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Lithium-Oxygen Batteries - A Comprehensive Finite Element Model

Martin Ayers and Dr. Hsiao-Ying Shadow Huang
Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, NC

Introduction and Background

The Needs for Li-O_2 Batteries:

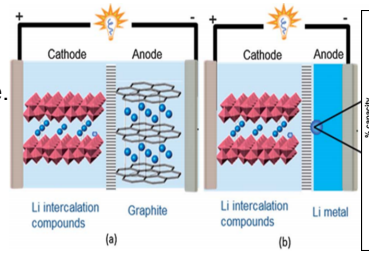
- Li-O_2 batteries possess 6-10 times greater energy densities compared to Li-ion batteries.
- Great for electric vehicles (EVs) or plug-in hybrid vehicles (PEHVs)
- Many energy potential energy storage uses.

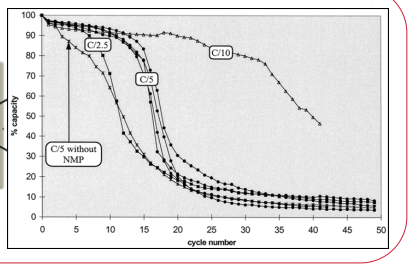
Motivations:

- Dendrite structures grow on anode surfaces.
- Precipitate growth in cathode leads to passivation.
- Identify determinant factors affecting battery performance.

Characteristics of Lithium-Oxygen Batteries:

- Utilizes a lithium metal anode.
- Carbon nanotube cathode structure.
- Oxygen enters and exits the cathode through an oxygen permeable membrane as needed.





Methods and Results

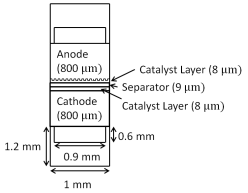
Fuel Cell Module ➔ Lithium-Oxygen Model

Anode Reactions

$$H_2 \longleftrightarrow 2H^+ + 2e^- \qquad 2Li \longleftrightarrow 2Li^+ + 2e^-$$

Cathode Reactions

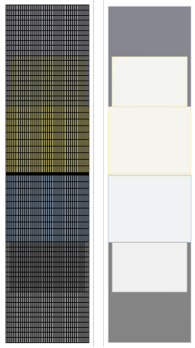
$$\frac{1}{2}O_2 + 2e^- + 2H^+ \longleftrightarrow H_2O \qquad O_2 + 2e^- + 2Li^+ \longleftrightarrow Li_2O_2$$



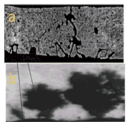
- Construct models of Li_2O_2 batteries with Fuel Cell module within ANSYS Fluent.
- Create models with dendrite growths of different lengths on anode surface.

A Comprehensive Finite Element Model

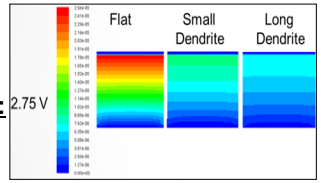
- Simulated discharge in theoretical models to observe several battery parameters such as anode homogeneity, mass fraction of oxygen, mass flow rate of oxygen, and cathode porosity, and their effects on battery discharge.
- Theoretical battery cells discharged at different voltages and their characteristics and performance were compared.
- Total of 150 battery finite element models tested from 2.75 V to 2.6 V.

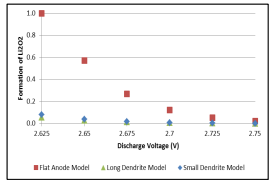


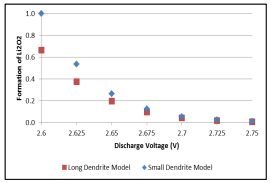
Anode Homogeneity:

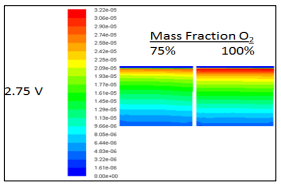


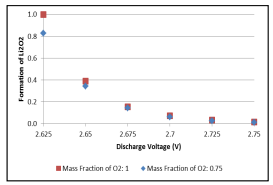
Mass Fraction of O_2:

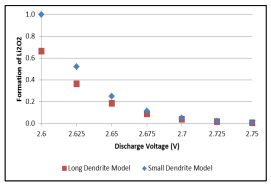












Discussions and Conclusion

- Found the anode homogeneity affected the discharge parameters of our lithium-oxygen battery greater than porosity or mass fraction of O_2.
- Cathode parameters (mass flow rate of O_2, mass flow rate, porosity) affected the performance of the battery cell to a lesser degree compared to the anode homogeneity.
- Lithium dendrite growth continues to pose a significant problem in the commercial development of lithium-oxygen batteries.
- Model can be further developed to incorporate differing reaction rates, different dendrite structures, dendrite spacing, and cell cycling (charging and discharging).

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