Understanding Multi-Ion Transport Mechanisms in Bipolar Membranes

Justin C. Bui[1,2], Alexis T. Bell[1,2], and Adam Z. Weber[2]

[1]Dept. of Chemical Engineering - University of California, Berkeley [2]Joint Center for Artificial Photosynthesis - LBNL

JCAP JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

Abstract:

A continuum model of multi-ion transport in a bipolar membrane (BPM) is developed and fit to experimental data. Specifically, concentration profiles are determined for all ionic species, and the importance of a water dissociation catalyst is demonstrated. The model describes internal concentration polarization and co- and counter-ion crossover in BPMs, determining the mode of transport for ions within the BPM and revealing the significance of ion crossover when operated with pH gradients relevant to electrolysis. Finally, a sensitivity analysis reveals that BPMs can be improved substantially by use of thinner dissociation catalysts, modulating the thickness of the BPM to control salt ion crossover, and increasing the ion-exchange capacity of the ion-exchange layers in order to amplify the water dissociation kinetics at the interface.

Introduction

- Because BPMs can operate under pH gradients, they enable favorable environments for catalysis at the individual electrodes for water splitting or CO_2RR.
- Transport in BPMs is poorly understood, and mitigating salt-ion crossover is vital to implementation in electrolyzers.
- The continuum model developed in this study captures water dissociation and crossover over a range of applied pH gradients relevant to various electrosynthesis reactions.
- The continuum model will inform the future design of bipolar membranes and water dissociation catalysts.

Broad Impact

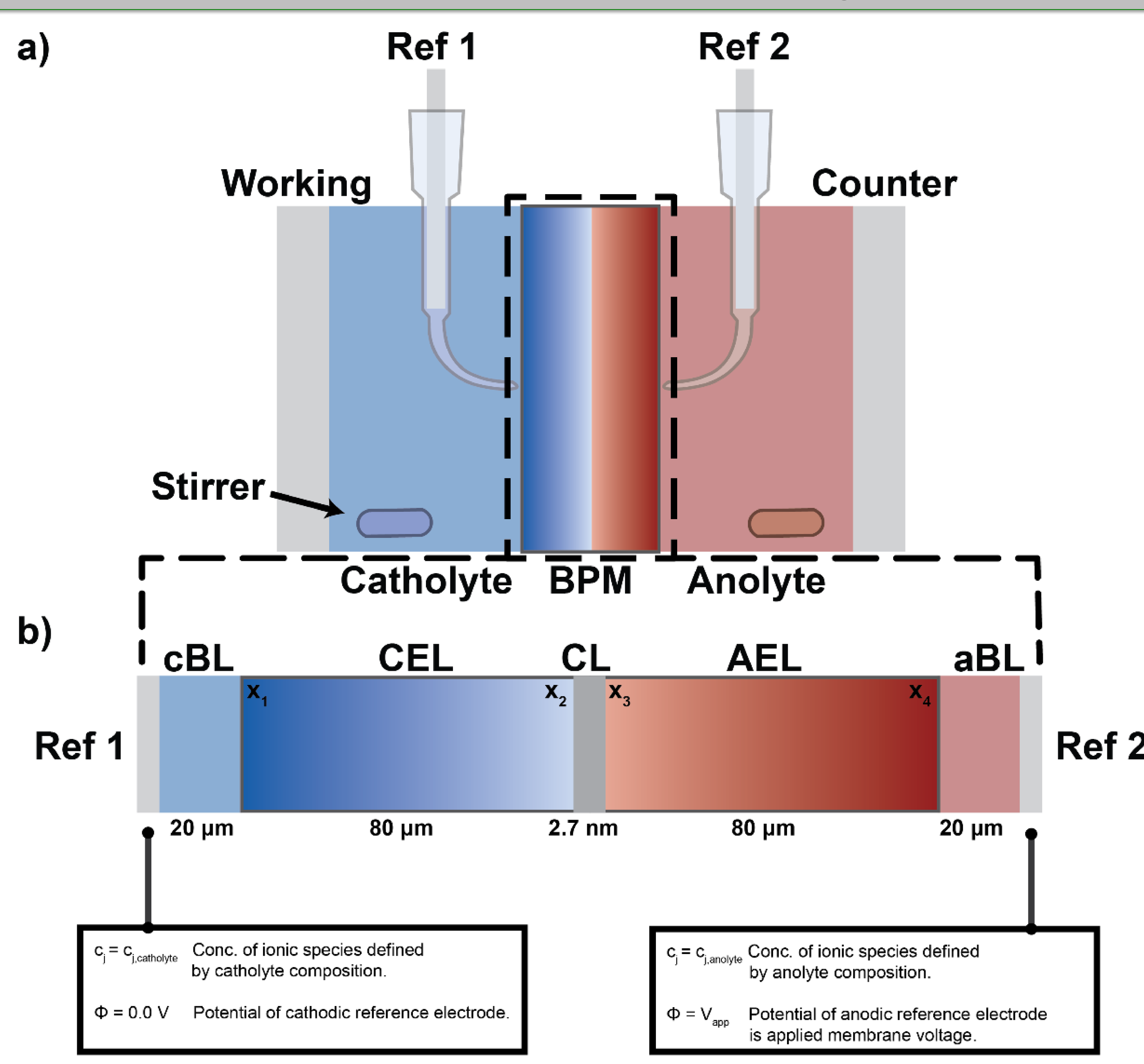
- Energy from renewable sources has become substantially **less expensive** and **more prevalent.**
- We can harness this energy to convert **affordable feeds** (water, air, CO_2) into **value-added chemicals and materials.**
- Many devices are limited by **expensive catalysts** or exhibit other **inefficiencies.**
- To reduce inefficiencies and lower cost, we can use a **bipolar membrane**, which enables device operation in environments most conducive to efficient use of **affordable catalysts.**
- We **simulate** a BPM to **optimize its performance** for a variety of different chemistries.

Acknowledgments

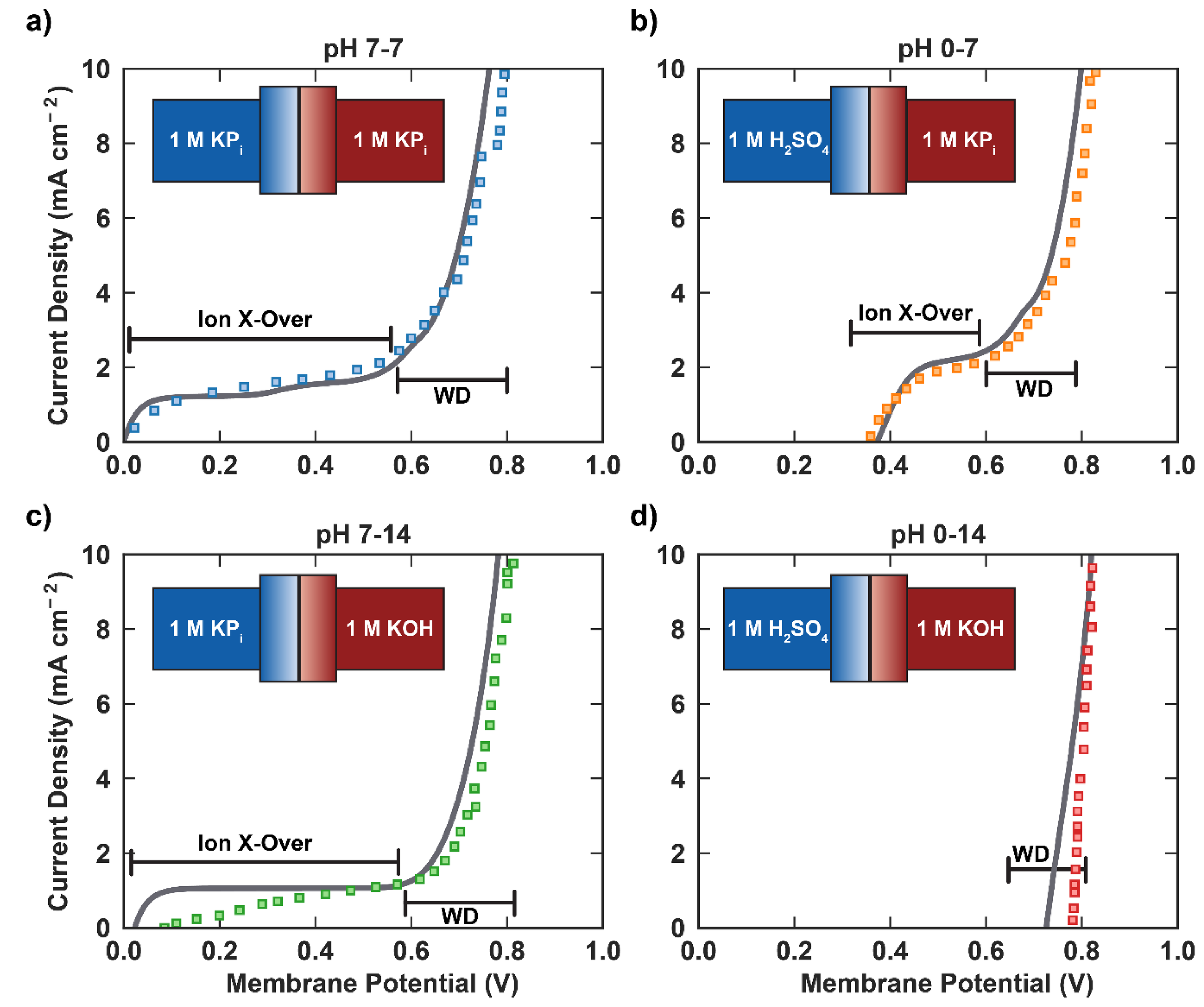
This material is based upon work performed by the Joint Center for Artificial Photosynthesis, a DOE Energy Innovation Hub, supported through the Office of Science of the U.S. Department of Energy under Award Number DE-SC0004993. JCB also acknowledges funding from the National Institutes of Health under Grant No. S10OD023532 and the National Science Foundation Graduate Research Fellowship under Grant No. DGE 1752814 .

Results, Highlights, and Accomplishments

Model Development and Boundary Conditions

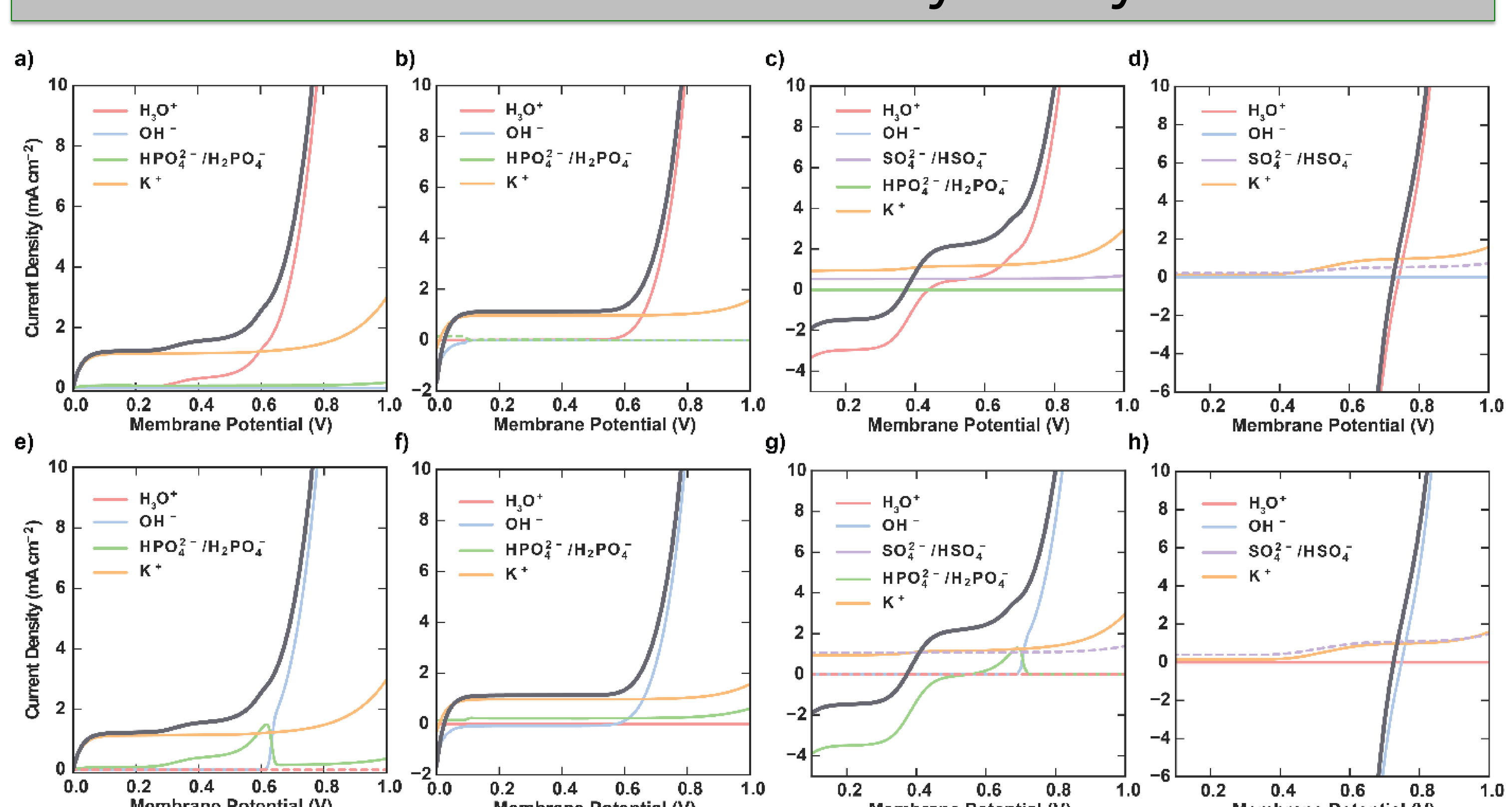


Polarization Curve Fitting



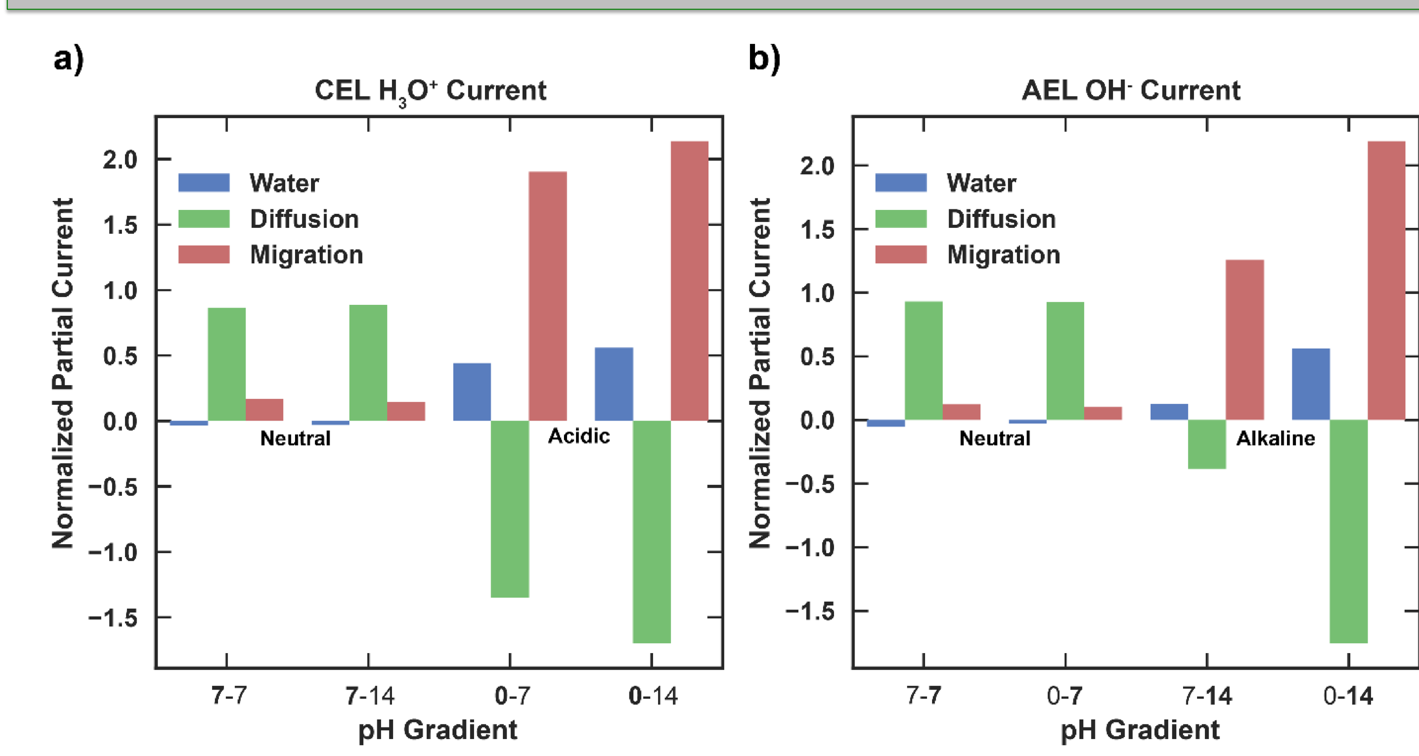
- Model displays solid agreement for **various applied pH gradients** over experimentally studied window of applied potentials.

Partial Current Density Analysis



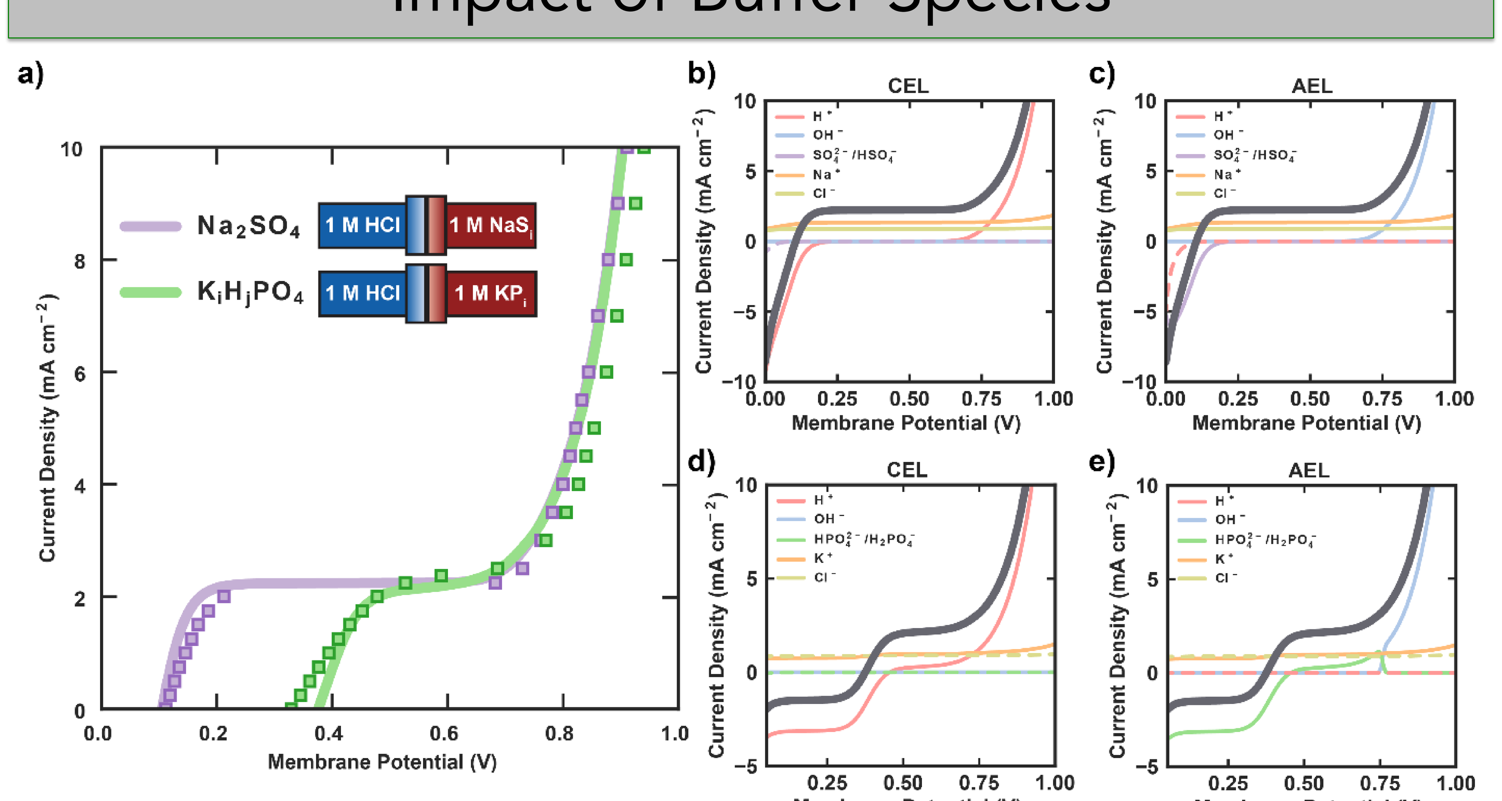
- **Salt-ion crossover** current dominates at **low applied potentials.**
- Water dissociation current density takes off **before 0.83** V.

Ion Transport Mechanisms



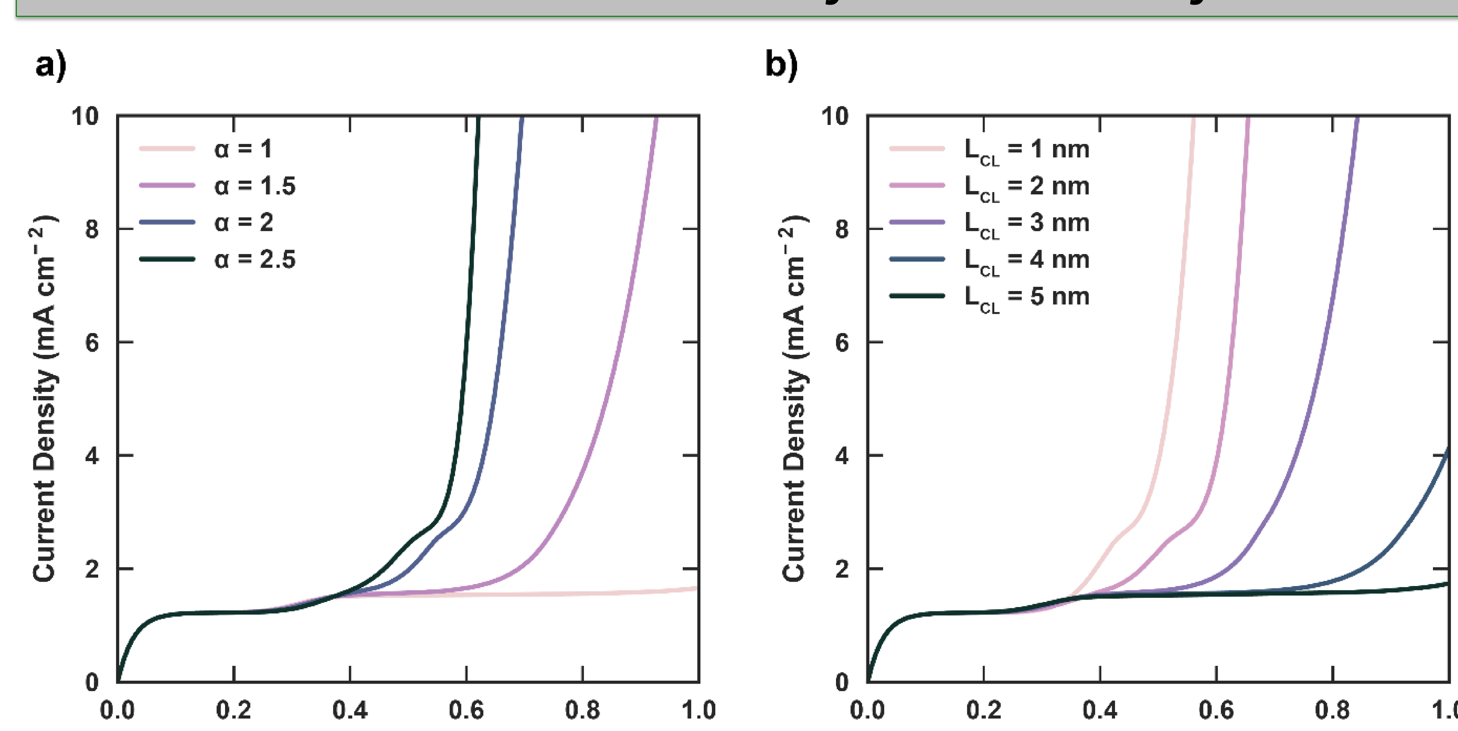
- Dominant mode of **transport depends on supporting electrolyte.**
- For highly alkaline or acidic electrolytes, dominant mode of transport is migration.
- For near neutral electrolytes, the mode of transport is diffusion.

Impact of Buffer Species



- Choice of buffer species affects measured open circuit potential.
- **Internal titration currents** heavily impact measured current densities at low potentials.

Dissociation Catalyst Sensitivity



- Water **dissociation catalyst is necessary** to achieve high currents.
- Will need **more effective, thinner catalyst layers** for optimal performance.