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Ammonia Oxidation at High Pressure as a Carbon Free Fuel

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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.
- NH_3 combustion characteristics are improved by mixing it with CH_4 and H_2, turning it into a suitable alternative fuel[2].
- Global chemical reactions for the formation of N_2, NO and NO_2.

$$NH_3 + \frac{3}{4}O_2 \rightleftharpoons \frac{1}{2}N_2 + \frac{3}{2}H_2O \quad r1$$
$$NH_3 + \frac{5}{4}O_2 \rightleftharpoons NO + \frac{3}{2}H_2O \quad r2$$
$$NH_3 + \frac{7}{4}O_2 \rightleftharpoons NO_2 + \frac{3}{2}H_2O \quad r3$$

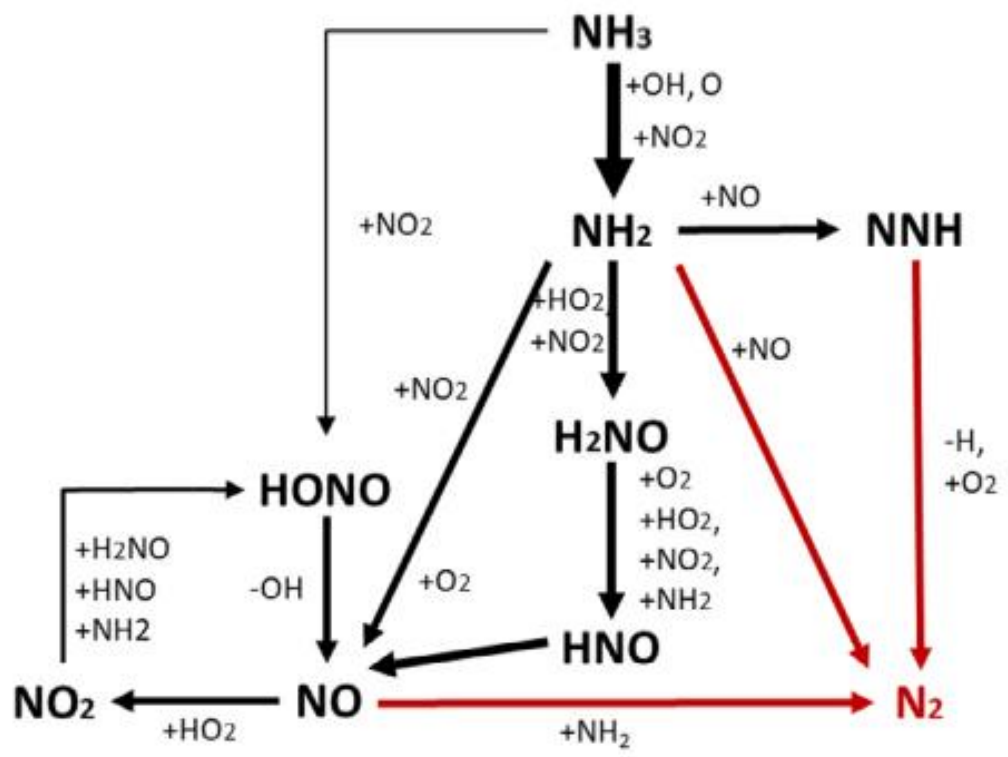
OBJECTIVES

- Increasing knowledge on the conversion of NH_3 at high pressures, as well as its mixtures with CH_4 and H_2 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 NH_3 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.

Kinetic model of Ammonia oxidation

Reaction set of Ammonia combustion cover reactions of NH_3 oxidation, NO_x/N_2O formation and reactions that involve other species formation such as HCN, HCNO, NCO, NH, N_2, NH_2. Kinetic models are reported by Glarborg[3], Konnov[4], Duynslaegher[5], Okafor[4], San Diego[4]…

Reaction pathway for NH_3 combustion (described at following figure) conditions based on the mechanism of Glarborg et al[3].



Outcomes

- Obtaining a data series that will allow us to increase the quality and quantity of knowledge about the combustion of NH_3 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.

References:
[1] Valera-Medina, A.; Xiao, H.; Owen-Jones, M.; David, W. I. F.; Bowen, P. J. Ammonia for Power. Prog. Energy Combust. Sci. 2018, 69, 63–102.
[2] Li, R.; Konnov, A. A.; He, G.; Qin, F.; Zhang, D. Chemical Mechanism Development and Reduction for Combustion of $NH_3/H_2/CH_4$ Mixtures. Fuel 2019, 257 (August), 116059.
[3] Glarborg, P.; Miller, J. A.; Ruscic, B.; Klippenstein, S. J. Modeling Nitrogen Chemistry in Combustion. Prog. Energy Combust. Sci. 2018, 67, 31–68.
[4] Han, X.; Wang, Z.; Costa, M.; Sun, Z.; He, Y.; Cen, K. Experimental and Kinetic Modeling Study of Laminar Burning Velocities of NH_3/Air, NH_3/H_2/Air, NH_3/CO/Air and NH_3/CH_4/Air Premixed Flames. Combust. Flame 2019, 206, 214–226.
[5] Duynslaegher, C. Experimental and Numerical Study of Ammonia Combustion. Univ. Leuven 2011, 1–314.

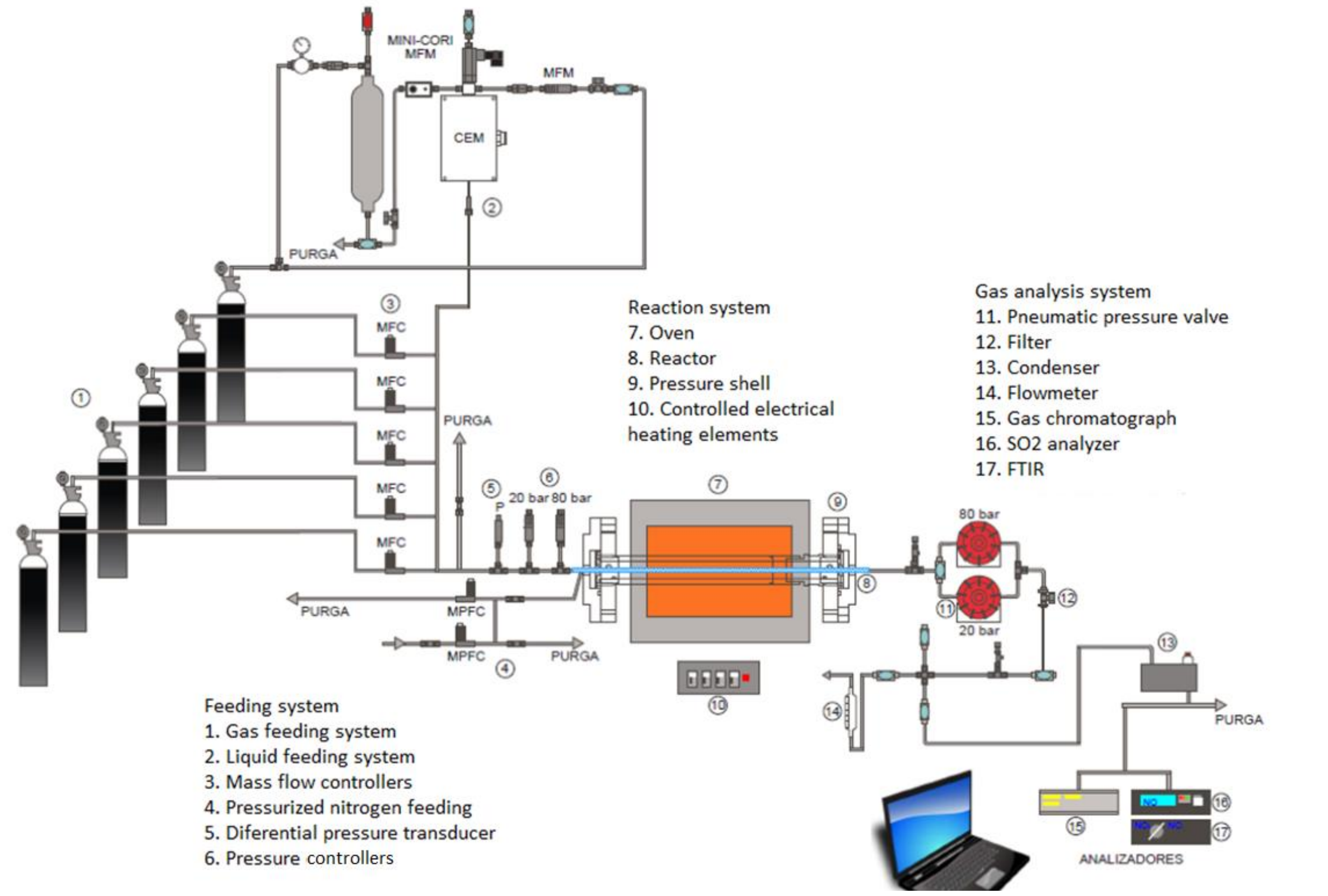
Advantages/Goals

- CO_2 free combustion
- Guaranteeing security of energy supply
- Suitable storage and transport characteristics
- Expertise in combustion facilities
- NH_3 production from renewable energy sources and raw materials

Disadvantages / Challenges

- Low combustion intensity
- NO_x/N_2O emission
- Minimization of NO_x and NH_3 emissions in the NH_3 oxidation

Methodology: laboratory scale high pressure PFR



Study of conversion of reactants and gas emissions produced from combustion of NH_3 and its mixtures in well-controlled experimental conditions in a quartz floe reactor at atmospheric and high pressure.

In the experiments, concentrations of NH_3, CH_4, H_2, CO, CO_2, hydrocarbons, NO, NO_2, N_2O 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 CH_4 and H_2 in the mixture, presence of pollutants such as NO, N_2O and NO_2 and air excess ratio from pyrolysis to highly oxidant conditions (**λ**). →

$$\lambda = \frac{[O_2]}{\frac{3}{4}[NH_3]} \quad \text{(refered to reaction r1)}$$

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