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Experimental and Simulated Study of Ammonia Combustion at High Pressures

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Introduction

Global chemical N_2 formation reaction

$$NH_3 + \frac{3}{4}O_2 \rightleftharpoons \frac{1}{2}N_2 + \frac{3}{2}H_2O \quad r1$$

Advantages: It can be burned directly [2] producing water and nitrogen (N_2) and it could be obtained using renewable energy sources and raw materials

Ammonia (NH_3) is an important carbon-free fuel carrier → combustion with no carbon dioxide (CO_2) emissions.

Applications: Security of energy supply and storage, transportation and gas turbines [1].

Objective:

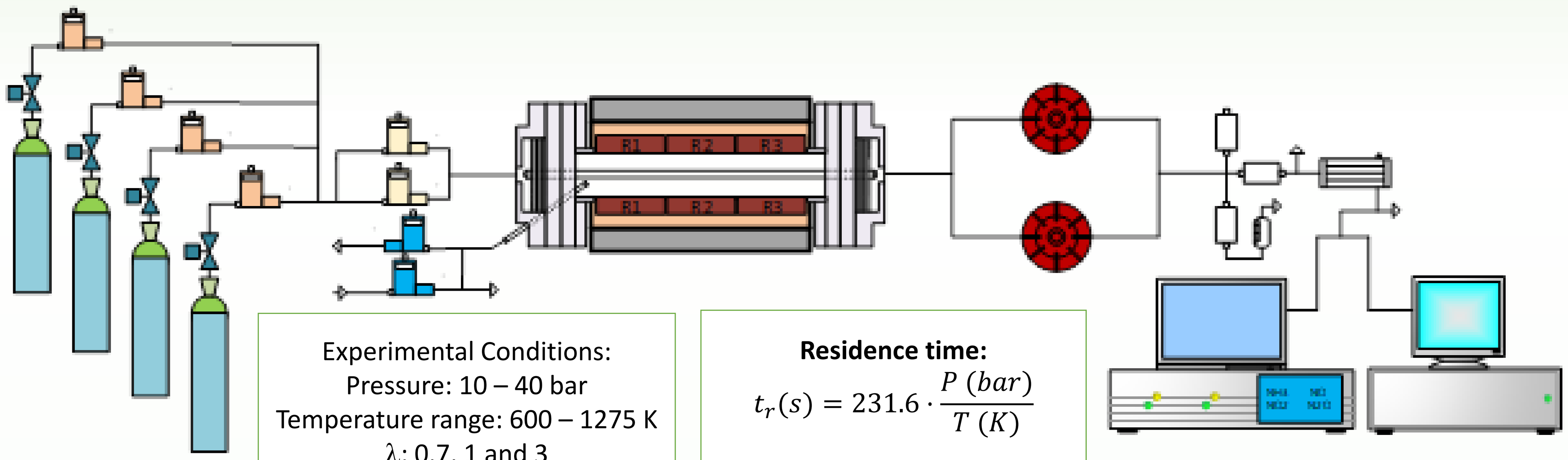
- Extending the knowledge of oxidation of pure ammonia at high pressure
- Development of a detailed reaction kinetic model

Global chemical NO formation reaction

$$NH_3 + \frac{5}{4}O_2 \rightleftharpoons NO + \frac{3}{2}H_2O \quad r2$$

Disadvantages: Obtained from CH_4 and nitrogen oxides (NO_x) can be formed from NH_3 oxidation [3].

Methodology



Experimental Conditions:
Pressure: 10 – 40 bar
Temperature range: 600 – 1275 K
λ: 0.7, 1 and 3
$[NH_3]$ = 1000 ppm
Quartz tubular reactor

Residence time:

$$t_r(s) = 231.6 \cdot \frac{P\ (bar)}{T\ (K)}$$

Oxygen excess ratio, Lambda:

$$\lambda = \frac{\left(\frac{NH_3}{O_2}\right)_{inlet}}{\left(\frac{NH_3}{O_2}\right)_{stoichometic}}$$

Table 1: Matrix of experimental conditions.

Set	NH_3 (ppm)	O_2 (ppm)	P (bar)	λ
1	1023	761	10	1,0
2	1019	2143	10	2,9
2R	983	2092	10	2,8
3	1053	745	20	1,0
4	1036	2230	20	3,0
5	1066	778	30	1,0
6	1068	2203	30	2,9
7	982	538	40	0,7
8	1070	765	40	1,0
9	1039	2265	40	3,0

- Chemical kinetic mechanism with **1468 reactions**
- Glarborg et al. development and our research group updates

Experimental Results

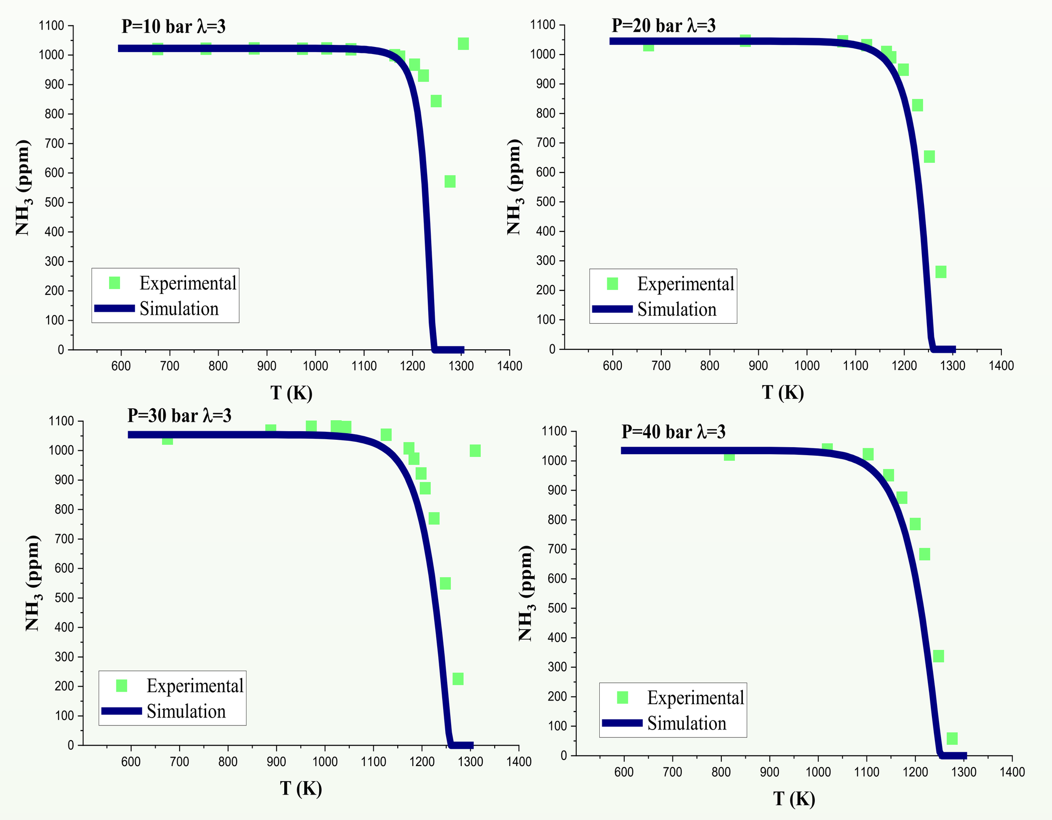


Figure 1: Comparison of experimental and simulated NH_3 concentration at 40, 30, 20 and 10 bar of pressure, λ=3.

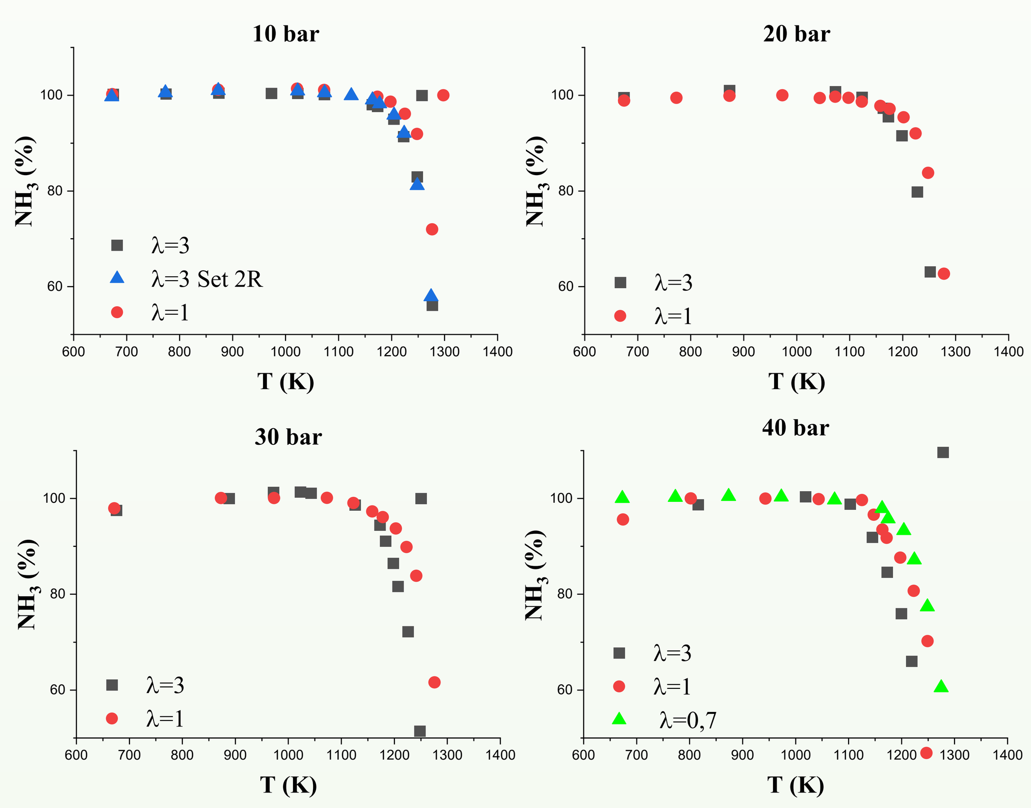


Figure 1: Experimental results of NH_3 concentration (ppm) as a function of temperature, all set of Table 1.

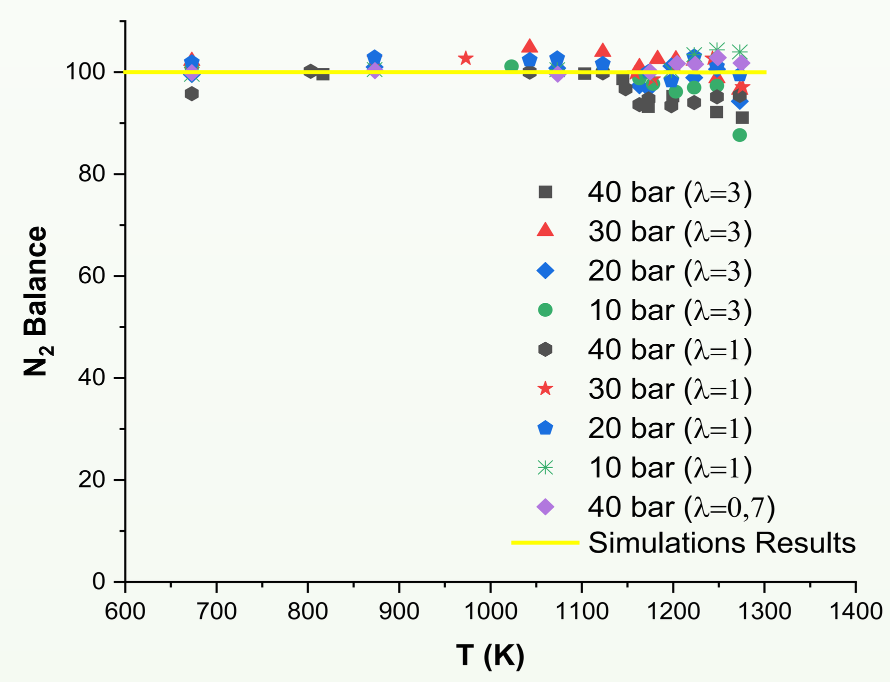


Figure 3: Comparison N_2 balance of experimental and simulated results as a function of the reactor temperature

- λ=3 (Figure 1): ↑ Pressure, ↓NH_3 oxidation onset temperature, 20 – 30 K
- N_2 is the main product of ammonia oxidation, no significant amounts of NO, NO_2, N_2O were produced.
- Modelling predictions show a good agreement with experimental results, full conversion of ammonia is overpredicted to occur at 1250 K approximately.

Conclusions

❖The main nitrogen containing product formed in NH_3 oxidation reaction is N_2, no significant amounts of NO, NO_2, or N_2O were formed.

❖At λ=1 and 3, NH_3 oxidation reaction starts at lower temperatures as the pressure increases.

❖The kinetic model reproduces well the experimental trends obtained, even though simulations slightly overpredict conversion of ammonia.

❖NH_3 conversion is higher at λ=3 than λ=1 at the same conditions of temperature and pressure.

References:

[1]. VALERA-MEDINA, A., XIAO, H., OWEN-JONES, M., DAVID, W. I.F. and BOWEN, P. J. Ammonia for power. *Progress in energy and combustion science*. 2018. Vol. 69, p. 63–102.

[2]. KOBAYASHI, H. Ammonia Combustion for Energy System. *Japan-Norway Hydrogen Seminar*. 2017.

[3]. GLARBORG, P., MILLER, J. A., RUSCIC, B. and KLIPPENSTEIN, S. J. Modelling nitrogen chemistry in combustion. *Progress in Energy and Combustion Science*. 2018. Vol. 67, p. 31–68.

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