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Mathematical Modeling of the Performance Degradation Mechanisms of Cation-Contaminated Proton-Exchange-Membrane Water Electrolysis

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The role of hydrogen as a commercial energy source is dependent on the development of robust processes to convert hydrogen into usable electricity as well as produce hydrogen at large scales. Proton-exchange-membrane water electrolysis (PEMWE) is the leading technology with the potential to produce hydrogen at projected consumption rates. In PEMWE, water is electrochemically split into hydrogen and oxygen gas using a membrane—electrode assembly, which uses a membrane capable of transporting both water and protons. Reactant water containing cationic impurities have been observed to degrade cell performance. Thus, developing an understanding of the influence of cationic contaminants is important to developing mitigation and recovery strategies for PEMWE systems.

In the current work, mathematical models were developed to provide insight into the mechanisms of performance degradation due to cationic contaminants. The models are non-isothermal continuum models that describe multi-phase porous flow, electrochemical reactions, and concentrated-species transport in both the gas membrane, and ionomer phases. Simulations were performed in steady-state and transient operational modes for various cationic species at several ionic concentrations. The calibration and fitting of the models were performed using experimental measurements performed by the National Renewable Energy Laboratory. The mathematical models suggest that gradients facilitate the adsorption of cationic contaminants in reactant water, which subsequently accumulate in the cathode catalyst layer, as shown in Figure 1(a), and inhibit the PEMWE hydrogen-evolution reaction (HER) that consume protons and electrons to produce hydrogen gas. The models suggest that protonic conductivity is not significantly affected by low-concentration cationic species, but access to the catalyst active sites in the cathode catalyst layer is severely impeded. As a result, the evolution of hydrogen then proceeds by hydrolysis pathway used in hydroxide-exchange-membrane water electrolysis (HEMWE), where water and electrons combine to produce hydrogen gas and hydroxide ions. An interpolated polarization curve shown in Figure 1(b) suggests that cell operation at high current densities favor the HEMWE hydrolysis HER reaction due to occlusion of the cathode catalyst layer active sites.

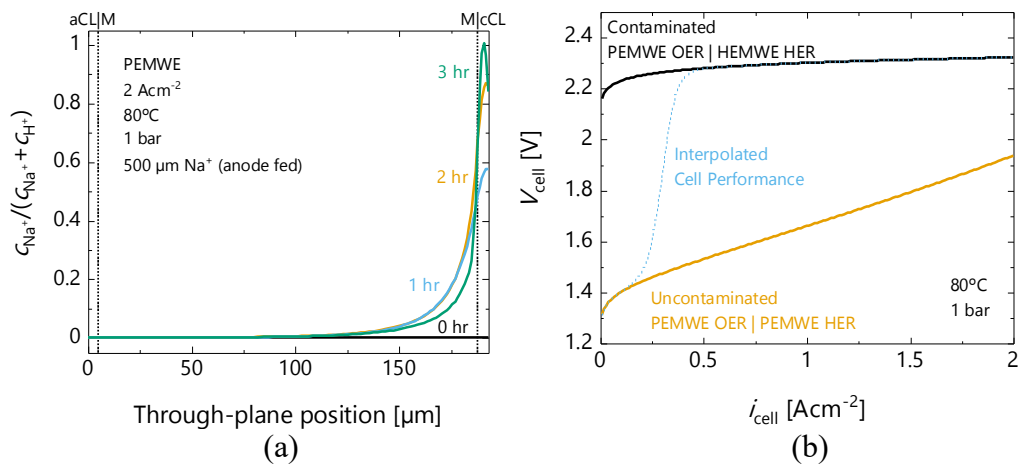


Figure 1 Simulated cell operation at 80°C with balanced 1 bar gas pressures. (a) Transient simulations of the distribution of sodium ions introduced to the anode-side of the cell at a concentration of $500 \mu\text{M}$. The concentration is scaled by the local cationic concentration in the catalyst and membrane phases as function of position with time as a parameter. (b) Polarizations curved of two electrochemical models, with one representing PEMWE oxygen and hydrogen evolution reactions (OER and HER) and the other representing a contaminated system where PEMWE OER and HEMWE HER occur. The interpolated polarization curve shown mimics experimental observations of contaminated PEMWE cells.

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