

Investigation of Surface Coverage on NH₃ Synthesis Catalysts by N₂-TPD

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Ammonia is one of the most significant products of the chemical industry as it is both an essential part of artificial fertilizer, but also as an energy carrier in Power-to-X technologies. Currently, ammonia is produced through the Haber-Bosch process at pressures up to 300 bar [1-2]. It is important to obtain information about the surface coverage of this catalytic process under industrial conditions. However, current studies have only made such analyses at atmospheric conditions. In this study, the behavior of the catalyst at higher pressures has been investigated by applying a quenching method developed in our research group [3].

The surface coverage on a doubly-promoted iron catalyst for ammonia synthesis has been investigated through a series of N₂-TPD experiments. The catalyst was prepared by co-precipitation from Fe(NO₃)₃ and Al(NO₃)₃ at pH 10 adjusted by aqueous ammonia. The dried powder was then impregnated by an aqueous solution of K₂CO₃ and dried again.

The experiments with the prepared catalyst were performed in a glass lined packed bed U-tube reactor. The catalyst was reduced in a 100 NmL/min flow of 5% H₂/Ar at 500 °C for 10 hours (excluding a temperature ramp of 2 °C/min) prior to adsorption of nitrogen. The basis for determining the surface coverage was a saturation of the surface by ramping the reduced catalyst from 500 °C to 25 °C by 2 °C/min (with a 1 h hold at 400 °C) in 1 bar of N₂ followed by an N₂-TPD with a 2 °C/min ramp. The N₂ content of the gas was monitored by mass spectroscopy. An example of data from such an experiment can be seen in Fig. 1.

The surface coverage of the working catalyst (treated with a synthesis gas mixture (3:1 H₂:N₂)) has been determined by rapid quenching of the working catalyst (at 400 °C and pressures up to 50 bar) followed by TPD in Ar. This data was fitted and extrapolated to industrially relevant conditions for the Haber-Bosch process.

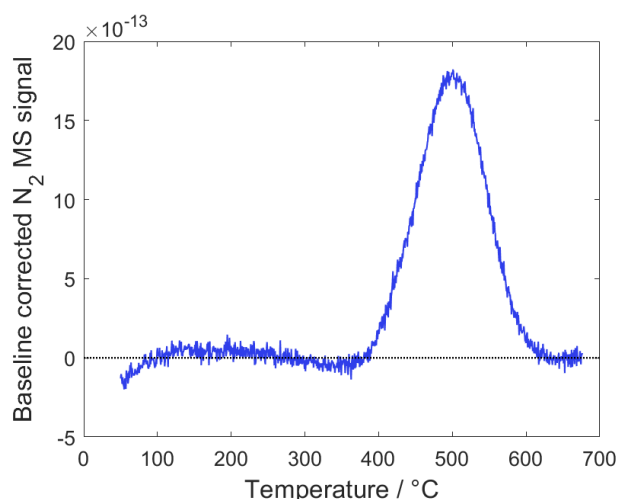


Fig. 1. Baseline corrected data from the N₂-TPD after adsorption in N₂ at 400 °C, 1 bar used as basis for determining the surface coverage of the catalyst after adsorption in a synthesis gas mixture (3:1 H₂:N₂) at different pressures.

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References

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