# Development and Analysis of Solid-State Batteries through Implementation of the COMSOL® Platform

R. Acacio[1], J. Neyra[1], S. Miorana[1], T. Garrison[1], C. Coddington[1], C. Scaduto[1], K. Baldwin[1], R. Integlia[1]
1.Florida Polytechnic University, IEEE Student Branch, Lakeland, FL. United States

**INTRODUCTION**: The objective is to investigate a variety of means by which COMSOL can be utilized to compare the effects of electrolyte potential, C-rates, and surface lithium ion concentration within a solid-state battery when modifying the dimensions of both an electrolyte and electrode. Simulations were conducted for several cases to determine the most desirable dimensions for battery components. Using COMSOL can reduce trial and error in the laboratory, which requires much greater resources and time.

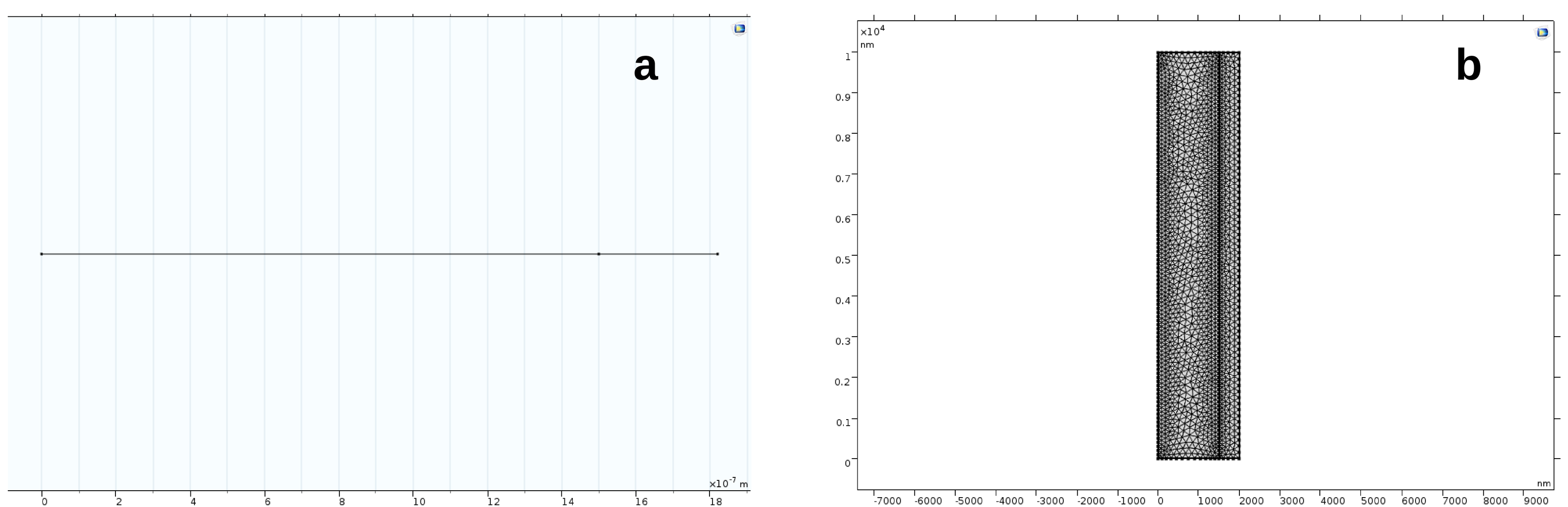
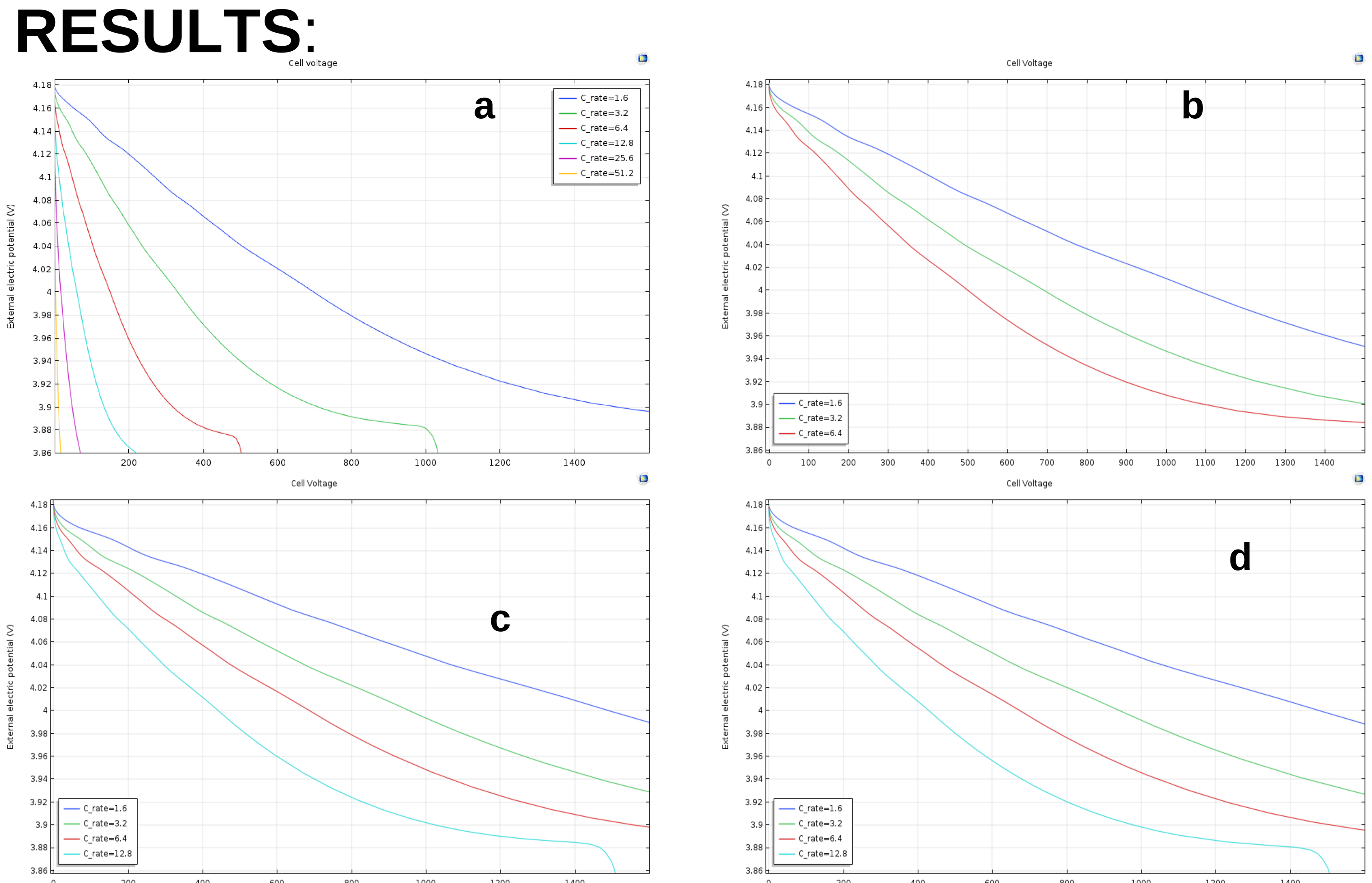



**Figure 3**. One-dimensional Solid State Battery (a) versus Two-dimensional Solid State Battery (b)

**Historical Background and Reasons for use of Solid-State Batteries:** Over the recent years, there has been an exponential demand for a higher energy storage, in which fluid typed electrolyte Lithium ion batteries aren't delivering. However, Solid State Batteries have been shown since the 1950's[1] to possess a higher energy density than fluid typed Lithium ion batteries. Solid State Batteries possess a solid electrolyte, proven to be much more eco-friendly, less flammable, and more durable than traditional fluid electrolyte based Batteries. Due to advancement in computer database, there has been an expensive influx in utilizing powerful software tools in performing stimulus runs. Using COMSOL allows for all the material to be tested before laboratory work, saving both time and yielding more reasonable results.

**COMPUTATIONAL METHODS**: Initially a one-dimension model of solid state was evaluated, to inspect the performance and functionality of this. However, a more reasonable and realistic approach was needed to test solid state batteries, but it allowed for a reference and baseline in further dimensions in working with the battery on the software. The solid- state battery was examined at a 2-Dimension model. In the stimulus run, electrochemical process was examined using positive electrode and electrolyte; however, the negative electrode was presumed to have a high conductivity. Certain parameters were set to have constant values, such as thickness of electrolyte, electrode, charge transfer coefficient, initial lithium concentration. For both the one-dimensional and two-dimensional simulations, it ulitized a solid $Li_3PO_4$ electrolyte and $LiCoO_2$ electrode. Various studies were performed to calculate electrolyte potential, C-rate, and surface concentration. Physics and electrochemical interfaces were used to calculate on Tertiary Current Distribution (TCD) in the positive electrode, and Transport of Diluted Species (TDS) in the electrolyte. Exceptional fine mesh was use to maximize accuracy and yield higher quality device to extricate information from.

**RESULTS**:




**Graph 1:** This illustrates the cell voltage over time, a is one-dimension, b is Case 1 two-dimension 1500 nm² and Electrolyte 500 nm² Electrode, c is Case 2 two dimension 900 nm² Electrolyte and 700 nm² Electrode, d is Case 3 two dimension 1500 nm² Electrolyte and 700 nm² Electrode.

The results of the various one-dimensional and two-dimensional solid-state simulations exhibit similar, but still distinct behaviour. Analysis of the cell voltage data shows a much more gradual descent of the external electric potential in the two-dimensional batteries. The graphs of the one-dimensional battery, however, show discharge rates of 6.4 V and 3.2 V dropping suddenly as they approach 0 seconds, while 1.6 V continues past 3.919 seconds. The two-dimensional batteries, conversely, show discharge rates continuing past 1600 seconds for these potential measures, indicating that it holds external electric potential for longer than the one-dimensional battery. The electrolyte transfer data suggests there are slight differences between the cases of the two-dimensional batteries, the primary distinction being the initial and terminal values of voltage. A larger electrolyte generally correlates to a broader the range of voltages, which is a possible signifier that the battery has a larger capacitance. The effects of slight changes in geometry were evidenced in discharge rate and the range of voltage, but were overall minimal and nondisruptive towards general performance.

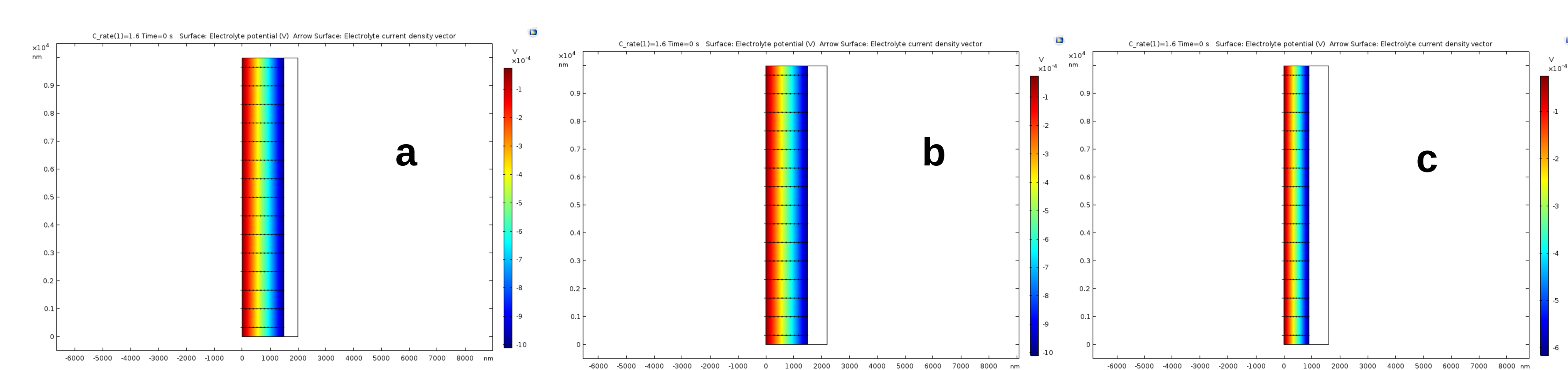



**Figure 4.** Electrolyte surface concentration of Lithium ions: Case 1, 2, and 3 represent a,b,c respectively

**FUTURE RESEARCH:**

The findings of these simulations provide a basis to investigate two-dimensional devices utilizing other COMSOL modules, and gives insight into the means necessary for the development of a three-dimensional solid-state battery. Finite element analysis can allow study of potential materials to compose a solid-state battery; furthermore, materials can be synthesized using extrapolated data to produce a superior alternative to current solid-state batteries.

**CONCLUSIONS**: Using COMSOL, a two-dimensional model of a lithium-ion solid-state battery could be created and used to generate accurate simulations of battery physics. Three two-dimensional solid-state batteries, each with electrodes of different sizes, were analyzed to compare the cell voltage and electrolyte ionic surface concentration. The two-dimensional battery Case 2 reached its maximum activity value of solid lithium concentration at higher time than compared to Case 1 and Case 3. This suggests that a solid-state battery with a smaller electrolyte layer may be best suited for future research, since the maximum activity value for solid lithium in the positive electrode is the maximum level of solid lithium the electrode is able to contain. A comparison of the electrolyte surface concentration indicates that the two-dimensional solid-state battery Case 3 with a 1500 nm² Electrolyte and 700 nm² Electrode has the greatest potential where the electrolyte and electrode meet. A solid-state battery matching these dimensions should be used for future research.

**REFERENCES**:

1.Owens B. and Munshi M., History of Solid State Batteries, Office of Naval Research, (1987)
2.The COMSOL Group, *All-Solid-State Lithium-Ion Battery*, COMSOL inc., Application Gallery