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Multiscale Modeling of Bubble Evolution on Gas-Evolving Electrodes

Amirreza Azad[1*], Ali Dolatabadi[1], Carlo Antonini[2], Mehdi Jadidi[1]
[1]Department of Mechanical and Industrial Engineering, University of Toronto, Toronto, Canada
[2]Department of Materials Science, University of Milano-Bicocca, Milan, Italy
*amirreza.azad@mail.utoronto.ca

ABSTRACT

Gas-evolving electrodes are integral to electrochemical systems, influencing processes such as hydrogen production, metal electrowinning, and fuel cells. The formation, growth, and detachment of gas bubbles on these electrodes play a crucial role in mass transport, electrolyte resistance, and overall system efficiency. Managing bubble dynamics is essential to optimize electrochemical performance, minimize overpotential, and enhance energy conversion efficiency. This research aims to develop a multiscale multiphysics modeling framework to study bubble evolution on electrode surfaces, integrating nanoscale nucleation mechanisms with microscale bubble dynamics for accurate prediction of bubble formation and detachment.

A hybrid numerical approach is adopted, combining transport-based models, computational fluid dynamics (CFD) simulations, and machine learning (ML)-based predictive tools. At the nanoscale, bubble nucleation is influenced by gas diffusion, ion migration, and electrochemical reactions near surface cavities. This study employs a transport-based nucleation model, incorporating electric double-layer effects, charge transport, and reaction kinetics to improve the estimation of bubble initiation sites. At the microscale, bubble growth is modeled using a Level-Set method, capturing bubble coalescence, detachment forces, and electrolyte flow interactions. A two-way coupling strategy connects nanoscale and microscale dynamics to investigate the impact of nanoscale gas pockets on microscale bubble distribution. This approach addresses a key research gap: the influence of surface wettability, nanobubble blockage, and bulk bubble formation on hydrogen production efficiency.

The study will explore optimized engineered surfaces by introducing specific patterns such as cavities and pillars, determining their optimal distribution to maximize nanoscale bubble nucleation. At the microscale, a combination of aerophobic and aerophilic surface modifications will be proposed to accelerate bubble detachment. Future experimental validation will measure hydrogen bubble generation rates and size distributions, allowing ML algorithms to predict water-splitting performance based on electrode surface variations. The final objective is to maximize system efficiency through data-driven optimization.

This research advances the fundamental understanding of bubble evolution on gas-evolving electrodes and establishes a robust computational framework for optimizing electrochemical systems. By integrating multiscale modeling with machine learning, this study provides a novel pathway for improving electrode designs, reducing energy losses, and enhancing gas evolution efficiency for sustainable energy applications.