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Controlling Gas Diffusion Layer Wettability via Additive Manufacturing and Simulation

Monday, 31 May 2021 15:10 (15 minutes)

Chemical exchange and energy storage devices utilize gas diffusion layers (GDLs) to facilitate the transport of gaseous reactants and liquid electrolytes to a catalyst site. The goal of the current work is to study the liquid-gas interface dynamics that result in flooding in GDLs in the context of electrochemical CO₂ reduction (CO₂R). In CO₂R reactors, flooding of the porous layer imposes a great challenge in expanding this technology to industrial applications. In fact, flooding of the GDL can happen within several hours of operation, leading to a reduction in selectivity toward CO₂R reaction products. Generally, flooding is inhibited by hydrophobic coating applied to internal surfaces of the GDL, such as polytetrafluoroethylene (PTFE). However, recent innovations in additive manufacturing and catalyst design have enabled high-performance reactors with unprecedented rates of product conversion. Wettability and the potential for flooding increases as lower surface tension CO₂R reaction products (e.g., formic acid, methanol, ethanol, and 1-propanol) are introduced in high concentrations into the flowing liquid streams, thus challenging existing GDLs. If the GDL becomes flooded and pores start to fill up with liquid, gaseous CO₂ is blocked from reaching the active site catalyst surface. It is hypothesized that the liquid electrolyte flooding the GDL under high-conversion reactor operation leads to suboptimal performance or even failure of the electrochemical reactor.

We will present a three-dimensional model incorporating the Hoffman expression for dynamic contact angle for CO₂R products. Next the governing equations will be discretized numerically using the volume of fluid technique in OpenFOAM and executed on a parallel computing platform. The CFD core of this simulation serves as foundation to an optimization algorithm that iterates over the surface texture and morphology of the GDL to study the liquid saturation as a function of capillary pressure. Three morphologies of gyroids, lattice structures, and tubular arrays in combination with three surface textures of triangular waves, Voronoi embossment, and finned embossments are selected for the purpose of study. The designs are constrained to have equal liquid-gas interface area and contact line length. However, surface texture parameters such as pattern density, chord height, and number of cells per unit volume are unconstrained variables that can be optimized. To update the geometry in each iteration, nTopology software has been used to create a new lattice structure with new sets of input variables. This unique software integration offers a significant advantage over geometry manipulation in OpenFOAM and could be applied to many similar problems involving complex geometry CFD calculations.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

Corral, D., Feaster, J., Sobhani, S. et al. "Advanced Manufacturing for Electrochemical CO₂ Reduction to Multi-Carbon Products." Under Review.

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