Ammonia oxidation at high pressure and intermediate temperatures - DTU Orbit (08/11/2017)

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Ammonia oxidation experiments were conducted at high pressure (30 bar and 100 bar) under oxidizing and stoichiometric conditions, respectively, and temperatures ranging from 450 to 925 K. The oxidation of ammonia was slow under stoichiometric conditions in the temperature range investigated. Under oxidizing conditions the onset temperature for reaction was 850–875 K at 30 bar, while at 100 bar it was about 800 K, with complete consumption of NH_3 at 875 K. The products of reaction were N_2 and N_2O, while NO and NO_2 concentrations were below the detection limit even under oxidizing conditions. The data were interpreted in terms of a detailed chemical kinetic model. The rate constant for the reaction of the important intermediate H_2NO with O_2 was determined from ab initio calculations to be $2.3 \times 10^{-2} T^{2.994} \exp(-9510\ K/T)\ cm^3\ mol^{-1}\ s^{-1}$. The agreement between experimental results and model work was satisfactory. The main oxidation path for NH_3 at high pressure under oxidizing conditions is $NH_3 \xrightarrow{+OH} NH_2 \xrightarrow{+HO_2,NO_2} H_2NO \xrightarrow{+O_2} HNO \xrightarrow{+O2} NO \xrightarrow{+NH_2} N_2$. The modeling predictions are most sensitive to the reactions $NH_2 + NO = NNH + OH$ and $NH_2 + HO_2 = H_2NO + OH$, which promote the ammonia consumption by forming OH radicals, and to $NH_2 + NO = N_2 + H_2O$ and $NH_2 + NO_2 = N_2O + H_2O$, which are the main chain-terminating steps.

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