Thesis project: **Investigating Dynamic CO2 electrochemical modelling along with extended electron transfer process**

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- Department: Process & Energy, 3mE
- Theme: Energy
- Is an external organization involved? No
- The thesis involves: Modeling (finite element)
- Prerequisite: Electrochemistry (basic),
  Finite element methods,
  Programming (preferably Python)

Background:

In recent years, CO_2 electrochemical reduction (CO_2ER) has emerged as one of the most promising technologies to mitigate the climate effects. The idea is to Electrify CO_2 with energy from renewable sources, resulting in many industrially relevant chemicals such as formic acid, methanol and CO. However, there are several challenges that arise while modelling such a process. For example, what is the most effective way to include the electrode charge transfer reactions within the framework of a continuum scale transport model? Does the reaction even occur at the electrode? How can we overcome the CO_2 mass transfer limitations that arise due the formation of dense electric double layer (EDL) on the electrode surface? These phenomena directly influence the overall cell performance and the maximum production rates. Hence, it becomes necessary to develop a modelling approach that accounts for these processes accurately.

Goals:

1. Investigate modelling techniques to include heterogenous electrode reactions within an existing continuum scale mass transport model, focusing specially on the possibility of extended electron transfer through tunnelling effect. Validate the results with existing experimental polarization curves.
2. Modify and analyse the model for dynamic operations. The idea is to perturb the input variables such as electrode potential to disperse the dense EDL resulting in an increased mass transfer for CO_2. Analyse the model under dynamic conditions and find the optimal dynamic conditions that result in maximum current densities and Faradaic efficiencies of desired product.

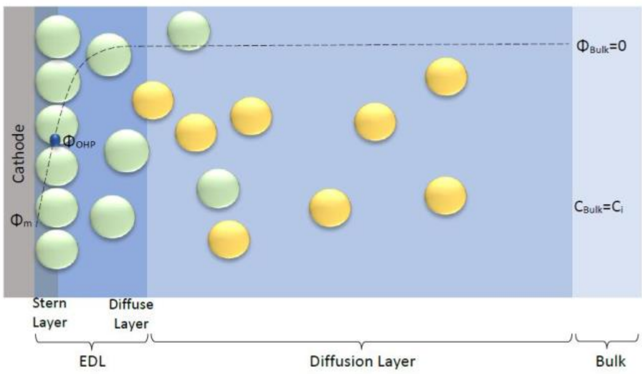

Figure 1: Schematic of CO2ER process including different mass transfer zones.

Bibliography

1. D. Bohra, J. H. Chaudhry, T. Burdyny, E. A. Pidko, W. A. Smith, Modeling the electrical double layer to understand the reaction environment in a co2 electrocatalytic system, Energy and Environmental Science 12 (2019) 3380–3389. doi:10.1039/c9ee02485a.

2. E.J.F. Dickinson, R.G. Compton, Influence of the diffuse double layer on steady state voltammetry, J. Electroanal. Chem. 661 (1) (2011) 198–212, https://doi.org/ 10.1016/j.jelechem.2011.08.002.