Ammonia Oxidation at High Pressure as a Carbon Free Fuel

BACKGROUND

- Ammonia can be burned benignly, making it a promising fuel for transportation and energy applications.¹
- Zero carbon and greenhouse gas emission → low-carbon economy, security of energy supply and effective replacement of fossil fuels.
- NH₃ combustion characteristics are improved by mixing it with CH₄ and H₂, turning it into a suitable alternative fuel.²
- Global chemical reactions for the formation of N₂, NO and NO₂:
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  \begin{align*}
  \text{NH}_3 + \frac{3}{4} \text{O}_2 &\rightarrow \frac{1}{2} \text{N}_2 + \frac{3}{2} \text{H}_2 \text{O } \text{r1} \\
  \text{NH}_3 + \frac{5}{2} \text{O}_2 &\rightarrow \text{NO} + \frac{3}{2} \text{H}_2 \text{O } \text{r2} \\
  \text{NH}_3 + \frac{7}{2} \text{O}_2 &\rightarrow \text{NO}_2 + \frac{3}{2} \text{H}_2 \text{O } \text{r3}
  \end{align*}
  \]

Kinetic model of Ammonia oxidation

Reaction set of Ammonia combustion cover reactions of NH₃ oxidation, NO/NO₂ formation and reactions that involve other species formation such as HCN, HCN0, NCO, NH, N₂, NH₂. Kinetic models are reported by Glarborg³, Konnov⁴, Duynslaegher⁵, Okafor⁶, San Diego⁷...

Reaction pathway for NH₃ combustion (described at following figure) based on the mechanism of Glarborg et al.⁸

OBJECTIVES

- Increasing knowledge on the conversion of NH₃ at high pressures, as well as its mixtures with CH₄ and H₂ under different operating conditions.
- Evaluating the pollutant emissions obtained during the use of ammonia in energy applications and determining the possible synergies due to the interaction of NH₃ and its mixtures with NO, which can result in a further reduction of this compound.
- Experimental results will be simulated and interpreted with a detailed kinetic reaction model, that allows us to describe the ammonia combustion process under the different operating conditions.

Outcomes

- Obtaining a data series that will allow us to increase the quality and quantity of knowledge about the combustion of NH₃ and its mixtures.
- Developing a good predicting kinetic model, design simulation models with Chemkin and another multiphysics simulation software. Furthermore, to obtain a proper correlation among the experimental results, the kinetic model and simulation modelling.

Advantages/Goals

- CO₂ free combustion
- Guaranteeing security of energy supply
- Suitable storage and transport characteristics
- Expertise in combustion facilities
- NH₃ production from renewable energy sources and raw materials

Disadvantages / Challenges

- Low combustion intensity
- NO/NO₂ emission
- Minimization of NOₓ and NH₃ emissions in the NH₃ oxidation

Methodology: laboratory scale high pressure PFR

Study of conversion of reactants and gas emissions produced from combustion of NH₃ and its mixtures in well-controlled experimental conditions in a quartz floe reactor at atmospheric and high pressure.

In the experiments, concentrations of NH₃, CH₄, H₂, CO, CO₂, hydrocarbons, NO, NO₂, N₂O and HCN will be analysed.

Ammonia combustion experiments accomplish under different operating conditions including: pressure from 1 to 60 bar; temperature from 400 to 800 °C, different concentration of CH₄ and H₂ in the mixture, presence of pollutants such as NO, NO₂, NO and O₂ and air excess ratio from pyrolysis to highly oxidant conditions (λ).

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\lambda = \frac{[O_2]}{[NH_3] (\text{referred to reaction r1})}
\]

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References: