Economic Evaluation of the Emerging Electrochemical Nitrogen Reduction to Ammonia Depending on Catalyst Performance

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Abstract

Electrochemical reduction of nitrogen to ammonia is a promising alternative to the conventional Haber-Bosch process to decarbonize ammonia production. Although there is a lot of work on catalyst development for this novel reaction, there is a lack of concise economic evaluations and rational goals for catalyst development.

Based on an economic evaluation, we estimate production cost based on catalyst performance in terms of achievable Faradaic efficiency at a certain production rate. By relating to benchmark cost, a function mapping Faradaic efficiencies and production rates to reach cost parity is derived, determining the feasible space for catalyst development.

All catalysts reported to date lie considerably below the cost parity curve. Even though recent catalyst developments achieve considerable high Faradaic efficiencies, the production rate remains too low, resulting in the investment cost alone being higher than the ammonia market price.

**Keywords**: Electrochemistry, Economic Evaluation, Ammonia, Catalyst Evaluation.

* 1. Introduction

Novel electrochemical reactions can aid in decarbonizing the chemical industry and transition away from using fossil fuels as feedstocks and energy sources (Luh et al., 2018). We evaluate the current status and the potential of the electrochemical nitrogen reduction reaction (eNRR) to ammonia, a novel reaction pathway to synthesize ammonia directly from water and air at near ambient conditions.

In developing these emerging electrochemical technologies, the focus is on identifying and improving suitable catalysts. However, there is a lack of rational goals for catalyst performance. Reported goals state the catalyst performance at one operating point (Soloveichik, 2016). This approach is insufficient as the required performance depends on the operating conditions.

We conduct an economic evaluation of the eNRR process to investigate the catalyst's influence on the performance of the overall process. We estimate production cost based on reaction rate and Faradaic efficiency, quantities reported in catalyst studies, and compare the production cost with benchmark prices. Based on this, we derive a curve mapping required production rates and Faradaic efficiencies to achieve cost parity with the benchmark.

* 1. Process model

In this work, we focus on evaluating the eNRR and thus model only the electrochemical reactor in more detail. Investigating the influence of downstream processes like product purification is out of the scope of this work. In the electrochemical cell, ammonia is formed at the cathode and the by-product oxygen at the anode. The anode reaction is the same as in alkaline water electrolysis, a mature technology. Therefore, no significant economic impact of an improvement of the anode catalyst is expected, and we focus on the cathode catalyst and the novel reaction. The performance of this catalyst determines the selectivity and reaction rate of the target product ammonia and the side product hydrogen. For a more detailed process description, the reader is referred to a recent literature review by Rezaie et al. (2023).

The levelized cost of ammonia (LCOA) is calculated as the sum of OPEX and annual CAPEX divided by the produced amount of ammonia. The CAPEX for the new process is estimated by transferring the CAPEX for alkaline water electrolysis to the proposed electrochemical reactor as they share the same basic setup.

OPEX of electrochemical processes is mainly determined by the cost of electricity (Hemauer et al., 2023). Additionally, fixed OPEX for operation and maintenance and variable OPEX for the educts are considered.

* 1. Results and discussion

We evaluate the catalyst studies reviewed by Rezaie et al. (2023) and calculate the respective LCOA at the reported production rate and Faradaic efficiency.

First, the minimal Faradaic efficiency is calculated by setting the investment cost to zero and equalizing the electricity cost with the benchmark price. Following this approach, the minimum Faradaic efficiency and thus the energy efficiency is calculated depending on the cell potential. Some studies achieve Faradaic efficiency higher than the minimal.

Second, the minimal reaction rate is calculated similarly by setting the electricity cost to zero and equalizing the CAPEX and fixed operation and maintenance cost with the benchmark price. All investigated reaction rates lie considerably below the minimal.

Third, we calculate the LCOA based on the experimental data. All results are well above the benchmark price. Even though some studies achieved Faradaic efficiencies higher than the minimal, the production rates and current densities are too low, resulting in capital cost being higher than the benchmark price. Higher production rates are required to reduce production costs considerably and to achieve cost parity.

The production cost calculation conducted in this work depends on the catalyst performance—the achieved Faradaic efficiency at a specific production rate. By equalizing this cost function with the benchmark price, a curve mapping required Faradaic efficiency to the production rate is derived. This curve can be used to evaluate new experimental data and to guide catalyst development towards a competitive process. As benchmarks to compare the LCOA, the ammonia market price as well as production cost of green ammonia produced via the Haber-Bosch process coupled with water electrolysis are used. Thus, electrochemical ammonia production can be compared to the conventional process and further possibilities to defossilize ammonia production.

* 1. Conclusion

In this work, we derived a function mapping operation conditions and Faradaic efficiency to achieve cost parity with a benchmark price. Competitive catalysts must reach or outperform the limit defined by this curve. Even though recent catalyst studies show considerable improvement in Faradaic efficiency, the production rates are still too low, resulting in CAPEX being higher than the ammonia market price.

The low reported production rates can be traced back to the nature of the experimental approach focusing on catalyst screening and improving Faradaic efficiencies at low potentials, resulting in low reaction rates. To enable a cost-competitive process, high Faradaic efficiencies at high production rates are required. Thus, catalyst research must transition into aiming for higher production rates.

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