Master Student Project:

"Designing an Industrial-Scale Electrochemical CO_2 Reduction Process"

Duration of the project	:	7-8 months
Earliest starting date	:	January 2022
Focus of the work	:	Process system design, simulation and optimisation (Aspen)
Daily supervisors	:	Asvin Sajeev Kumar (PhD student, *3mE*, A.SajeevKumar@tudelft.nl)
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Main supervisor	:	Wiebren de Jong / Ruud Kortlever

Project description

The continuous increase in the level of CO_2 in the atmosphere and the need to develop an alternate source of energy have steered researchers to explore several mitigation measures such as CO_2 capture, CO_2 storage and CO_2 conversion. Among the various proposed CO_2 conversion technologies, the electrochemical CO_2 reduction (ECR) is considered to be promising owing to its operational convenience and the possibility to store renewable energy, such as wind and solar, in the form of chemical bonds [1]. The CO_2 feedstock for the purpose of ECR could be obtained from chemical industries or power plants. However, one of the major drawbacks is the presence of impurities such as SO_2, NO_2, H_2S, COS and other volatile organic compounds. These gaseous contaminants may corrode the system or poison the electrocatalyst [2, 3]. The deactivation of catalyst can also occur due to the presence of trace amounts of heavy metal contaminants such as Fe^{2+} and Zn^{2+} in the liquid electrolyte [4]. Therefore the feed streams from the industries undergo a series of cleaning processes to remove the undesirable contaminants. The cleaned CO_2 stream is fed into the ECR reactor, where it is electrochemically reduced to high energy density fuels and chemicals which are either gaseous or dissolved in the liquid electrolyte (see list of products in Figure 1). The gaseous products are separated from the unreacted CO_2 in a separation unit and the latter is either directly recycled back to the ECR reactor or fed to the gas cleaning unit depending on the purity of the CO_2 stream. Similarly, the liquid products are separated from the electrolyte and the latter is either directly recycled back to the ECR reactor or fed to the liquid cleaning unit depending on the purity of the electrolyte steam. The concentrated gaseous and liquid products are finally extracted from their respective separation units (see block diagram in Figure 1).

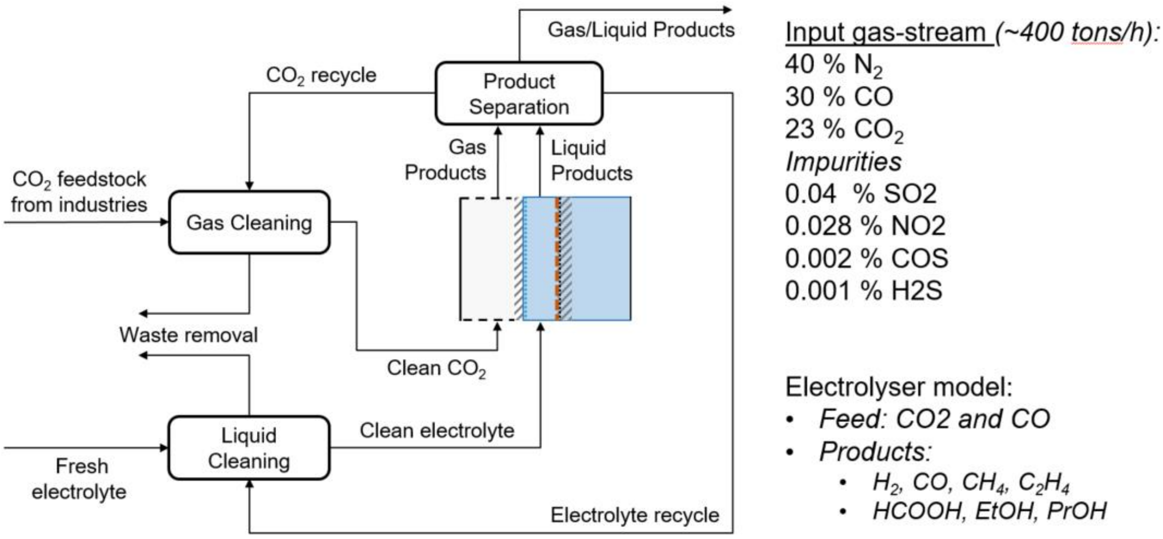

Figure 1: Block diagram of ECR process with industrial feedstock composition and electrolyser product distribution.

An initial design for the ECR process was developed in Aspen by a group of students, which highlighted some technology choices as the primary bottlenecks. Namely, the liquid and gaseous cleaning steps for impurities removal and the separation of formate from the liquid product stream. Further, a highly basic electrolyte stream (pH > 14) at the outlet of the electrolyser was also found to be challenging.

Research objective

TU Delft, in collaboration with the E2CB consortium, is working to design an industrial-scale ECR process that utilises the industry-supplied CO_2 feedstock for the production of high energy density fuels and chemicals. Therefore, the objective of this student project is to identify energy efficient technologies for the removal of impurities in the gaseous feedstock and liquid electrolyte, and develop a detailed process design in Aspen. The developed process model will be used for a techno-economic and sensitivity analysis, which can then be used to identify bottlenecks and lay the foundation for an optimization study of process and design choices for the ECR. Also, the future case where the ECR process will be powered by renewable energy sources such as wind/solar will be studied, accounting for the intermittency of these sources.

Getting started

- Prepare a time planning for the coming month including milestones
- Literature research (Electrochemical CO_2 reduction, techno-economic studies of ECR processes, system design for ECR processes) [5, 6, 7, 8]
- Install Aspen, MATLAB and Excel; get introduction on how to couple modelling tools

Literature to get started:

[1] S. Liang, N. Altaf, L. Huang, Y. Gao, and Q. Wang, "Electrolytic cell design for electrochemical CO2 reduction," *Journal of CO2 Utilization*, vol. 35. Elsevier Ltd, pp. 90–105, 01-Jan-2020, doi: 10.1016/j.jcou.2019.09.007.

[2] G. V. Last and M. T. Schmick, "Identification and Selection of Major Carbon Dioxide Stream Compositions," Richland, WA (United States), Jun. 2011.

[3] T. E. Graedel, G. W. Kammlott, and J. P. Franey, "Carbonyl sulfide: Potential agent of atmospheric sulfur corrosion," *Science (80-.).*, vol. 212, no. 4495, pp. 663–665, May 1981, doi: 10.1126/science.212.4495.663.

[4] Y. Hori *et al.*, "'deactivation of copper electrode' in electrochemical reduction of CO2," *Electrochim. Acta*, vol. 50, no. 27, pp. 5354–5369, Sep. 2005, doi: 10.1016/j.electacta.2005.03.015.

[5] M. Jouny, W. Luc, and F. Jiao, "General Techno-Economic Analysis of CO2 Electrolysis Systems," *Ind. Eng. Chem. Res.*, vol. 57, no. 6, pp. 2165–2177, Feb. 2018, doi: 10.1021/ACS.IECR.7B03514.

[6] W. A. Smith, T. Burdyny, D. A. Vermaas, and H. Geerlings, "Pathways to Industrial-Scale Fuel Out of Thin Air from CO2 Electrolysis," *Joule*, vol. 3, no. 8, pp. 1822–1834, Aug. 2019, doi: 10.1016/J.JOULE.2019.07.009.

[7] S. K. Nabil, S. McCoy, and M. G. Kibria, "Comparative life cycle assessment of electrochemical upgrading of CO2 to fuels and feedstocks," *Green Chem.*, vol. 23, no. 2, pp. 867–880, Feb. 2021, doi: 10.1039/D0GC02831B.

[8] A. Zimmerman *et al.*, "Techno-Economic Assessment & Life-Cycle Assessment Guidelines for CO2 Utilization," 2018, doi: 10.3998/2027.42/145436.