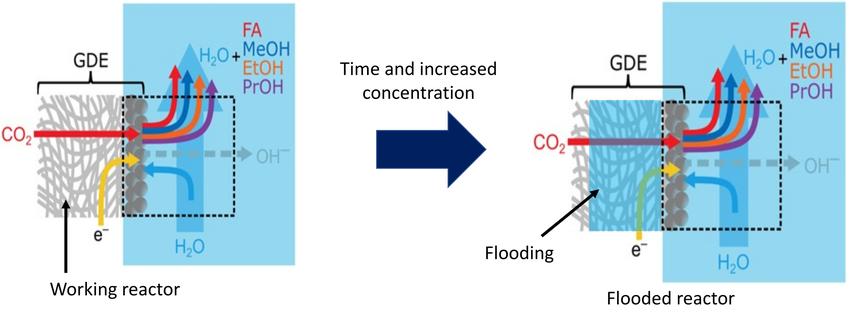
CornellEngineering
Sibley School of Mechanical and Aerospace Engineering

Simulation and Topology Optimization for Additive Manufacturing of Gas Diffusion Layers

Joshua Krsek*, Sadaf Sobhani

Introduction

- Gas diffusion layers (GDL) are a porous medium through which carbon dioxide (CO_2) diffuses in vapor-fed aqueous electrolyte carbon dioxide reduction reactors (CO2RR)
- CO2RRs can help transition to a more sustainable future by allowing energy produced by renewables to be stored as chemical fuel
- Atmospheric CO_2 diffuses through the GDL into a porous catalyst layer where it interfaces with an aqueous electrolyte solution. Electrical current is supplied through the porous medium triggering an electro-chemical reaction, resulting in a conversion of the atmospheric CO_2 into valuable industrial chemicals and fuels, such as formic acid.
- A current drawback of CO2RRs is ”flooding”, which is when the aqueous electrolyte solution flows upstream, into the GDL, preventing CO_2 to flow into the reactor

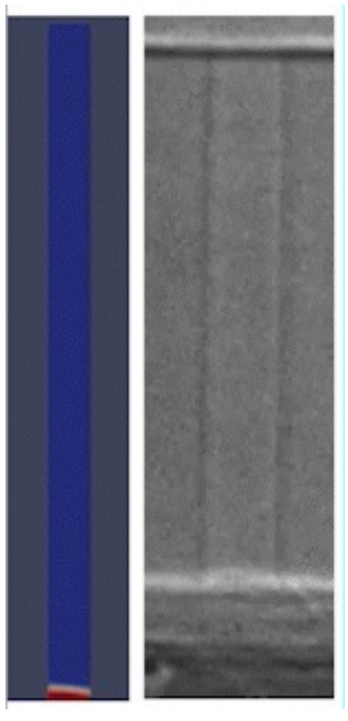


Click the button to talk to me about my poster!
April 29. 3:10 - 4:00 pm

- A solid understanding of the physics at the gas-liquid-solid interface is needed to predict when flooding occurs

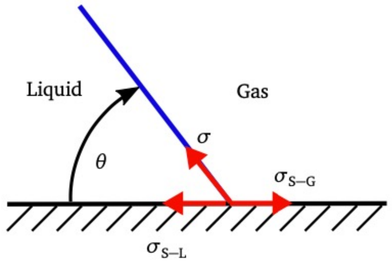
Methodology & Current Results

- The complex geometry of GDLs in operational CO2RRs is computationally intensive to model; therefore, the 3-D geometry is simplified to 2-D channels



Axisymmetric simulation vs radiography for flow through a 50-micron diameter, 400-micron height, capillary tube with applied pressure gradient

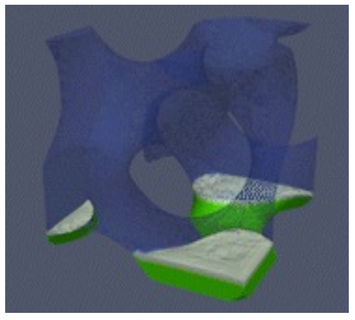
- An algebraic volume of fluids method is utilized in the open-source CFD software package OpenFOAM to multi-phase flow



- Dynamic contact angle models are implemented to capture the motion of the three-phase interphase

Future Work

- Once confidence is established in the agreement of 2-D channel simulations with experiment, we will move to modeling more complex 3-D geometry unit cells



- Optimization techniques will be applied to the topology of the porous medium to minimize the amount of “flooding” that occurs at typical operating conditions
- 2-photon polymerization will be used to 3-D print the complex topology of the optimized GDL
- Once optimized for the hydrodynamics, simulations will transition to simultaneously optimizing the electro-chemical reactions

References:
[1] McLain E. Leonard et al 2020 J.Electrochem.Soc. 167 124521
[2] Rettenmaier, Daniel. (2019):Numerical Simulation of Shear Driven Wetting.Darmstadt, Technische Universität, [Ph.D. Thesis]