Porous Transport Layer CFD Simulation

Master Project (30 ECTS)/Semester Project (10 ECTS)

Administrative

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Location: Sion or remotely (travel allowance offered)

Project description:

Anion exchange membrane water electrolyzers (AEMWE) are electrochemical devices that split the water molecule into H_2 and O_2 when a DC current is applied. AEMWE are a novel yet promising technology for hydrogen production due to their low cost and relatively high efficiency. A simple representation of the AEMWE cells is shown in figure 1, where the membrane is situated between the anode and the cathode, each containing a catalyst layer (CL) and a porous transport layer (PTL). The CL is where the electrochemical reaction happens (half-cell reaction equations written in figure 1), while the PTLs are responsible for evacuating the produced gases from the cell.

As part of HyPrAEM [1], a European project of the Horizon Europe initiative, the objective is to image different PTL samples using computed micro-tomography, then to retreive the imaged PTL samples, compute their microstructural properties (using an in-house-developed code) and use them in a CFD study. The study includes simulating the 2-phase flow in the electrodes and finding the most important PTL parameters that contribute to the bubble evacuation. Then, a PTL porosity gradient needs to be investigated (figure 2), to study non-homogenious PTL structructes. In the end, the goal is optimize the PTL microstructure. To achieve this goal, an existing multi-physics model developed in the lab needs to be improved to account for non-homogeneities and different PTL microstructures.

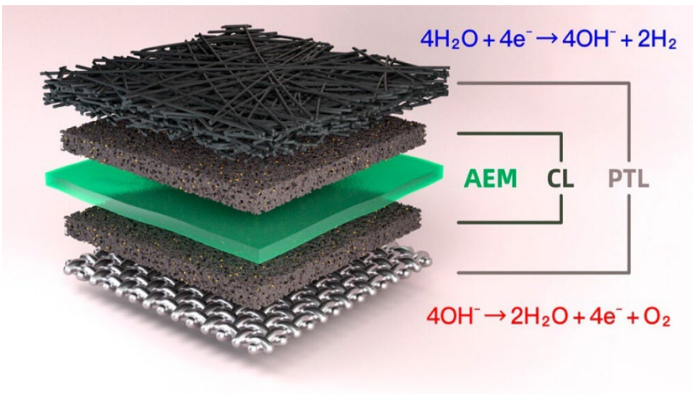

Figure 1: AEMWE cell structure with half-cell reactions [2]

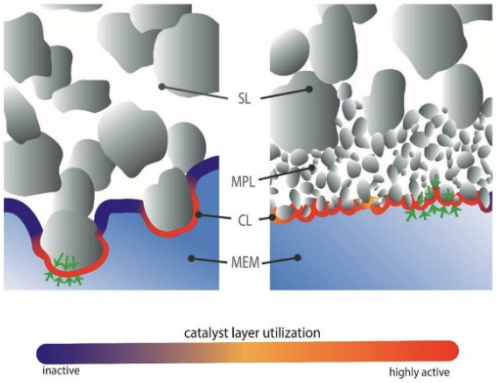

Figure 2: Non-homogeneous PTL microstructure [3]

Your tasks:

The student tasks for this project are:

1. Import the imaged samples from the computed micro-tomography into COMSOL
2. Compute the microstructural properties of the samples
3. Conduct a CFD study using the different imaged samples
4. Simulate non-homogeneous PTL structrures
5. Optimize PTL microstructure

References

[1] cordis.europa.eu CORDIS, “High-pressure anion exchange membrane electrolyzers for large-scale applications,” *CORDIS | European Commission*, Dec. 20, 2024. https://cordis.europa.eu/project/id/101192442 (accessed Jun. 20, 2025).

[2] Q. Li *et al.*, “Anion Exchange Membrane Water Electrolysis: The Future of Green Hydrogen,” *The Journal of Physical Chemistry C*, vol. 127, no. 17, pp. 7901–7912, Mar. 2023, doi: https://doi.org/10.1021/acs.jpcc.3c00319.

[3] T. Schuler *et al.*, “Hierarchically Structured Porous Transport Layers for Polymer Electrolyte Water Electrolysis,” *Advanced Energy Materials*, vol. 10, no. 2, p. 1903216, Nov. 2019, doi: https://doi.org/10.1002/aenm.201903216.