

Modeling and Optimization of a Microfluidic Electrochemical Cell for the Electro-Reduction of CO₂ to CH₃OH

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Abstract : First, an electrochemical model for the reduction of CO₂ into CH₃OH is developed in which mass and charge transfer, reactions at the surface of the electrodes and fluid flow of the electrolyte are considered. This mathematical model is developed in COMSOL Multiphysics® where both secondary and tertiary current distribution interfaces are coupled to consider concentrations and potentials inside different parts of the cell. Constant reaction rates are assumed as the fitted parameters to minimize the error between experimental data and modeling results. The model is validated through a comparison with experimental data in terms of faradaic efficiency for production of CH₃OH, the current density in different applied cathode potentials as well as current density in different electrolyte flow rates. The comparison between model outputs and experimental measurements shows a good agreement. The model indicates the higher hydrogen evolution in comparison with CH₃OH production as well as mass transfer limitation caused by CO₂ concentration, which are consistent with findings in the literature. After validating the model, in the second part of the study, some design parameters of the cell, such as cathode geometry and catholyte/anolyte channel widths, are modified to reach better performance and higher faradaic efficiency of methanol production.

Keywords : carbon dioxide, electrochemical reduction, methanol, modeling

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