

## Numerical Investigation of Gas Pocket Stability in CO<sub>2</sub> Electrolyzers

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- **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). No COMSOL experience required

### Background

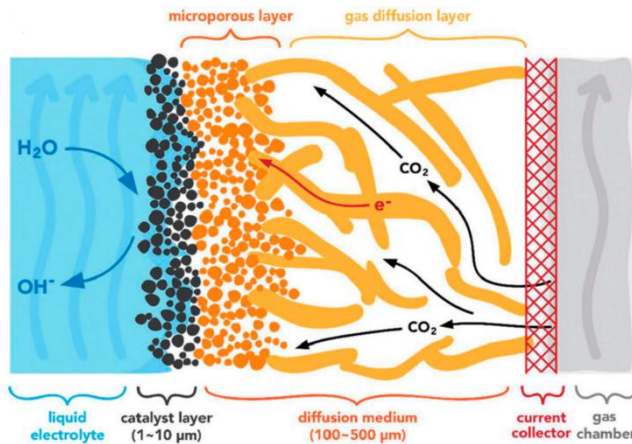


Figure 1: **Diagram of a cathodic GDE for CO<sub>2</sub> electrolysis** (<https://dx.doi.org/10.1021/acscatal.0c03319>)

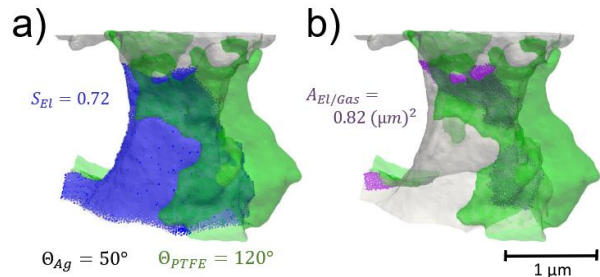


Figure 2: **Simulated triple-phase region inside a GDE pore.** (a) Electrolyte (in blue) saturation  $S_{EI}$  is mainly determined by capillary wetting on solid materials (defined with contact angles  $\theta$  on the catalyst in grey, and hydrophobic additive in green). (b) Surface CO<sub>2</sub>R reactions occur in a triple-phase region near the electrolyte/gas interface (area  $A_{EI/Gas}$  marked in purple) ([https://doi.org/10.1149/osf.io/ahdux\\_v1](https://doi.org/10.1149/osf.io/ahdux_v1))

**CO<sub>2</sub> reduction (CO<sub>2</sub>R)** refers to the electrochemical conversion of CO<sub>2</sub> into valuable chemicals. To circumvent slow CO<sub>2</sub> transport through the liquid phase, cathodic **gas-diffusion electrodes (GDEs)** are used to bring CO<sub>2</sub> gas close to catalytic reaction sites (figure 1). CO<sub>2</sub>R occurs in **triple-phase regions** (figure 2) inside the catalyst layer, close to both catalyst surfaces and electrolyte-gas interfaces.

In mass-transfer simulations, **trapped gas pockets** leftover from the initial electrolyte saturation are sometimes ignored. However, due to reactant gas input from the main electrolyte/gas interface, and degassing of product gases, **these pockets may be stable**, obstructing the electrolyte or acting as reactant gas reservoirs. Alternatively, by storing reactant gases, **these pockets may destabilize the local environment** through transient reaction hotspots.

In this project, you will conduct multiphase simulations in **COMSOL** in idealized catalyst layers and pores to **investigate the stability of trapped gas bubbles in GDEs under operating conditions.**

### Goals

- **By the end of the literature review**, you will:
  - Explain mass-transfer limitations in GDE catalyst layers for CO<sub>2</sub>R (in particular due to trapped gas pockets) from a literature review and simple analytical models,
  - Formulate a research question and plan to investigate trapped gas pocket stability in GDEs.
- **By a midterm review halfway through the thesis**, you will:
  - Develop a multiphase mass-transfer simulation framework in COMSOL that flexibly integrates gas and solute transport, chemical reactions, and electrolyte/gas interface movement,
  - Simulate trapped gas pockets in simplified reaction environments to validate your previous analysis.
- **By the end of the thesis**, you will:
  - Model trapped gas pocket stability in COMSOL under representative operating conditions and simplified 2/3D geometries,
  - Breakdown the effects of trapped gas pockets in GDEs for CO<sub>2</sub>R under steady or pulsed operation,
  - Advise on modeling trapped gas pockets in fully resolved 3D simulations.