# Pressure Effects on NOx Emission in Ammonia/Hydrogen Swirl Flames: a Comparison of Kinetic Mechanisms using LES-CRN Approach

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## Abstract

Non-premixed combustion of ammonia/hydrogen blends is a promising approach for low-carbon energy applications. This study presents a numerical investigation using Large Eddy Simulations (LES) to analyse the combustion characteristics and NOx emission in a swirl-stabilized burner. LES results are validated against experimental data based on flame morphology. Subsequently, an analysis of NOx formation mechanisms is conducted using a LES-Chemical Reactor Network (LES-CRN) approach. This methodology leverages time-averaged LES fields to evaluate different chemical kinetics mechanism, providing a comprehensive comparison of NOx formation. Among the different kinetic schemes investigated, the Otomo et al. scheme provides the best agreement with experimental data with less then 10% error.

## Introduction

The use of ammonia ($NH_3$)/hydrogen ($H_2$) fuel blends in gas turbine applications has gained increasing attention as a potential pathway toward carbon-free combustion [1, 2]. The adoption of these blends presents significant challenges, particularly concerning the NOx formation mechanisms. The accurate numerical prediction of $NO_x$ emissions in $NH_3/H_2$ combustion remain key research challenges [2] even when using high-fidelity LES [3, 4]. In fact, existing CFD methodologies either underpredict or overpredict $NO_x$ emissions, depending on the chosen chemical kinetic scheme and turbulence-chemistry interaction model. These considerations highlight the need for a systematic investigation of available chemical kinetic mechanisms aiming at assessing their accuracy in predicting $NH_3/H_2$ combustion under relevant gas turbine conditions. The objective of this study is to provide an assessment of $NO_x$ formation mechanisms by comparing different kinetic models. To achieve this, high-fidelity LES simulations are firstly validated against experimental data based on flame morphology and employed to generate time-averaged flow and species fields, which are then utilized as input for a Chemical

Reactor Network (CRN) model [5]. By leveraging the LES-CRN methodology, this work aims to identify the strengths and limitations of different kinetic models, ultimately contributing to the development of more reliable $NO_x$ prediction frameworks for $NH_3/H_2$ combustion in gas turbines.

## Materials and methods

Experimental tests are carried out in the Cardiff University's High Pressure Optical Combustor (HPOC). Details of the experimental systems are described by Ansari et al. [3]. A blend made of 75% $H_2$ – 25% $NH_3$ (% vol.) is burnt using air as oxidizer at 500 K. Fuel and air mass flow rates are imposed at the combustor inlet equal to 0.275 and 6.8 g/s, respectively. Three test points were carried out as the pressure changed. Specifically, the operating pressures analysed are 1.1, 3, and 5 bar. The thermal power (12.5 kW) and the equivalence ratio (0.54) are kept constant in the three test points. LES results shown in this work are obtained through Ansys Fluent 2023R1. The Wall-Adapting Local Eddy-Viscosity (WALE) model is employed at the turbulence sub-grid scale. The chemistry of the $H_2/NH_3$ mixture is modeled using a tabulated chemistry approach based on non-premixed flamelet approach. The detailed chemical kinetic scheme by Stagni et al. is used, alongside additional transport equations for NO and $NO_2$. Furthermore, a Chemical Reactor Network (CRN) model was developed in Cantera [6] based on time-averaged LES fields.

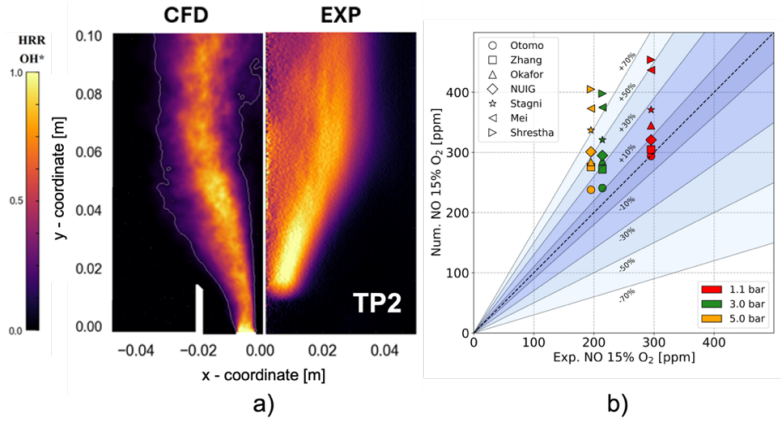


**Fig. 1:** a) Flame morphology validation of LES results with experimental OH* chemiluminescence images; b) predicted NO emissions from the LES-CRN framework: comparative analysis of the chemical kinetic schemes evaluated.

## Results and discussion

LES results show good agreement with experimental OH* chemiluminescence images at 2 bar (TP2), as shown in Fig. 1a, even if the experiment exhibits a more intense OH* emission concentrated on the centreline of the burner. Fig. 1b shows the NO emission comparison using the LES-CRN approach. At 1.1 bar, mechanisms such as Otomo, Zhang and NUIG provide the best agreement with experimental data

with less then 10% error. At 3 and 5 bar (TP2 and TP3), the deviation among mechanisms becomes more pronounced: the Otomo scheme continues to show reasonable accuracy due to the more accurate prediction of the reactions characterizing the NO formation via fuel-bound pathways, whereas the others tend to overestimate NO formation, especially in TP3 when Mei and Shrestha mechanisms show the largest discrepancies, exceeding +50%. This is explained by the Rates of Production (ROP) in Fig. 2, where the main reactions are compared. The most significant difference is observed in the Main and IRZ reactors in the $NO_2$ dissociation reaction, NO + O (+M) ⇌ $NO_2$ (+M), which is identified as the main contributor to the overestimation of NO prediction, while in the Pilot reactor there is no particular difference between the mechanisms analyzed. These results highlight the significant pressure dependence of NOx formation and emphasize the importance of selecting appropriate kinetic schemes. The LES-CRN methodology [5] proves effective in evaluating the performance of each mechanism, offering an efficient tool to assess chemical model reliability under pressurized conditions.

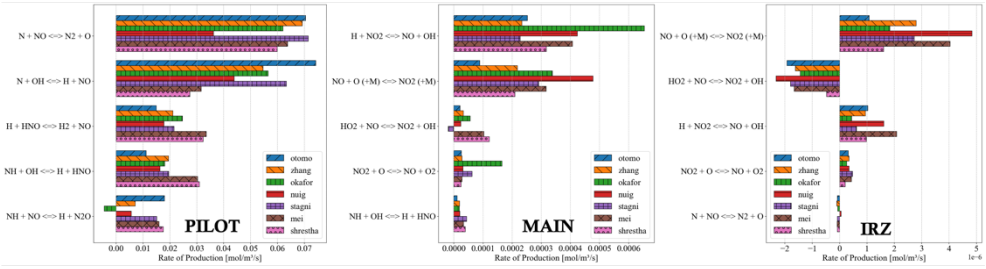


**Fig. 2:** NO Rate of Production analysis in Pilot, Main and IRZ reactors at 3 bar.

## References

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