Experimental and Simulated Study of Ammonia Combustion at High Pressures

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Abstract

Ammonia can be burned directly without CO_2 emissions. The present work deals with the experimental and simulated study of the NH_3 conversion at high pressures at two oxygen excess ratios (lambda, λ) 1 and 3, and different pressures (from 10 to 40 bar).

Introduction

Nowadays, ammonia (NH_3) plays an important role in the decarbonization of energy resources because it does not produce carbon dioxide (CO_2) emissions. Ammonia has been studied as an alternative fuel for several applications including energy storage, transportation and gas turbines [1, 2]. Although it is mainly produced from natural gas, it can also be obtained using renewable energy sources and raw materials. Ammonia represents a clean energy carrier because it could be burn directly [3] producing water and nitrogen (N_2) but, as a disadvantage, nitrogen oxides (NO_x) can be formed from NH_3 oxidation [4]. The present work pursues extending the knowledge of high-pressure oxidation of pure ammonia and the development of a detailed reaction kinetic model in order to describe the conversion of ammonia under various operating conditions.

Methodology

Conversion of reactants and produced emissions during the combustion of NH_3 are studied under well-controlled experimental conditions. The present work is performed considering the effect of main variables: oxygen excess ratio (stoichiometry λ=1 and oxidizing λ=3), pressure (10, 20, 30 and 40 bar), temperature (from 600 to 1300K). In the experiments, concentrations of NH_3, N_2, H_2, O_2, NO, NO_2 and N_2O are measured and analysed. The experimental setup is a laboratory-scale high-pressure reactor used with success in previous works. The experiments have been simulated using the kinetic model proposed in a recent work [5] updated and completed with the model proposed in a previous work of our research group [6].

Results and Discussion

Experimental results are obtained at specific conditions: 40, 30, 20 and 10 bar of pressure, λ=1 and 3, and a range of temperatures from 600K to 1300K for 1000ppm of pure NH_3.

For both λ= 1 and 3, NH_3 oxidation reaction starts at lower temperatures as the pressure is increased. For example, at λ=3 (Figure 1) NH_3 conversion is produced about 30K less, for the experiment at 40 bar compared to experiment at 30 bar, while the experiment at 30 bar stars 25K earlier than at 20 bar, and the same difference is found between the experiment at 20 and 10 bar. The decrease in temperature at which NH_3 initiation reaction occurs as pressure is increased is slightly more relevant at λ=1.

The oxidation of NH_3 did not produce amounts of NO, NO_2, N_2O significantly. The main product of ammonia conversion is N_2. The nitrogen balance is shown in figure 1 and, as can be seen, the number of nitrogen atoms is roughtly conserved.

The results of NH_3 conversion as a function of temperature for λ=3 are shown in figure 2 as an example. Similar observations can be made for λ=1. In this figure, both experimental results (symbols) and simulations made with the kinetic model (lines) are represented at 10, 20, 30 and 40, bar, in a range of temperatures from 600K to 1300K.

Calculations do folllow the same trends as observed experimentally, even though conversion of ammonia is predicted to occur at lower temperatures compared to the experimental data, about 20-40K.

Conclusions

The results in this experimental study can be summarised as follows:

1. The main nitrogen containing product formed in NH_3 oxidation reaction is N_2, no significant amounts of NO, NO_2, neither N_2O were formed.
2. At λ=1 and 3, NH_3 oxidation reaction starts at lower temperatures as the pressure increases. At a given temperature, the NH_3 conversion is also larger at higher pressure.
3. The effect of pressure is slightly more important at λ=1 than at λ=3.
4. NH_3 conversion is higher at λ=3 than λ=1 at the same conditions of temperature and pressure.
5. The kinetic model reproduces well the experimental trends obtained, even though simulations slightly overpredict conversion of ammonia.

ACKOWLEDGEMENTS

The authors acknowledge the funding from the Aragón Government (Ref. T22_17R), co-funded by FEDER 2014-2020 "Construyendo Europa desde Aragón “, to MINECO and FEDER (Project RTI2018-098856-B-I00, and MINECO PRE2019-090162 for financial support.

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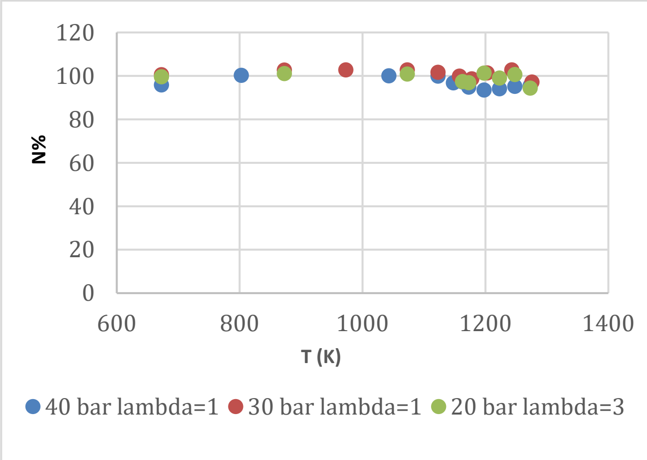

Figure 1: Nitrogen atoms (N) balance (percentage).

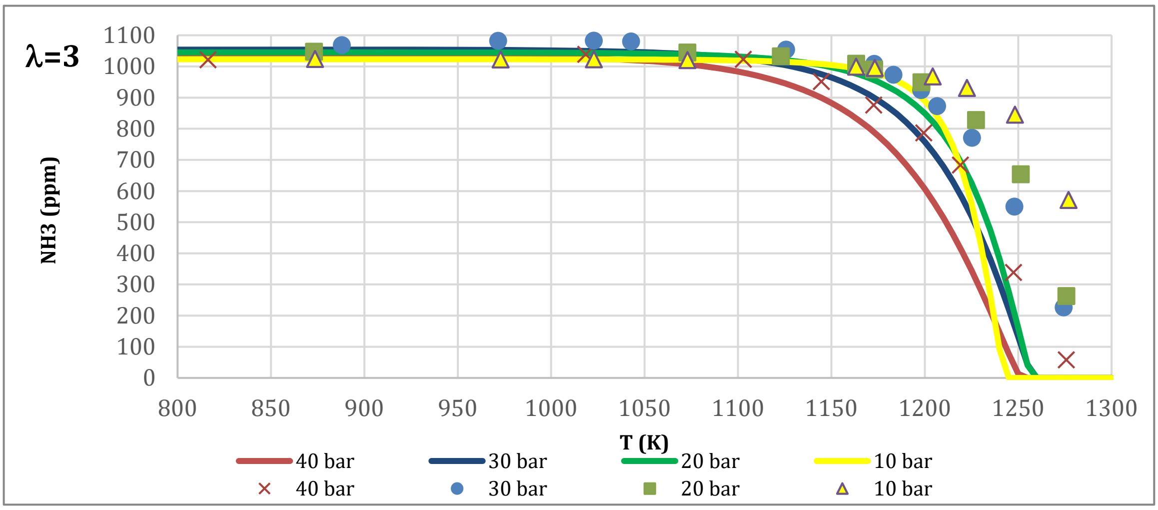

Figure 2: Experimental (symbols) and simulated (lines) NH_3 (ppm) at 40, 30, 20 and 10 bar of pressure, lambda=3