#494 / Oral Communication
TOPIC : Energy

# Ammonia cracking under high pressure conditions for a hydrogen fuel cell: reactor conditions and kinetics


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## PURPOSE OF THE ABSTRACT

Introduction

Hydrogen (H2) as a carbon-free energy source is considered to be one of the energy sources of the future. However, because of its low volumetric energy density and its small molecular size, there is no H2 transport and storage technology available that can satisfy the practical requirements of usage of hydrogen as an energy source e.g., for fuel cell application [1]. The on-site production of hydrogen by decomposition of hydrogen-vectors is therefore seen as a promising, practicable technology. Ammonia (NH3) is a potential hydrogen-vector candidate for, e.g., usage in fuel cells that is easy to be stored, transported, and distributed and is thus a safe, and cheap long-term hydrogen handling method [1]. The conversion of ammonia to hydrogen can take place directly in harbours or wherever additional energy is required.

Materials and Methods

Endothermic ammonia cracking can be operated at temperatures of 700 - 900°C and, unlike ammonia synthesis, low pressure is favoured [2]. The use of a catalyst can significantly reduce the reaction temperatures and improve the ammonia conversion rates. Various catalysts are applicable to catalytic ammonia cracking, but ruthenium (Ru) appears to be the best one [1].

To maximize the activity, selectivity, and stability of chemical reactors, the latter are subject to continuous improvement. While experimental optimization entails high expenses in terms of cost and time, virtual optimization is a promising alternative. This paper describes a combined experimental and theoretical investigation of catalytic NH3 cracking using a Ru catalyst. Detailed micro-kinetic analysis is a powerful method that allows for insights into the catalyst that are inaccessible via real experiments.

In this work, a method to develop detailed kinetic mechanisms valid over a broad range of boundary conditions based on experimental investigations of a Ru-based NH3 cracker is presented. A 1D model, LOGEcat [3] is utilized to carry out the simulations. The model has been successfully applied and tested in past studies [4] of after-treatment catalytic processes, as well as chemical reactor modelling.

Typical energetic hydrogen applications often require high-pressure hydrogen. Thus, even if low pressures are favoured during ammonia cracking, a high-pressure operation can make it possible to dispense with expensive

pumps. In this work, the conversion efficiency of NH3 cracking under different inlet pressures and temperatures is investigated. The experimental campaign aims to understand the kinetics of ammonia cracking in detail. To that purpose, the temperature along the fixed bed reactor is monitored.

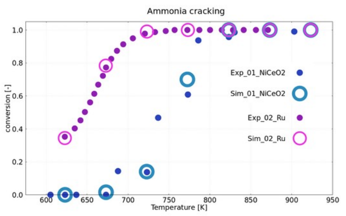
Results and Discussion

The detailed surface reaction mechanism used in the present study involves three gas phase and five surface phase species and consists of 12 reactions based on [5]. Reaction kinetics are taken into account using the Arrhenius approach with prefactor, temperature dependency, and activation barrier. The simulation results of the kinetic model reflect the observed experimental behaviour such that conclusions can be drawn on intermediate surface species, surface coverage and rate determining steps under the investigated operating conditions.

Significance

Within this investigation, we show the predictive capability of a cost-effective reduced order 1D simulation tool using detailed surface chemistry to investigate the production of hydrogen from NH3 for a fuel cell application. The virtual investigation allows us to study the rate-limiting reactions in function of the inlet conditions and catalyst properties.

## FIGURES




## FIGURE 1

## FIGURE 2

## KEYWORDS

NH3 cracking | carbon free energy | heterogeneous catalysis | 1D modelling

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