Numerical Investigation of Electrowetting in CO_2 Electrolyzers

- **Supervisors**: Ezra Käs (daily supervisor e.kas@tudelft.nl), Dr. R.M. Hartkamp (Process & Energy, ME)
- **Prerequisites**: ME Advanced Fluid Mechanics (or equivalent), *some* numerical modeling experience (ME Multiphysics transport in Energy Materials **or** ME CFD for Engineers **or** AE CFD1/2 **or** WI Numerical Analysis **or** relevant personal/educational project).

Interested in multiphase CFD, electrochemistry, and directly contributing to ongoing research at the P&E department? Send an email to e.kas@tudelft.nl !

Background

CO_2 reduction (CO2R) refers to the electrochemical conversion of CO_2 into valuable chemicals. To circumvent slow CO_2 transport through the liquid phase, cathodic **gas-diffusion electrodes (GDEs)** are used to bring CO_2 gas close to catalyst sites (figure 1).

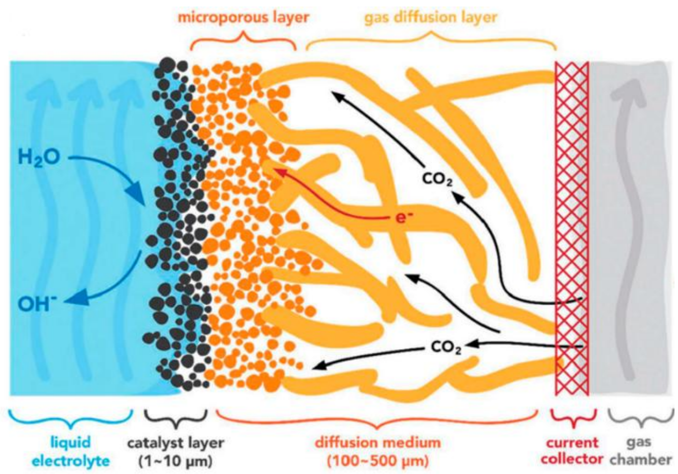

*Figure 1: **Diagram of a cathodic GDE for CO_2 electrolysis** (https://dx.doi.org/10.1021/acscatal.0c03319)*

GDE flooding refers to **inadequate electrolyte management** leading to electrolyte intrusion into the gas diffusion layer, and the lengthening of CO_2 diffusion paths. As an electric potential is applied and affects all layers of the GDE, **electrowetting (figure 2) makes gas diffusion layer (GDL) surfaces less hydrophobic, and can cause flooding.** This effect can worsen as otherwise chemically inert carbon or polymer surfaces become activated.

Young's equation:

$$\gamma_{sl} = \gamma_{sv} + \gamma_{lv}\ \cos(\alpha)$$

Lippmann's equation:

$$\gamma_{sl}(\phi) = \gamma_{sl}(\phi = 0) + \frac{1}{2} C_D \phi^2$$

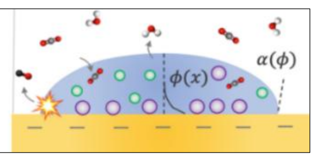

*Figure 2: Macroscopic description of electrowetting according to Lippmann's equation. **The liquid-solid interface develops a capacitance C_D** due to the presence of ions in the electrolyte. **This capacitance** responds to applied potential, and **modifies surface energy and the contact angle α.***

In this project, you will conduct pore-scale electrowetting simulations in **COMSOL** in idealized gas diffusion layers to **investigate the dependence of GDL saturation and flooding on applied potential and electrolyte concentrations.**

Goals

- **By the end of the literature review**, you will be able to:
  - Explain how electrowetting affects CO_2 electrolyzers and how this is modeled in the literature,
  - Identify relevant conditions in the GDL (applied potential, electrolyte concentrations, etc.),
  - Assess which multiphase model available in COMSOL is best for electrowetting simulations,
  - Recommend 2D geometries with available validation data as representative GDL models,
  - Formulate a research question and plan to investigate electrowetting-sensitive GDL saturation.
- **Halfway through the thesis**, you will have:
  - Validated chosen 2D geometries against effective medium correlations and saturation data,
  - Determined how to include electrowetting effects in multiphase simulations in COMSOL,
  - Developed a systematic framework in COMSOL to evaluate electrowetting-sensitive GDL saturation.
- **By the end of the thesis**, you will have:
  - Modeled electrowetting-sensitive GDL saturation in COMSOL in representative 2D geometries,
  - Evaluated GDL saturation sensitivity and saturation due to electrowetting effects,
  - Theorized how electrowetting affects 3D GDLs under steady or pulsed operation,
  - Presented your findings in a thesis report that forms the basis of a scientific publication.