MSc thesis topic: A feasibility study: Electrochemical ammonia synthesis versus the old and conventional Haber-Bosch process

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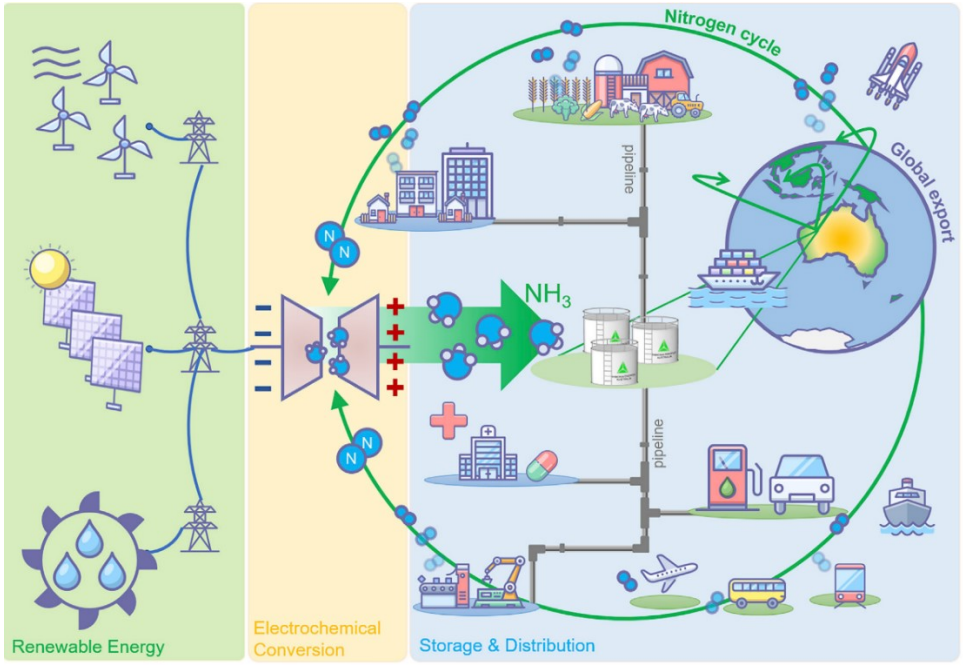

Figure 1 Vision of the ammonia economy [1]

The world market size for ammonia is estimated to be 171 million tonnes in 2020 with an expected annual growth rate of 3-5% [2]. Therefore, it belongs to the group of highest produced synthetic chemicals. It is mainly used as fertilizer and contributes to the nitrogen nutrition demand of agriculture. Ammonia is for 90% produced by the energy intensive Haber-Bosch process [3], which is responsible for 1.8% of the global CO_2 emissions and contributes highly towards climate change.

Recently, a lot of research interest focusses on finding sustainable alternatives for the energy intensive Haber-Bosch process. Using an electrolyzer to produce ammonia electrochemically, where the conversion of nitrogen, water and electrons (Nitrogen reduction) into ammonia, seems a promising alternative since no emissions are involved and it could be produced on small scale in a decentralized manner.

While most research focusses on finding an active electrocatalysts to accelerate nitrogen reduction (NRR), less is known about the implementation, design and feasibility of this new process on large scale. An initial process model has been implemented in Aspen by a former MSc student and this project will be a continuation of the former, wherein the existing model will be expanded and further optimised. This gives insights into the electrolyzer design, important electrochemical parameters and its techno-economic feasibility compared to Haber-Bosch ammonia plants.

This thesis project will mainly involve process modelling and simulation in MATLAB and Aspen custom modeler. **The main deliverables at the end of this project entail:**

- An extensive literature screening and documentation of related electrochemical ammonia articles.
- Expanding the model by adding different types of electrolyzers and separation technologies to gain high purity ammonia
- Techno-economic feasibility of the plant by parameter sensitivity analysis.

We are looking for: Motivated MSc. Students with affinity towards modelling, process design and simulation, and with a showing interest in electrochemical technologies. Prerequisite knowledge of Aspen and MATLAB is necessary. Understanding electrochemistry fundamentals is a pre, but not required.

What's in it for you? Gaining research experience in a multidisciplinary group, become an expert in electrochemical process modelling and simulation, setting the boundaries for an entirely new and not existing renewable ammonia process.

For more information, please contact: Boaz Izelaar (b.izelaar@tudelft.nl)

[1] MacFarlane et al. Joule 4, 1–20, June 17, 2020
[2] The Catalyst Group, "Ammonia Production: Recent Advances in Catalyst and Process Technology and Impacts on the Competetive Lanscape," 04 2018.
[3] M. Appl, "Ammonia," in *Encyclopedia for industrial chemistry*, Wiley-VCH, 2006, p. 155.