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Modelling and Simulating CO2 Electro-Reduction to Formic Acid Using Microfluidic Electrolytic Cells: The Influence of Bi-Sn Catalyst and 1-Ethyl-3-Methyl Imidazolium Tetra-Fluoroborate Electrolyte on Cell Performance

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Abstract : A modified steady-state numerical model is developed for the electrochemical reduction of CO₂ to formic acid. The numerical model achieves a CD (current density) (~60 mA/cm²), FE-faradaic efficiency (~98%) and conversion (~80%) for CO₂ electro-reduction to formic acid in a microfluidic cell. The model integrates charge and species transport, mass conservation, and momentum with electrochemistry. Specifically, the influences of Bi-Sn based nanoparticle catalyst (on the cathode surface) at different mole fractions and 1-ethyl-3-methyl imidazolium tetra-fluoroborate ([EMIM][BF₄]) electrolyte, on CD, FE and CO₂ conversion to formic acid is studied. The reaction is carried out at a constant concentration of electrolyte (85% v/v., [EMIM][BF₄]). Based on the mass transfer characteristics analysis (concentration contours), mole ratio 0.5:0.5 Bi-Sn catalyst displays the highest CO₂ mole consumption in the cathode gas channel. After validating with experimental data (polarisation curves) from literature, extensive simulations reveal performance measure: CD, FE and CO₂ conversion. Increasing the negative cathode potential increases the current densities for both formic acid and H₂formations. However, H₂ formations are minimal as a result of insufficient hydrogen ions in the ionic liquid electrolyte. Moreover, the limited hydrogen ions have a negative effect on formic acid CD. As CO₂ flow rate increases, CD, FE and CO₂ conversion increases.

Keywords : carbon dioxide, electro-chemical reduction, ionic liquids, microfluidics, modelling
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