Thesis project
Theme: Energy

Thesis title: "Investigating charge transfer reactions inside a gas diffusion electrode for CO_2 electrochemical reduction"

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Is an external organization involved? No

The thesis involves: Modelling

Prerequisite courses and/or knowledge: Electrochemistry (basic), Finite element methods, Coding

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 electrically convert CO_2 using energy from renewable sources. This process allows for the production of many industrially relevant chemicals, such as formic acid, methanol and CO. However, there are several questions 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 a 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. Investigation of a microkinetic modelling approach for CO_2 reduction to determine the adsorbate coverages and current densities inside a 2D catalyst pore.
2. Coupling the kinetic approach with an already existing continuum scale mass transport model.
3. Validate the model with existing experimental polarization curves.

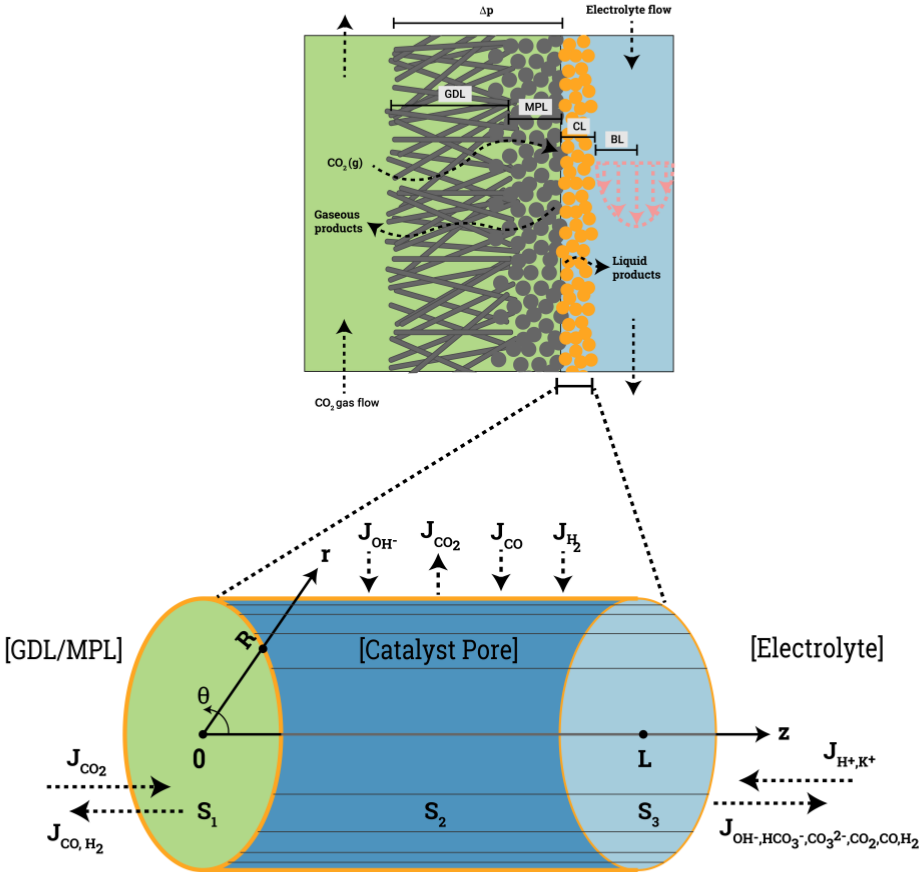

Figure 1: 3D representation of a cylindrical catalyst pore [2].

Bibliography

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2. Bohra D, Chaudhry J, Burdyny T, Pidko E, Smith W. Mass Transport in Catalytic Pores of GDE-Based CO2 Electroreduction Systems. *ChemRxiv* (2020). doi: 10.26434/chemrxiv.13073348.v1
3. Xinwei Zhu, Jun Huang, and Michael Eikerlin ACS Catalysis 2021 11 (23), 14521-14532 DOI: 10.1021/acscatal.1c04791