ALTERNATIVE FUELS

(643) - (*) - DEVELOPMENT AND VALIDATION OF A CHEMICAL REACTOR NETWORK MODEL FOR NH3/H2/AIR FLAMES IN A SWIRL BURNER TOWARDS A RICH-QUENCH-LEAN IMPLEMENTATION

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Ammonia (NH3) has recently emerged as an interesting alternative fuel for several combustion applications. Its carbon-free chemical composition allows for zero-CO2 burning, therefore having a much lower impact in terms of greenhouse gases when compared with conventional fuels. However, low reactivity and the emission of nitrogen oxides (NOx) are still the biggest issues concerning its combustion. Additionally, unburnt ammonia presents a serious problem due to its toxic nature. Some well-known drawbacks of the use of ammonia as fuel - weak reactivity, low flame speed, high ignition delay time and hard flame stabilization - can be partially overcome by adding hydrogen (H2), which results in a mixture with notable properties. To study the combustion of this type of mixture, a swirl and bluff-body stabilized burner was developed at Instituto Superior Técnico (IST) and experiments were performed for flame stabilization, emissions and temperatures, for both lean and rich premixed flames, for a range of NH3/H2 fuel compositions, showing good performance. The main objective of the present work is to create a Chemical Reactor Network (CRN) model to represent the burner and fit to experimental results, in order to better understand the underlying phenomena present in the burner, as well as to define the best theoretical conditions for the lowest NOx and unburnt NH3 emissions. To accomplish this, an in-house model of Perfectly Stirred Reactors (PSR) and a Plug-Flow Reactor (PFR) was developed, taking into account aerodynamic and geometric characteristics of the burner and being able to predict temperature, residence time, species concentrations and combustion efficiency. The model was validated by experiments from previous works as well as RANS simulations. Although the tendencies of the predicted results are in accordance with the experiments, those results present a discrepancy when compared to the experimental ones, which can be explained by the kinetic mechanism limitations and heat losses in the burner, as well as possible hydrogen diffusion effects not accounted for in the simplified model. In the end, the CRN is extended to include a secondary air injection stage, to theoretically predict optimal conditions for a rich-quench-lean (RQL) combustor, a method that decreases NOx at the first stage while securing high overall combustion efficiency.

Palavras-chave : Ammonia combustion, Hydrogen, Swirl burner, NOx emissions, Chemical Reactor Network