Finite Element Analysis of Bipolar-Electrochemistry based Water Sensor

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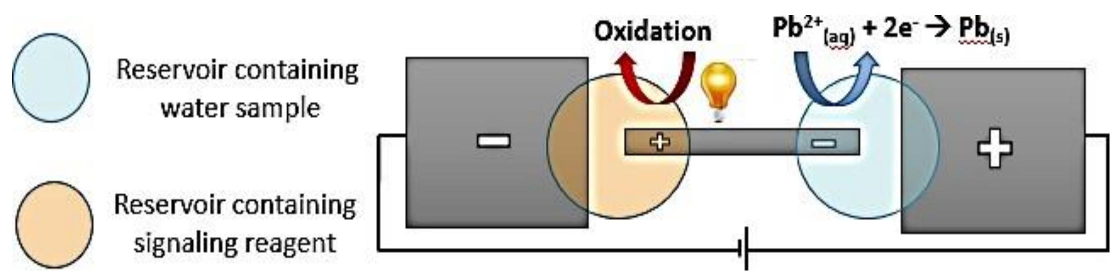
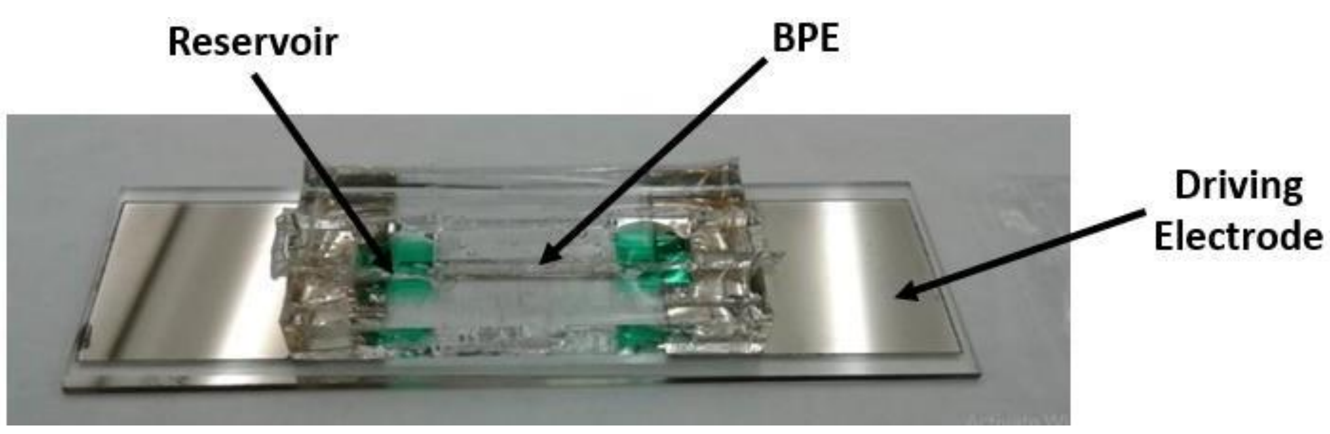
Motivation

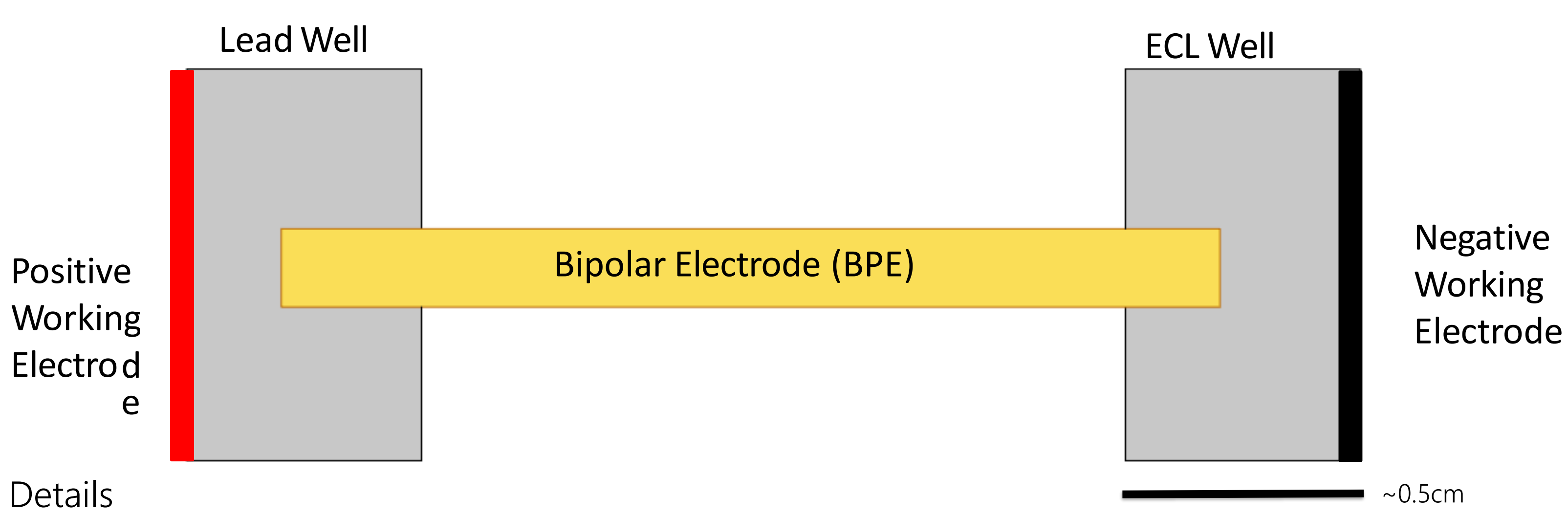
Bipolar Electrochemistry is an emerging and increasingly popular area of research with many potential applications. A promising technique uses what is known as "Closed-Cell" Bipolar-Electrochemistry (BPE), in which two sets of electrochemical processes are physically isolated from each other, having only an electrode allowing current flow in between. In the context of the Flint Water Crisis, the need for accessible water sensors is highlighted. This laboratory set on to create such a device with the principles of Bipolar Electrochemistry and Cathodic Electrochemiluminescense.





The Model

The prototype was modelled utilizing COMSOL Multyphysics 5.3a



Details
-2D Geometry
-Secondary Current Distrbution coupled with Transport of Dilluted Species
- Depositing/Dissolving Species at lead side of BPE.
- Time Dependent Study (no initialization)
-Electroneutrality Assumption
-Concentration-dependent Kinetics
-Electrode-Electrolyte interfaces defined at boundaries, insulation elsewhere.

Properties Modelled and Results

Many crucial aspects of this technique have not been studied, and further understanding of underlying aspects of Closed-Cell BPEs is needed to optimize designs and maximize usefulness of applications.

Potential Drop Across the BPE and at the BPE/Electrolyte interface.

A. B.

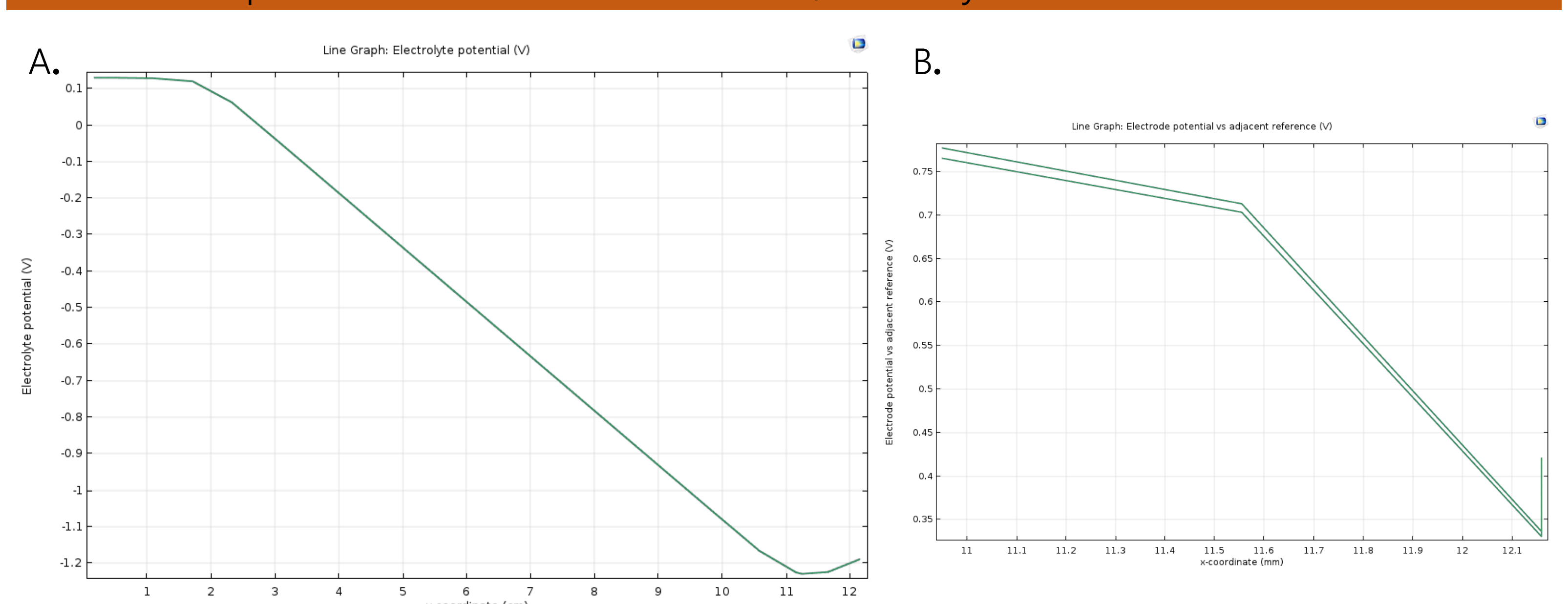


Figure A) Potential Drop Across BPE B) Potential Drop Across ECL side of BPE

Determinants of Line of Zero Potential (LZP)

C.

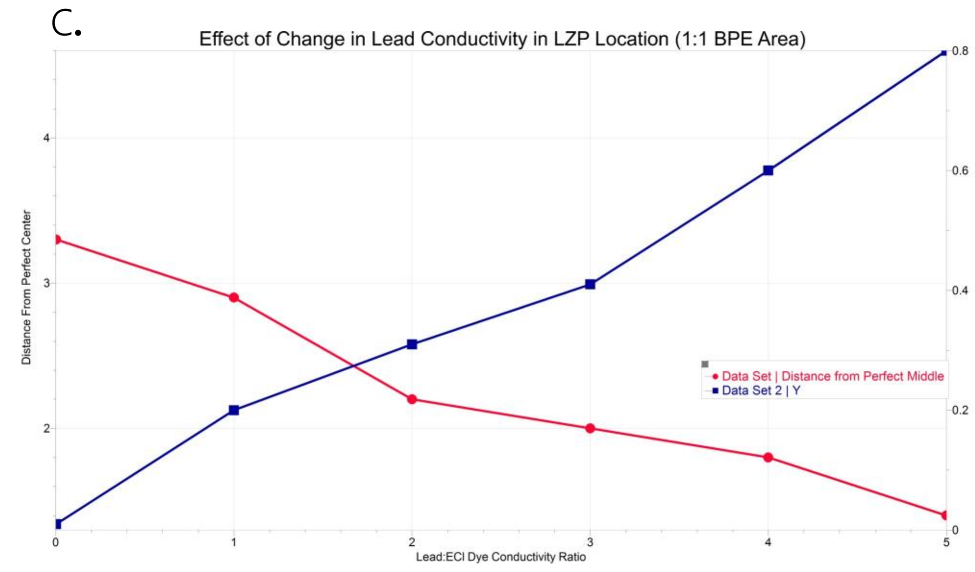


Figure C) Effect of Change in Ratio of Conductivities of Electrolytes in LZP Location (deviation from perfect center).

D.

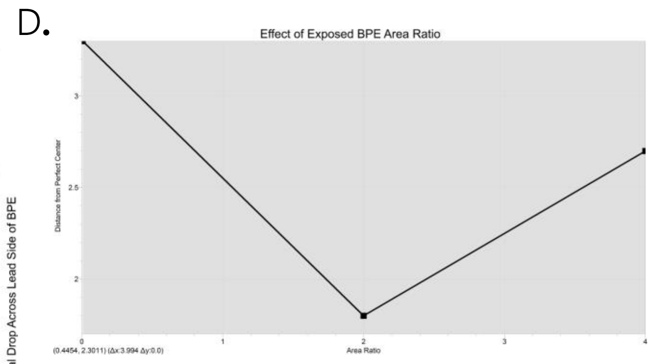


Figure D) Effect of Change in Ratio of Exposed BPE in LZP Location (deviation from perfect center).

Others: Type of Electrode Kinetics (ie. concentration of active species and presence/absence of Supporting Electrolyte)

Geometric Considerations (size and shape).

E.

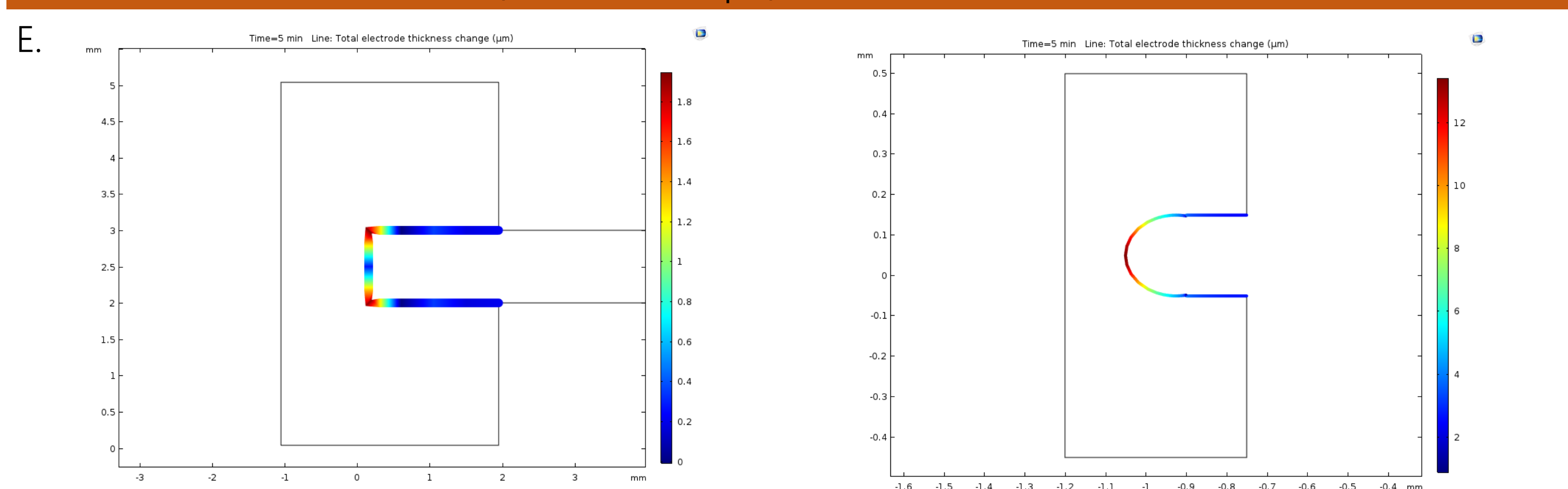
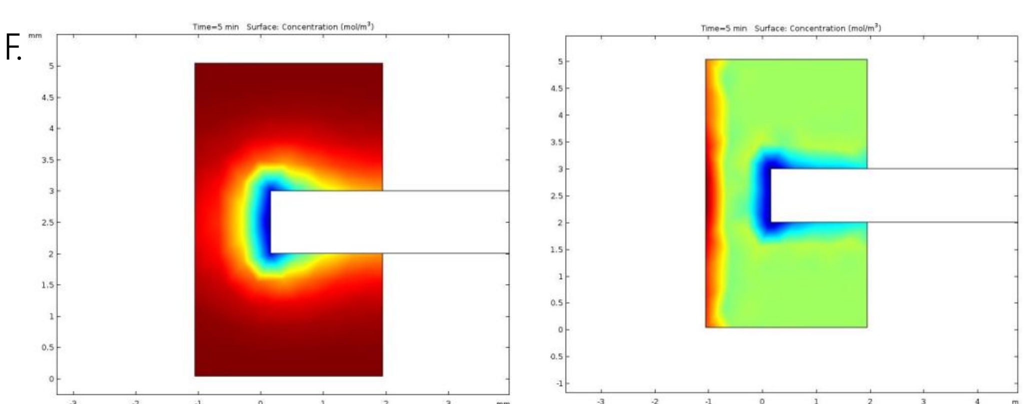


Figure E) Comparison of Potential Distribution in Different-Shaped BPEs irrespective of size (round BPE is 4.5x smaller, same voltage.

Chemical Considerations

F.



G.

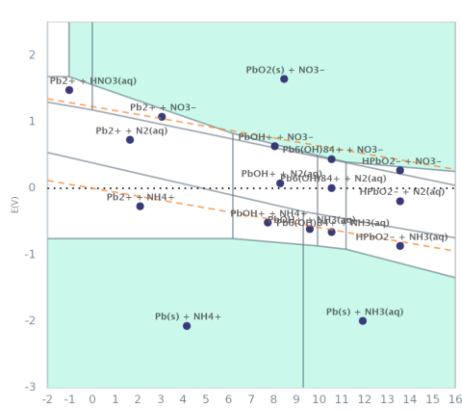


Figure F) Comparison of Pb^{2+} distribution at pH 7 and measured pH (4.3) at 5V
Figure G) Pourbaix Diagram of Lead Electrolyte.

Physical Considerations

H.

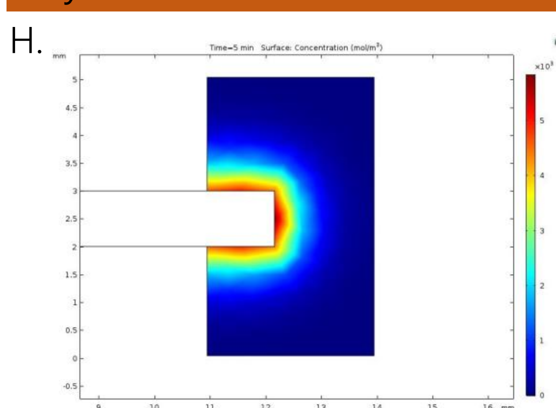


Figure H) Localizing Effect of very large Conductivities.

I.

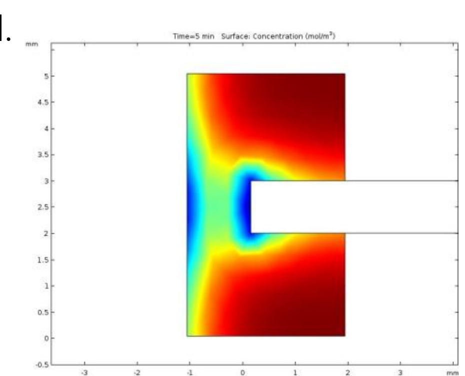


Figure I) Diffusion issues with multiple active species in constrained space

Discussion

-The discrepancy between the model and the experimental data, primarily on the ECL side point to the fact that the chemistry is very complicated and more than one reaction is occurring at the potential applied (besides the limitations faced when constructing the model). The model provides a framework for testing further ideas on cathodic ECL. 3D Modelling would also improve accuracy.

-Experimental validation and theory development are not too complicated and would greatly benefit the BPE field. In particular, experimentation with determinants of LZP would be particularly insightful.

References & Acknowledgements

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