

# CHEMICAL REACTOR NETWORK FOR PREDICTION OF NO<sub>x</sub> EMISSIONS FROM PREMIXED NATURAL GAS AND HYDROGEN ENRICHED FLAMES STABILIZED WITH A LOW-SWIRL BURNER

## MOTIVATION

In this study a flame stabilized with a low swirl burner (LSB) serves as the platform for the analysis of the NO<sub>x</sub> formation in gas turbines fueled with **hydrogen enriched fuels and natural gas**. Hydrogen enrichment decarbonizes the fuel and can reduce the production of greenhouse gases and carbon based pollutant emissions, such as CO<sub>2</sub>, CO, unburned hydrocarbons, soot particles and volatile organic compounds (VOC); moreover the addition of hydrogen to the fuel can stabilize ultra-lean hydrocarbon flames with fuel concentrations well below the corresponding lean blow off limit of natural gas

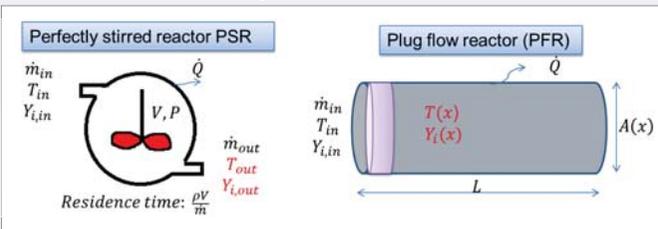
## GOALS

The current research aims to study the following:

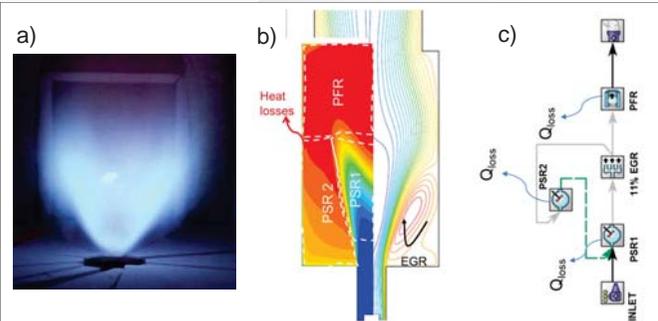
- Provide a simple numerical model to identify the underlying mechanisms controlling the formation of NO<sub>x</sub> in the LSB stabilized reaction using a chemical reactor network (CRN).
- Run parametric analysis to understand the effect of the fuel composition, pressure, exhaust gas recirculation and heat losses on the emissions of nitrogen oxides.
- Compare the numerical prediction using CRN to the experimental data and other numerical predictions using Computational fluid Dynamics.
- Test the result sensitivity to different reaction mechanisms.

## APPROACH

The CRN is a set of interconnected ideal reactors, perfectly stirred reactors (PSR) and plug flow reactors (PFR), representing a “simplified and equivalent” flow field, volume of the chamber and energy flow. This simplified version of the combustion application allows the use of detailed chemistry (Complete reaction mechanism) while reducing the computational cost.



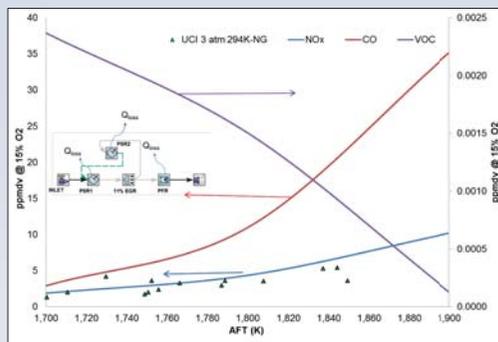
F1: PSR describes highly turbulent-mixed reacting flows (L). PFR: Describes unidimensional reacting flows (R)



F2: a) Characteristic low swirl reaction. b) Classification of the zones using CFD results. c) Equivalent CRN

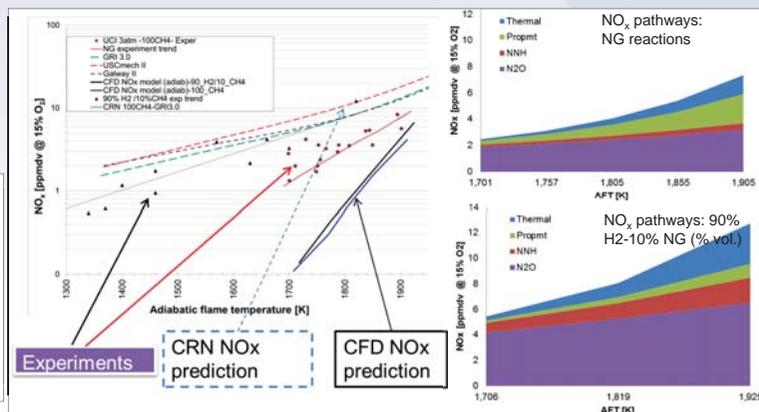
## RESULTS

The results obtained with the CRN indicate that most of the NO<sub>x</sub> is formed through the N<sub>2</sub>O route for the LSB, regardless of the fuel composition or the reaction mechanism used. The CRN predicts similar trends to those observed experimentally, regardless of the reaction mechanism. The results also show that fuel enrichment with hydrogen promotes the production of NO<sub>x</sub> through the Zeldovich, NNH and N<sub>2</sub>O routes while hindering the prompt route, when compared to the NG flames.



F3: Prediction of NO<sub>x</sub>, CO and VOC using CRN. Comparison with experimental NO<sub>x</sub> data at 3 atm.

## COMPARING STRATEGIES (CFD vs. CRN)



F4: Comparing the prediction of NO<sub>x</sub> with different strategies (CFD and CRN) (L). NO<sub>x</sub> pathways as predicted with GRI 3.0 (R)

## CONCLUSION

The CRN model is able to predict the changes in the emissions with variable parameters as the fuel composition, equivalence ratio, pressure, exhaust gas recirculation and heat losses. The methodology demonstrated that prediction is sensitive to the selection of the reaction mechanism.

## RECENT PUBLICATIONS & PAPERS

Andrés Colorado, Vince McDonell. “Reactor network analysis to assess fuel composition effects on NO<sub>x</sub> emissions from a recuperated gas turbine”. Proceedings of ASME Turbo Expo 2014: Turbine Technical Conference and Exposition GT2014 June 16 – 20, 2014, Düsseldorf, Germany

## PERSONNEL

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