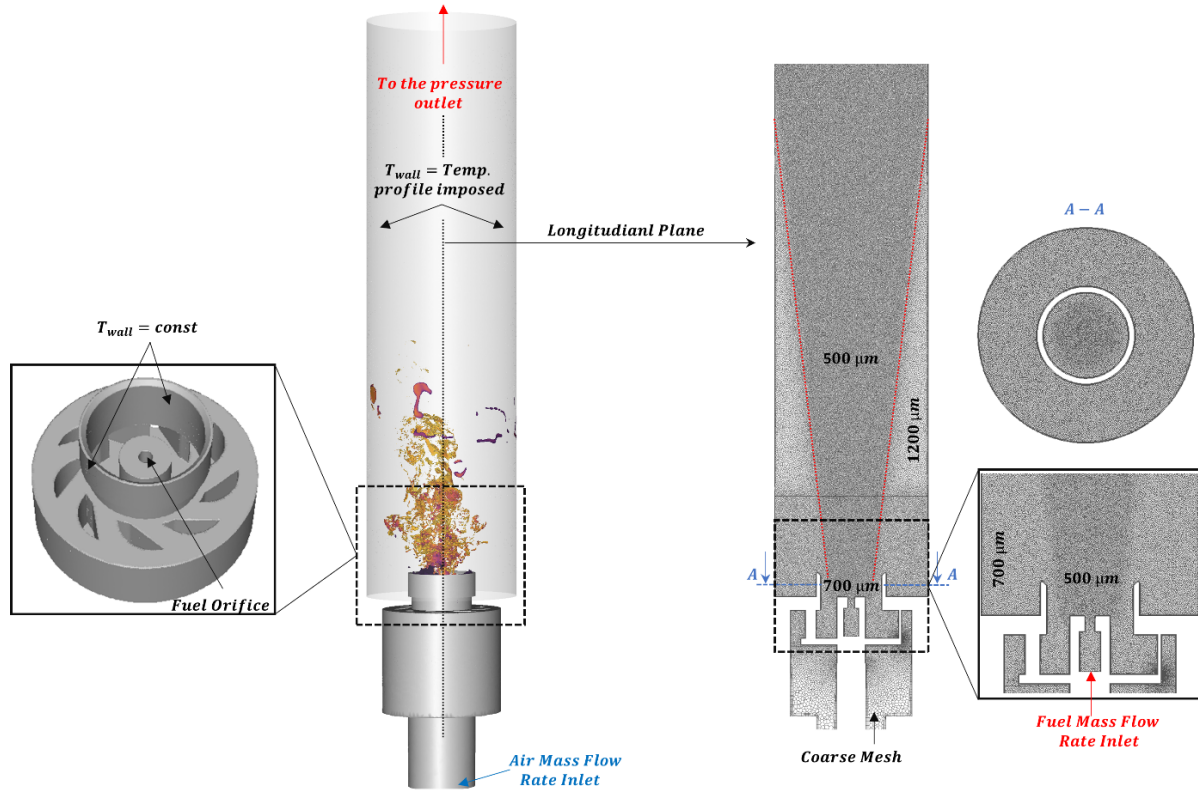


Figure 2. Computational domain adopted in this study (left) and the corresponding mesh with detailed views (right).

3. TEST RIG AND OPERATING CONDITIONS

A dedicated test campaign is executed in the high pressure rig of GTRC. Figure 3 shows a simplified sketch of the system. A containment vessel encloses the tubes through which both air and fuel are delivered inside the flame tube and the flame tube itself, made of quartz. Multiple windows on the vessel allow the visualization of the primary zone of the combustor through which detailed flame imaging can be executed. No secondary air stream is used to cool down the flame tube.

The fuel is delivered through a central lance, coaxial to the tube where the air flows and, as stated above, it is injected in the primary zone with a post-orifice of 5 mm in diameter. So, non-premixed conditions are investigated in this test campaign, providing a dominantly diffusive combustion regime. The flame tube is engaged with a metal tube downstream (not visible in Figure 3) that supports the backpressure valve and the exhaust gas sampling probe, installed at about 540 mm from the dome plate. The temperature of the probe is water-conditioned using an external heat exchanger. In this way, the temperature of the sampled gas is maintained at about 430 K.

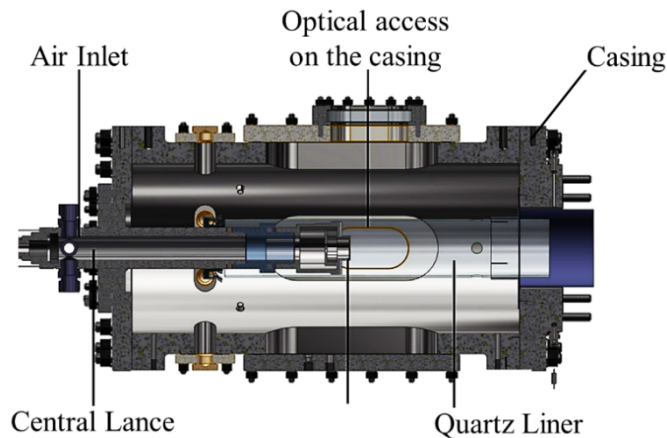


Figure 3. Sketch showing the main components of the high pressure rig.

Regarding the instrumentation, NO_x emissions (NO , NO_2) are measured using a heated vacuum chemiluminescence technique performed with a Signal 4000VM. NH_3 slips are quantified through a NO converter (Signal 410 instrument). Emissions are normalized measuring the dry O_2 concentration in the exhaust gas through a Signal 9000 MGA. Additional information on emission measurement is available in [21]. Moving to the flame characterization, a LaVision camera coupled with a high-speed intensifier and UV lens is used to acquire chemiluminescence of several excited radicals, like OH^* , NH^* and NH_2^* . For each species a different bandpass filter was used to isolate the corresponding wavelength. In all the operating conditions the camera parameters are kept constant in terms of acquisition frequency, gain and exposition time for a meaningful comparison among them.

The investigated operating conditions are recorded along a fuel gas mimicking the 99% of cracked ammonia: this corresponds to a composition made of 1% NH_3 , 17.5% H_2 and 81.5% N_2 by weight. The choice to implement a 99% cracking level was motivated by its representation of optimal combustion performance, where ammonia is nearly fully converted into hydrogen and nitrogen. This minimizes the formation of fuel NO_x while maintaining high reactivity. For lower cracking levels (e.g., 50–80%), the presence of unreacted ammonia increases fuel NO_x production, resulting in higher overall NO_x and unburned ammonia emissions. In contrast, near-complete cracking (e.g., 99%) shifts the NO_x formation mechanism toward thermal NO_x , which becomes dominant due to the hydrogen-rich fuel and high combustion temperatures. The global equivalence ratio Φ is kept constant all along the experimental campaign and equal to around 0.54. A pressure sweep is performed rising the operating value from 1.1 up to 6 bar. Neither the combustion air nor the fuel mass flow rate are changed rising with the pressure, meaning that:

- 1) the residence time inside the flame tube increases linearly;
- 2) the Reynolds number remains approximately constant since the viscosity weakly depends on the pressure.

Table 1 summarizes the remaining parameters of the test campaign.

99% Cracked NH_3 fuel Campaign

Air temperature	[K]	500					
Operating pressure	[bar]	1.1	2	3	4	5	6
Air mass flow rate	[g/s]	11.8					
Fuel mass flow rate	[g/s]	1.06					
Thermal Power	[kW]	23					

Flame Temperature	[°C]	1515					
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Table 1. Main operating parameter characterizing the test campaign.

Numerically, three out of six test conditions are simulated to limit the computational effort and preserve the ability to investigate the impact of the operating pressure onto both the flame morphology and the pollutant emissions. Specifically, the test points at 1.1 bar, 3 bar and 6 bar are simulated. In the following paragraphs they will be named TP1, TP2 and TP3, respectively.

4. RESULTS AND DISCUSSION

4.1. Experimental Results

The experimental characterization of the flame morphology rising with the operating pressure is reported in Figure 4 where the Abel-transformed pictures calculated from the OH^* chemiluminescence are presented. Each figure is normalized with the absolute maximum value, recorded at the lowest operating pressure: as investigated in [22], this behavior is related to the increased collisional quenching at higher pressures. The isoline of the OH^* intensity at 40% of the peak value is also reported in each picture as a measure of the flame length. Regarding the furthest point from the burner exit, the flame elongation is subjected to a slight reduction in the range 1.1 to 4 bar while a further rise of the pressure hasn't a significant impact on that. Conversely, looking at what happens along the combustor axis, an elongation of the flame is observed moving from 1.1 to 3 bar, while at higher pressures the iso-line reaches always an axial extension close to 32 mm.

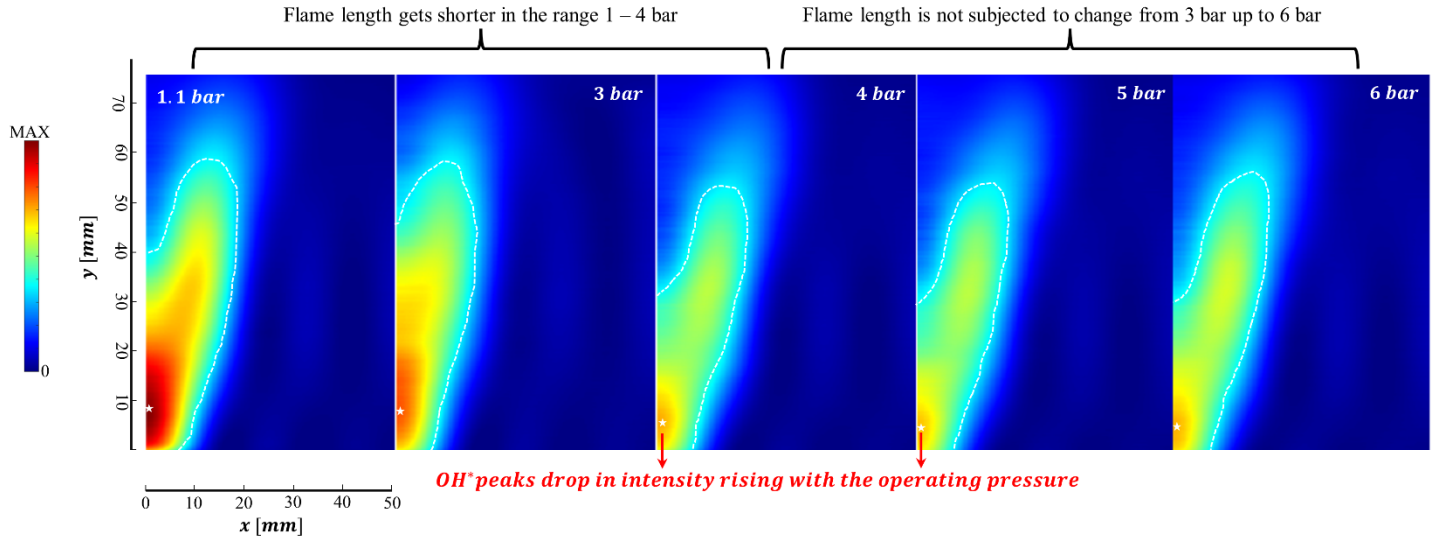


Figure 4. Experimental Abel-transformed OH^* chemiluminescence as HRR marker rising with the rig operating pressure. The maps at 2 bar is omitted for sake of simplicity

Regarding the location of the OH^* peak, the maximum value falls approximately at the same location at 5 and 6 bar, while it gets closer and closer to the burner exit moving from 1.1 bar up to 4 bar. Overall, it can be stated that despite a significant pressure sweep, the flame morphology doesn't change so much considering the OH^* as representative of the HRR. This is primarily due to the small variation of the integral Reynolds number.

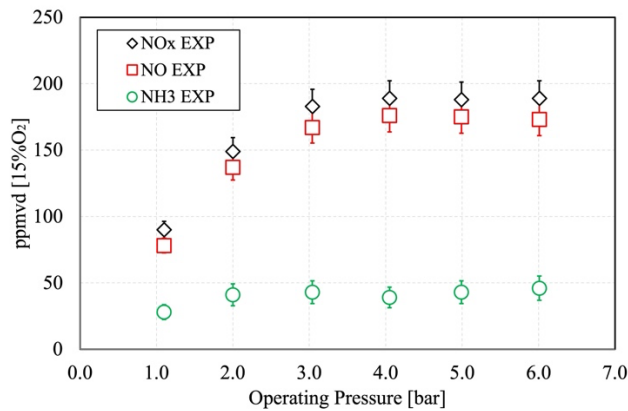


Figure 5. Pollutant emissions measured as a function of the operative pressure.

Moving to the pollutant emissions, the graph in Figure 5 summarizes the measured values. The NH_3 slip remains practically constant over the investigated pressure range (at around 40 ppmvd) with the exception of the minimum reached at 1.1 bar, equal to 28 ppmvd. Coming to the NO_x emissions, a rising trend from 1.1 bar (90 ppmvd) up to 3 bar (183 ppmvd) is recorded. Eventually, the curve becomes

flat from 3 bar on, remaining close to around 190 ppmvd. It is worth noting that reporting NO_x emissions in terms of volume concentration (ppmv at 15% O₂, dry) may introduce challenges when comparing hydrogen-rich fuels with conventional hydrocarbons. As highlighted in recent studies [23 - 25] the high-water vapor content in the exhaust, along with differences in volumetric flow rates and specific heat capacities, affects NO_x dilution and normalization in post-processing. These factors can make hydrogen blends appear to have a higher NO_x penalty compared to traditional fuels, whereas a comparison based on specific NO_x mass emissions (e.g., g/MJ) could provide a more balanced evaluation. In Figure 5, can be also observed that the NO emission represents the majority of the NO_x, with NO₂ playing a marginal role. This trend can be seen as the combination of different factors. First of all, a non-negligible fraction of the NO_x emission is surely produced by the thermal pathway that linearly increases with the residence time (i.e., with the operating pressure). Regarding fuel-bound NO_x, there are two competing mechanisms having an impact on the global emission. First of all, it is well known that the third-body effect contributes more and more to the NO_x reduction rising with the pressure: reactions like $H + O(+M) \leftrightarrow OH(+M)$ and $H + OH(+M) \leftrightarrow H_2O(+M)$ are enhanced at higher pressure, decreasing the oxygen availability for NO_x formation. Conversely, the *HNO* pathways seems to have the opposite trend. Figure 6 shows the NH_2^* field measured for TP1, TP2 and TP3. These maps reveal a higher and higher emission of this excited species meaning that also the NH_2 concentration is favored with the pressure rise. As a consequence, NO_x formation can be promoted through the reactions chain $NH_2 + O \rightarrow H + HNO$, $HNO + H \rightarrow NO + H_2$.

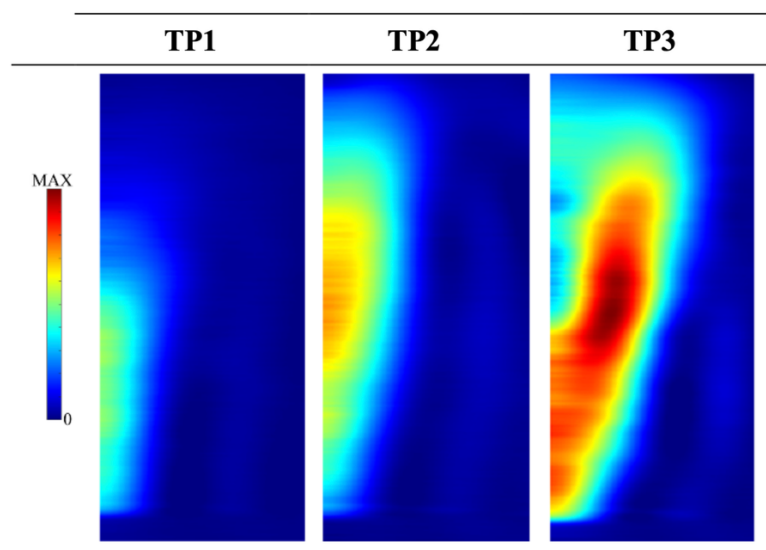


Figure 6. NH_2^* maps for TP1, TP2 and TP3.

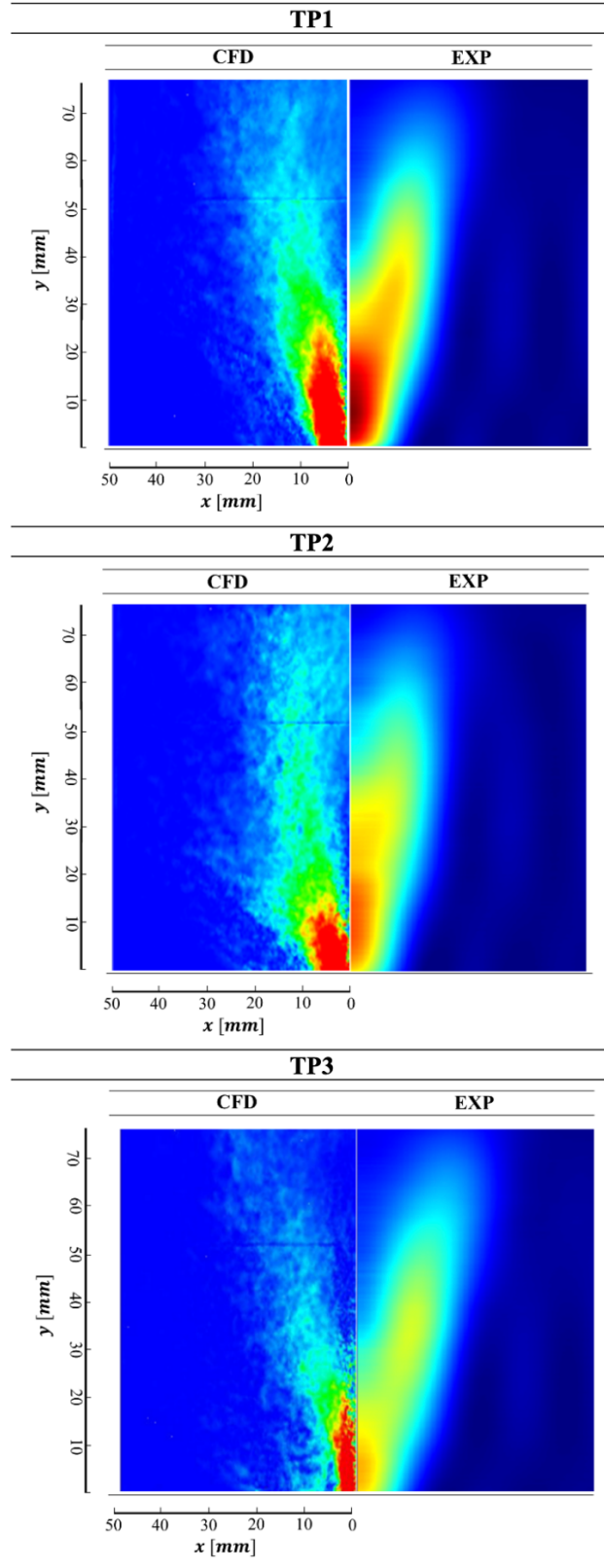


Figure 7. Comparison between numerical HRR and experimental OH^* .

4.2. Flame Morphology Validation from the Ext-FR

In Figure 7 the *HRR* from the CFD simulations is reported side by side with the experimental map for each simulated test point. It must be said that, for different reasons, the direct comparison of the numerical with the experimental results is not possible. First of all, in a pre-tabulated chemistry context, the inclusion of OH^* in the chemical mechanism doesn't represent a meaningful choice since the numerical time scale is far greater than the OH^* existing time. This means that only the *HRR* can be post-processed as representative of the flame. But, for high hydrogen content fuels, comparing directly the *HRR* with OH^* can be misleading, as demonstrated by Schiavone et al. in [26]. This behavior is mainly related to the chain branching nature of hydrogen combustion that is characterized by the highest OH^* emission in the post-flame region where the *HRR* is instead quite low, being the majority of the heat already been released. Considering the different nature of these two quantities, only a qualitative comparison among the experimental and the CFD maps can be addressed. So, it is surely more meaningful focusing only on the numerical results to verify their ability in reproducing the trend discussed in the previous paragraph. Considering the regions characterized by the highest reactivities in the numerical maps (colors from green (50% of the peak) to red (peak value)), it can be stated that the numerical results correctly predict the shortening of the flame length rising with the pressure. Especially in TP3 conditions, a significant drop of the heat release can be observed for $y > 40\text{ mm}$ compared to TP1 and TP2. Additionally, the CFD seems to be characterized by a narrower and more elongated *HRR* distribution at the highest pressure: this is quite evident looking at the region close to the highest reactivity value. Finally, the numerical simulations are able to correctly capture also the inclination of the heat release region with respect to the combustor axis, meaning that the complex interaction between the fuel jet, the related combustion and the flow field seems to be correctly captured. From this point of view, Figure 8 reports in the left-half of each picture the time-averaged axial velocity with the corresponding iso-line at 0 m/s. The definition and characterization of the Central and External Recirculation Zones (IRZ and ERZ) are based on the investigation detailed in Mazzotta et al. [27]. The axial velocity iso-lines are overlapped with the *HRR* whose color map has been clipped to focus mainly on what happens right after the fuel injection (not visible in Figure 7). Looking at the *HRR*, it can be seen that the flame gets always stabilized in the shear layer between the fuel stream and the surrounding air, right after the fuel injection. But at lower pressure, the high velocity of the fuel jet leads to an enhancement of the strain rate with a consequent lower value of Γ_k compared to the other conditions (right-half of each picture, as instantaneous field). This is a factor promoting the elongation of the flame at 1.1 bar together with the well-known kinetic effect (the higher the pressure, the higher the rate leading the reactants toward the combustion products). The jet-flame interaction has also a major effect onto the inner recirculation zone, as it can be seen from the position of the iso-line. At the lowest pressure, the inner recirculation region lifts downstream compared to the higher pressure cases: in the latter, the iso-lines get firstly attached to the burner tip (TP2) and eventually rises its extension operating at even higher pressure (TP3).

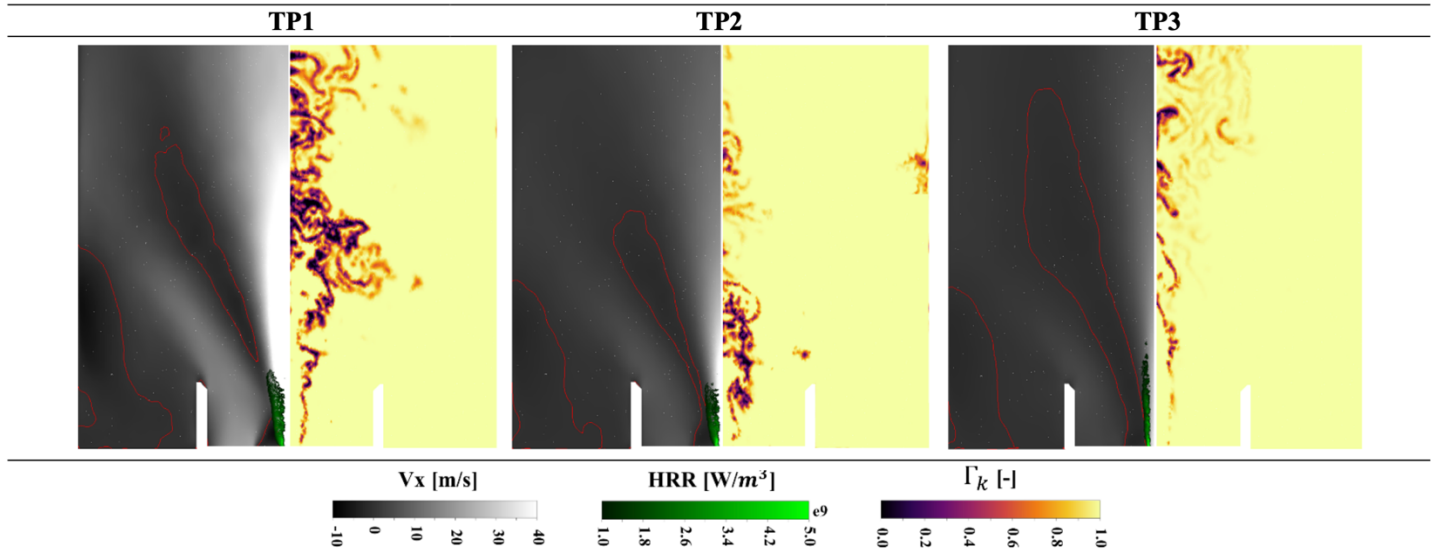


Figure 8. Correlation between the axial velocity field and HRR. The red iso-line identifies the recirculation regions ($V_x=0$ m/s)

4.3. NO_x emission prediction through the CFD-CRN approach

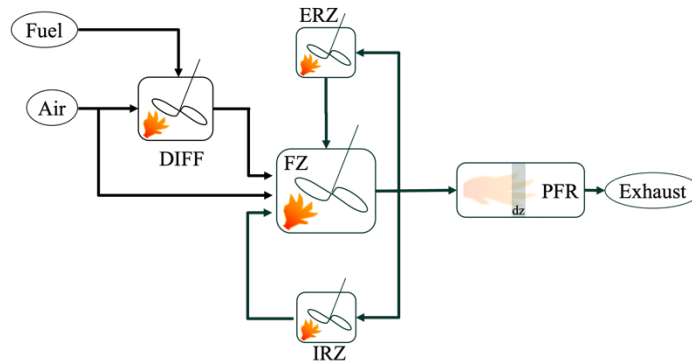


Figure 9: Chemical Reactor Network schematic and volumes discretization employed.

A Chemical Reactor Network (CRN) model was employed alongside the CFD simulations previously described to quantify and assess the influence of pressure on NO_x emissions. This methodology serves as a powerful framework for analyzing and optimizing reactor systems by integrating the detailed flow-field predictions from CFD simulations with the simplified reaction dynamics of CRN models. By exporting the time-average fields from the CFD simulations described in the previous sections and reading them into a bespoke Cantera code [18], it was possible to obtain the volumes, and subsequently the residence times and thermal boundary conditions, of each individual reactor. Further information about the methodology can be found in [12]. To capture the reactions occurring at the flame front, a reactor with a diffusive configuration (DIFF) was incorporated. This addition is crucial for the evaluation of emissions, as the flame

front is subject to temperature increases as a result of diffusive effects. Although the main emissions are from the fuel-bound NO_x pathway [28-29], Zeldovich mechanism [30], which are fundamental to the formation of thermal NO_x. Figure 9 illustrates the configuration of the CRN employed in which three perfectly stirred reactors (PSRs) were employed to represent the flame zone (FZ) and the inner and external recirculation zones (IRZ and ERZ), respectively. Furthermore, a plug flow reactor (PFR) was incorporated to represent a unidirectional flow zone or a region where axial velocity is equal to the magnitude one. The volume of the PSR and PFR reactors was found to change in accordance with the pressure, resulting in the precise reactor cell volume from CFD simulations.

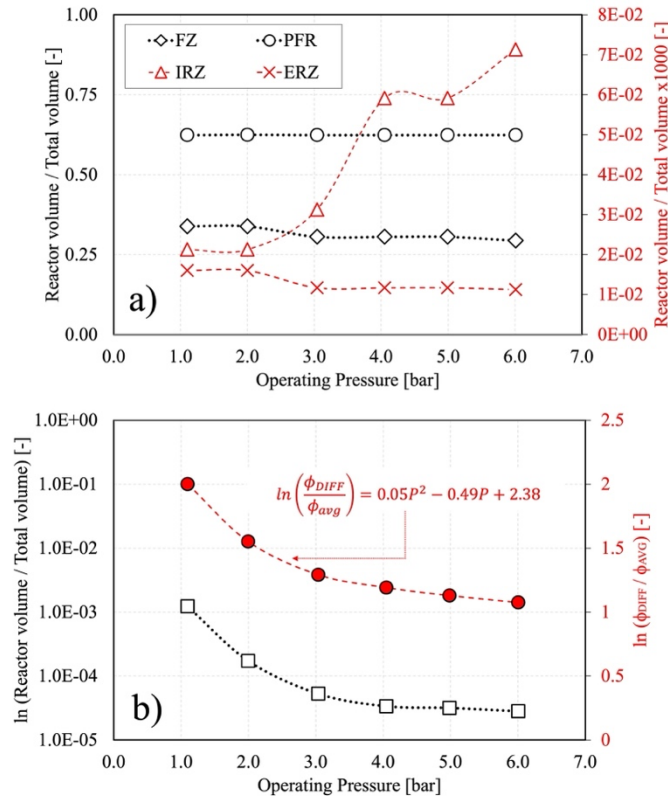


Figure 10: Reactor volume distribution derived from CFD analysis as a function of operating pressure (a). Trend of diffusive reactor (DIFF) volume distribution (black squares) and CRN calibration via ϕ_{DIFF} (red circles) (b).

This was achieved by accounting for changes in flame morphology, as evidenced by the chemiluminescence data (Fig. 7), axial velocity and HRR contours (Fig. 8).

The kinetic model developed by Stagni et al. [14] was adopted, comprising 31 species and 203 reactions, where the major reactions involved in NO_x formation are present. This kinetic scheme was selected based on results from a previous 0D–1D comparative study

[27]. Figure 10 focuses on the relationship between operating pressure and the volumetric distribution of distinct reactor zones: the Flame Zone (FZ), the Plug Flow Reactor (PFR), the Inner Recirculation Zone (IRZ), and the External Recirculation Zone (ERZ). Figure 10a represents the normalized reactor volumes as fractions of the total reactor volume across a range of operating pressures. Notably, the FZ, ERZ and PFR zones remain relatively constant, suggesting that their volumetric contributions are minimally affected by pressure. This is confirmed also by CFD results, in particular when compared to OH* maps (Fig. 7) and axial velocity contours (Fig. 8). However, the IRZ exhibits significant variation, with the IRZ volume increasing substantially at higher pressures, especially when pressure is higher than 4 bar, due to enhanced mixing and reaction intensities. This is also confirmed when compared to axial velocity contours in Fig. 8. Figure 10b offers a more detailed assessment of the volumetric trends observed in the diffusive reactor in black squares, presented in logarithmic scale. As pressure increases, there is a corresponding decrease in the volume of the DIFF reactor. Prior research [12] has demonstrated that the most efficient calibration parameter for non-premixed applications is the equivalence ratio within the diffusive reactor. On this basis, the quadratic equation of the curve resulting from the CFD-derived volumes was also used to calibrate the equivalence ratio within the DIFF reactor.

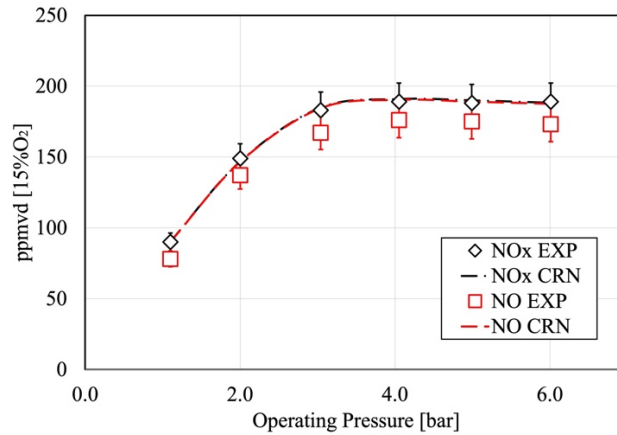


Figure 11: NOx and NO emissions results derived by CRN and compared to experimental data.

The red curve in Fig. 10b represents a quadratic relationship between the normalized equivalence ratio in the diffusive reactor on the averaged one ($\phi = 0.54$), as a function of operating pressure. The regression equation is as follows:

$$\ln(\phi_{DIFF}/\phi_{AVG}) = 0.05P^2 - 0.5P + 2.4 \quad (11)$$

This equation was then applied to calibrate ϕ_{DIFF} , where the first value (at $P = 1.1$ bar) is the one resulting from CFD. This calibration parameter is thus consistent with the volume trend and not arbitrary. The resulting equivalence ratio value was then used to quantify the NO and NOx emissions and compare them with the experimental data.

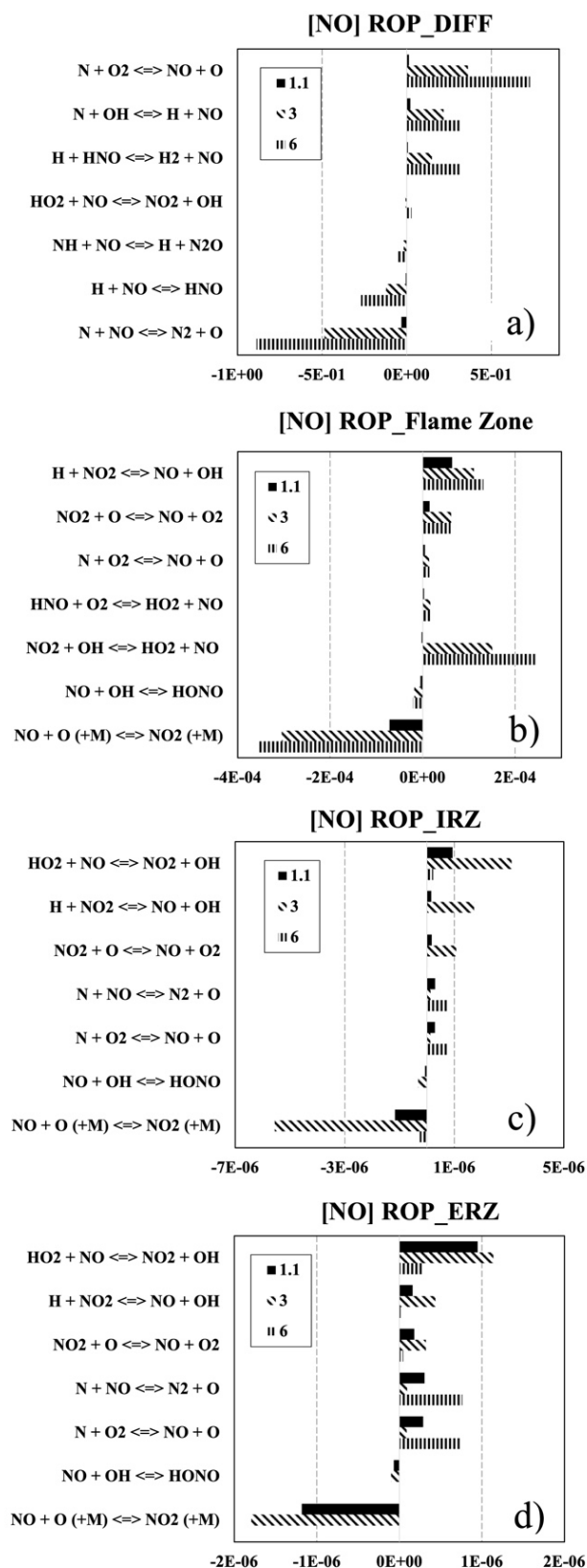


Figure 12: Comparison of the NO Rate of Production related to the three test points investigated.

Figure 11 shows the NO_x emission outcomes from the CRN analysis, compared with experimental data previously discussed in Fig. 5. The figure compares experimental and simulated NO and NO_x emissions, focusing on identifying trends and potential deviations between the datasets. Experimental data for NO_x emissions, represented by black diamond markers, show an initial increase with pressure from 1 to approximately 3 bar, then stabilizes around 190 ppmvd, suggesting a saturation effect where further pressure increases yield minimal impact. CRN predictions, depicted by a black dashed line, follow the same trend, showing a pressure-driven increase that levels off around 190 ppmvd, with minimal discrepancy from the experimental values. The NO emissions experimental data (red squares) follow the same trend, with levels rising up to 3 bar before plateauing near 170 ppmvd. The CRN model (red dash-dot line) exhibits a slight tendency to overpredict these values, failing to discern a substantial difference between NO and NO_x. This was due to the inability of the model to accurately predict NO₂ emissions, which were practically close to zero. The results highlight the CRN model's effectiveness in predicting experimental trends with minimal error thanks to the calibration used.

Following the calibration and validation of the CRN model, the effect of pressure on the rate of production (ROP) of NO in the Diffusive (DIFF), Flame Zone (FZ), Inner Recirculation Zone (IRZ), and External Recirculation Zone (ERZ) reactors is analyzed in Fig. 12 and reflects the intricate relationship between chemical reaction kinetics and operating pressure. At lower pressures, such as 1.1 bar, there is no evidence of NO emissions in the diffusive zone when compared to those at higher pressures. At higher pressure (3 and 6 bar), the most important NO formation route is thermal NO, specifically in:



corresponding to part of the Zeldovich mechanism [30]. Reaction 12 is favored only at high temperatures requiring a high activation energy to break the tight N–N bond, usually considered to be relevant when the gas temperature is higher than 1800 K. Reaction 13 becomes relevant when abundant O₂ is available. The production of NO via the thermal NO route linked to the diffusive reactor is the predominant process within the entire system. This is due to the high concentration of hydrogen in the 99% cracked ammonia mixture. In the Flame Zone, at lower pressure (1.1 bar) the formation of NO is predominantly driven by reactions involving dissociation of NO₂ reacting with O/H radicals with third body effect, in particular $NO + O (+M) \rightleftharpoons NO_2 (+M)$ and $H + NO_2 \rightleftharpoons NO + OH$. As pressure rises to 3 and then 6 bar, these radical-driven pathways resulting in a significant increase in the rate of NO production. At 3 and 6 bar, the $NO_2 + OH \rightleftharpoons HO_2 + NO$ reaction also plays a substantial role in NO production, while at low pressures it is negligible. In both the diffusive reactor and the flame zone reactor, the discrepancy in NO production between the low-pressure test point (1.1 bar) and the test points at 3 and 6 bar is significant, whereas the difference between the tests at 3 and 6 bar is relatively minor. The Inner and External Recirculation zones (I/ERZ) exhibit a more balanced and generally lower NO production and destruction of NO compared to the Diffusive and Flame

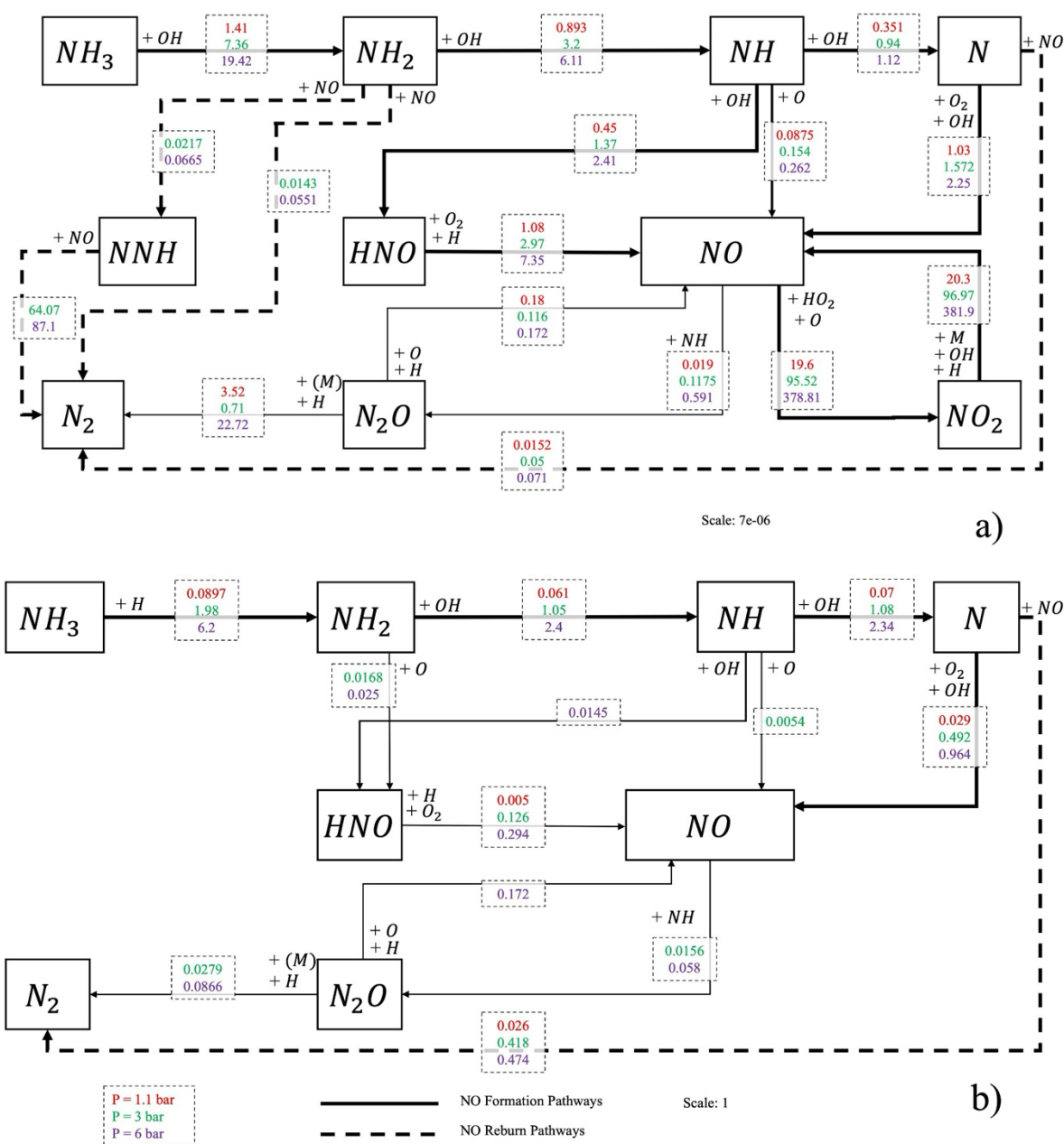


Figure 13: NO formation pathways in the Flame Zone (a) and Diffusive (b) reactors.

Zone. This can be attributed to the intrinsic characteristics of the recirculation zone. At elevated pressures (6 bar), a reduction in NO production is evident, balancing the higher production observed in the DIFF and FZ reactors.

Figure 13 shows the NO formation and reburn pathways within the Flame Zone (FZ) (Fig.13a) and Diffusive (DIFF) (Fig. 13b) reactors under varying pressures (1.1 bar, 3 bar, and 6 bar) according to the three test points investigated. The differences between the pressures reflect how elevated pressure impacts both the forward and reburn pathways in NO kinetics. The diagram provides valuable insights into the intricate interactions among various nitrogen-containing radical species. The flow of reactions within the diagram is illustrated

by directed arrows, with each arrow indicating the direction of the reaction and connecting lines emphasizing the relationships between species. The NO formation pathways are organized to reflect key reaction mechanisms, beginning with the conversion of ammonia (NH_3) to NO. Once NOx has been formed, it can be reduced to N_2 , through interaction with NH_i , with $i=0,1,2$, and NNH , forming the reburn (or DeNOx) route [28].

The formation pathways shown in Fig. 13 are consistent with the ROPs analyzed in Fig. 12. With regard to the flame zone reactor, the dissociation of NO_2 and the interaction with a third body via the $\text{NO}+\text{O}(\text{+M}) \rightleftharpoons \text{NO}_2(\text{+M})$ reaction, as well as the interaction with OH/H radicals via $\text{H}+\text{NO}_2 \rightleftharpoons \text{NO}+\text{OH}$, $\text{NO}_2+\text{OH} \rightleftharpoons \text{HO}_2+\text{NO}$, have been confirmed as the primary factors responsible for the observed increase in NO formation as a result of pressure changes.

Regarding to the effect of pressure in the diffusive reactor, the formation of HNO for the test point at 1.1 bar is less pronounced than at higher pressures (3 and 6 bar). Consequently, the formation of NO via $\text{HNO}+\text{H} \rightleftharpoons \text{NO}+\text{HO}_2$ at low pressures can be considered negligible. Furthermore, the effect of pressure is significant with regard to the formation of NO from thermal NO, as described in reactions 12 and 13 above, with negligible impact at 1.1 bar in comparison to higher pressure. N_2 formation by DeNOx route is only consistent for higher pressures with similar impact.

Finally, nitrous oxide (N_2O) emissions are strongly influenced by the equivalence ratio, particularly under lean combustion conditions for ammonia/hydrogen and cracked ammonia mixtures. High N_2O emissions can occur in these regimes due to incomplete nitrogen conversion pathways. However, the combustion conditions considered in this study, which involve a high ammonia cracking rate (99%) and the specific equivalence ratio employed ($\phi = 0.55$), result in negligible N_2O emissions. As a result, the formation of N_2O does not significantly offset the environmental benefits of reduced NOx emissions in this scenario.

5. CONCLUSIONS

This study investigated NOx emissions and flame morphology in a semi-industrial burner operating with 99% cracked ammonia as fuel. A combination of experimental measurements and numerical simulations was used to explore the effects of operating pressures on combustion characteristics and pollutant formation. The key findings and conclusions are as follows:

- Experimental results revealed a non-linear relationship between operating pressure and NOx emissions. NOx levels increased from 1.1 bar to 3 bar, plateauing at approximately 190 ppmvd for pressures beyond 3 bar. Experimental chemiluminescence imaging showed that the flame morphology remained stable over the pressure range, with the OH^* peak decreasing while increasing in pressure.

- Three test points at three different pressure levels (1.1, 3 and 6 bar) were numerically analyzed using Large-Eddy Simulations (LES). LES successfully captured the flame morphology and the position and trend of the OH* peaks.
- A CRN based on the time-averaged LES solutions is implemented. The calibration of the CRN is achieved by varying the equivalence ratio within the diffusive reactor in accordance with the observed trend in diffusive reactor volume. The CRN model's predictions were found to align well with experimental data, demonstrating its effectiveness in capturing the underlying chemical kinetics and their dependence on pressure.
- Higher pressures enhanced the NO production in diffusive reactor, driven by thermal NO pathways, while in the flame zone the fuel-bound NO_x resulted to be more relevant, particularly via the HNO and NO₂ dissociation process involving a third body.
- The combined CFD-CRN methodology provided an effective framework for predicting NO_x emissions and assessing flame dynamics. This approach offered a computationally efficient alternative to direct CFD-based pollutant prediction, particularly for complex non-premixed ammonia combustion scenarios.

This research contributes to the advancement of knowledge regarding ammonia-based fuel systems, establishing a foundation for future studies aimed at refining numerical models, optimizing ammonia cracking processes and addressing challenges associated with large-scale implementation in industrial gas turbines.

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