End Term Report: Sodium Ion Battery

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Introduction:

The primary objective of the project is to analyse and model the Sodium ion Battery. A study has been done on a research paper working on the development of a Single Particle Model (SPM) for sodium-ion batteries (SIBs), offering a computationally efficient alternative for the conventional P2D model, which is accurate but comes with a huge computational constraint. Understanding the model and its implementation is essential for future work in battery simulation, design optimization , and developing complex battery management systems.

A 1D isothermal sodium-ion battery model was modelled using COMSOL Multiphysics 6.3, following the official application library documentation. From this model, solid and liquid phase currents, overpotential of both the electrodes and reaction current was extracted to further plot the Heat flux and energy using MATLAB.

Implementation of a piecewise function on this 1D isothermal sodium-ion battery model was also done to obtain cell voltage and current density relation with respect to time for different load cycles, i.e., for charge and discharge cycles, similar to that of a Lithium ion battery model.

Summary of Research Paper:

(https://iopscience.iop.org/article/10.1149/1945-7111/acb01b/pdf)

The paper introduced a reduced-order electrochemical model based on single-particle assumptions for SIBs. It simplifies complex electrochemical processes while maintaining predictive accuracy for key battery parameters such as terminal voltage and electrode potentials. The model was validated by comparing its results with experimental data and the P2D model for various discharge conditions.

Key Findings and Results of Research Paper:

- Accuracy of Predictions:
    - The SPM showed a maximum terminal voltage error of 1.78%
    - Accurate predictions for negative electrode voltages; slightly larger deviations for positive electrode voltages at higher discharge rates
- Performance Across Current Densities:
    - Results aligned with experiments through discharge rates from 1 to 12 A/m²
    - Minor deviations observed at higher currents accounting for neglected concentration polarization.
- Comparison with P2D Model:
    - SPM predictions closely match P2D results, confirming the model's reliability along with improved computational efficiency.
- Practical Implications:
    - The model is computationally efficient, making it suitable for generating design iterations and error handling for complex battery management systems.

Methodology for 1D Sodium Ion Battery Model:

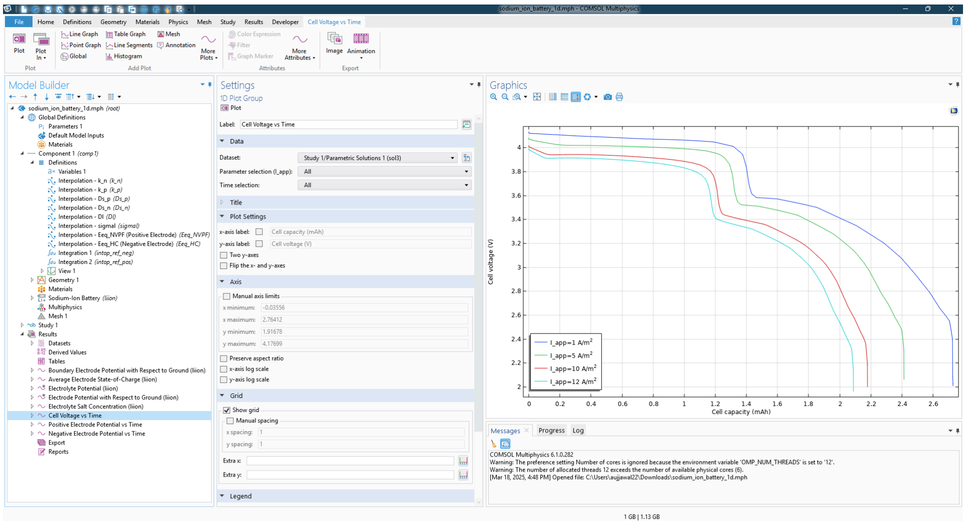
- Software Used : COMSOL MultiPhysics 6.3
- Battery modelled as a 1D cross-section:
    - Negative porous electrode: 64 µm
    - Separator: 25 µm
    - Positive porous electrode: 68 µm
- Key model inclusions/assumptions:
    - Electronic and ionic conduction
    - Mass transport within electrode particles
    - Butler–Volmer kinetics
- Materials used:
    - Negative electrode: Hard carbon (HC - Li_xC_6)
    - Positive electrode: NVPF ($Na_3V_2(PO_4)_2F_3$)
    - Electrolyte: 1.0 M $NaPF_6$ in EC:PC (1:1 by weight)
- Boundary Conditions:
    - Negative terminal grounded at 0 V.
    - Average current density applied at the positive terminal.
    - Contact resistances included at both terminals.
- Simulations run for discharge rates: 1, 5, 10, and 12 A/m²
- End-of-discharge voltage: 2 V

Results:

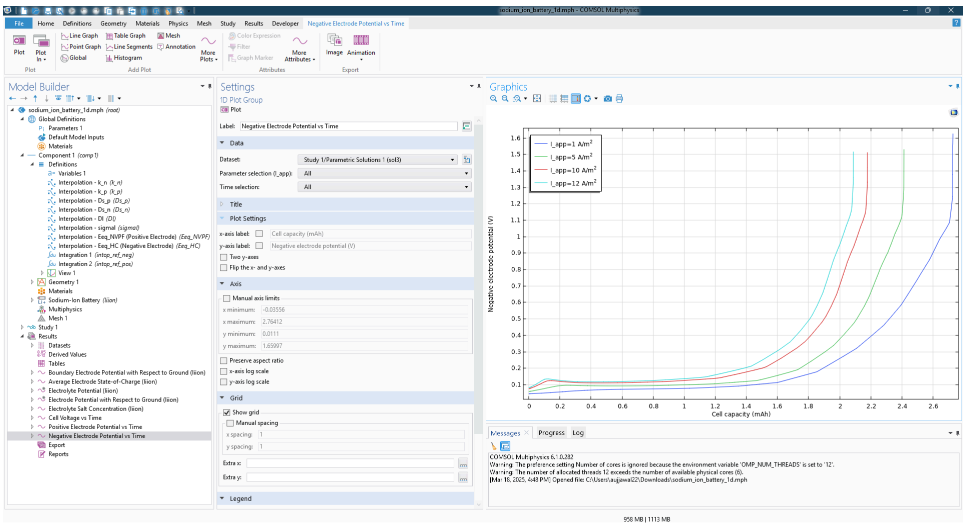
- Voltage vs. Capacity curves obtained.
- Higher discharge rates resulted in quicker voltage drops and reduced overall capacity.
- Positive electrode potential was found to be negatively correlated with capacity.
- Negative electrode potential was found to be positively correlated with capacity.

Graphs:

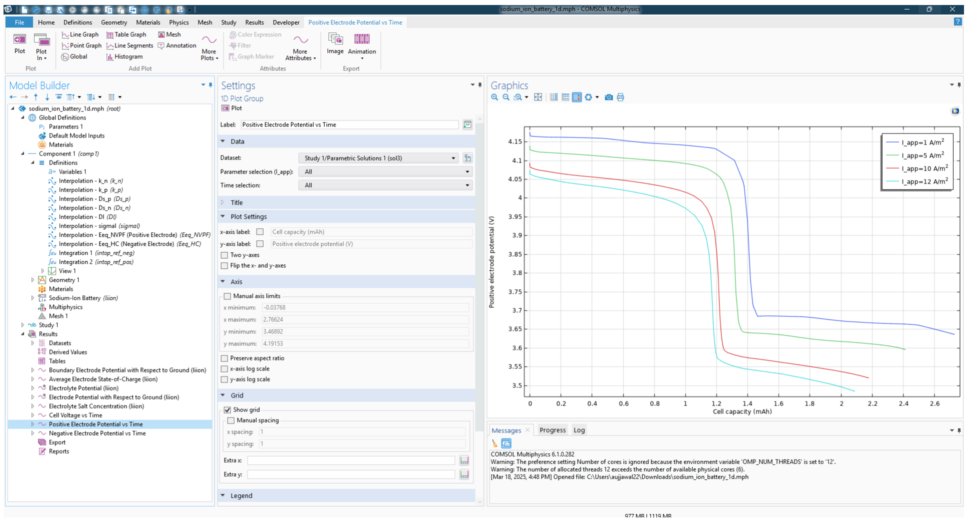
1. Cell Voltage v/s Cell Capacity:



2. Negative Electrode Potential v/s Cell Capacity:

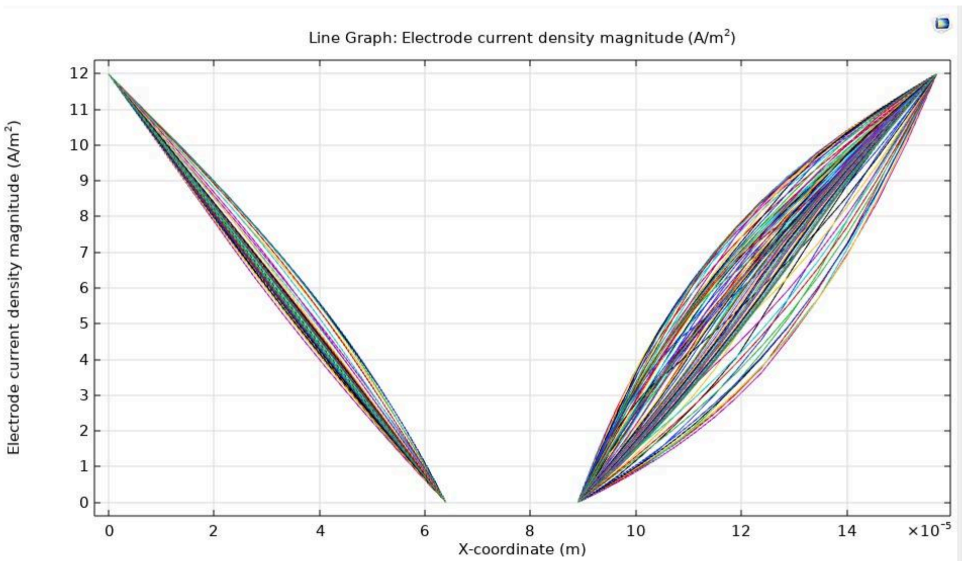


3. Positive Electrode Potential v/s Cell Capacity:

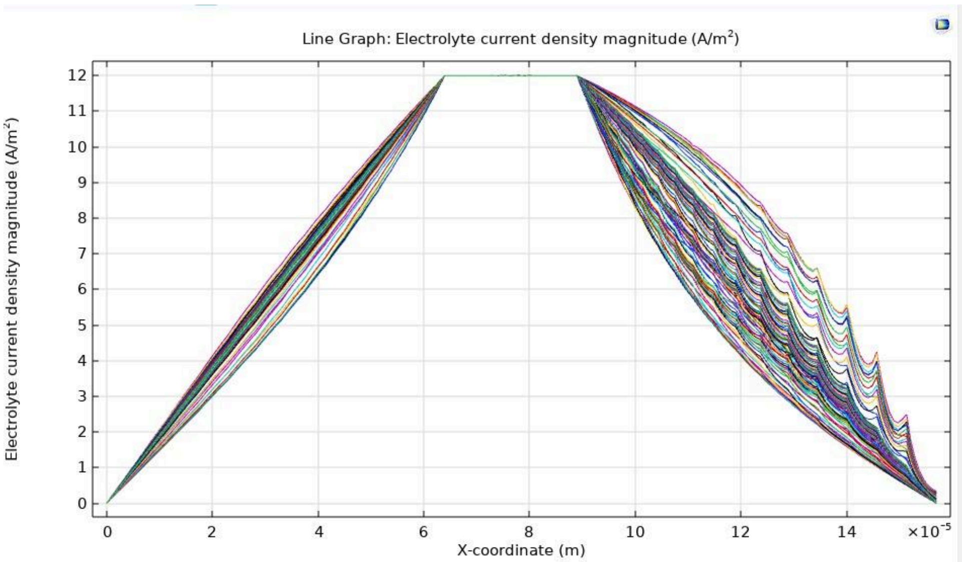


Extracted Variables:

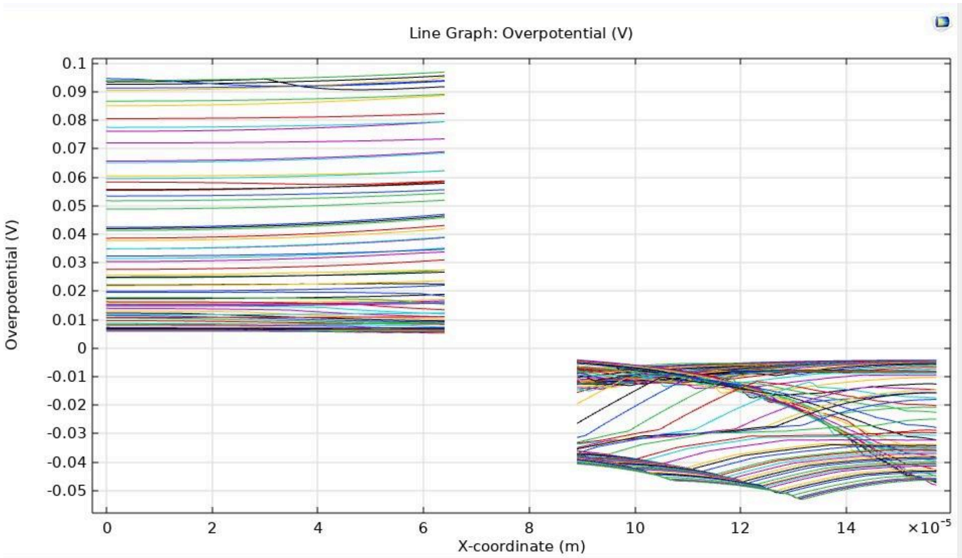
1. Electrode (Solid Phase) Current Density:



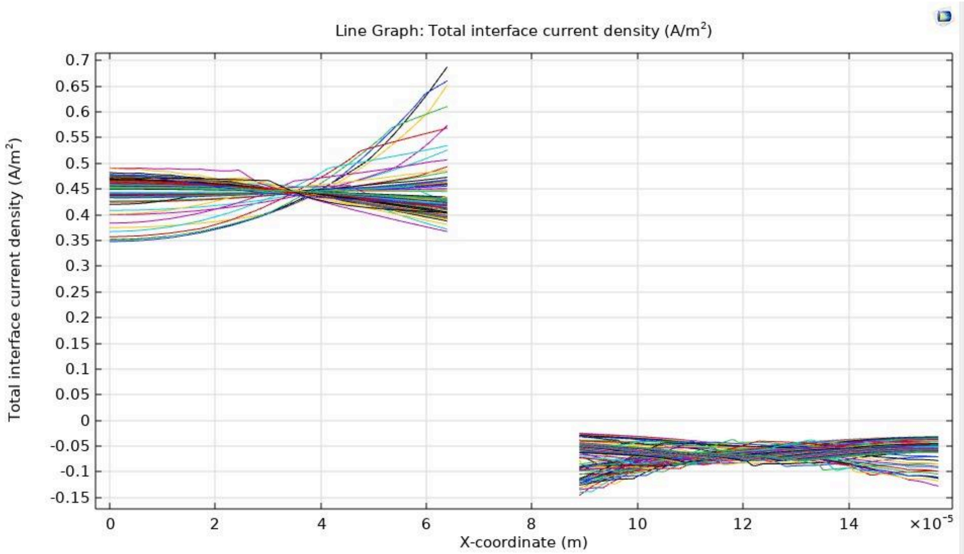
2. Electrolyte (Liquid Phase) Current Density:



3. Overpotential:



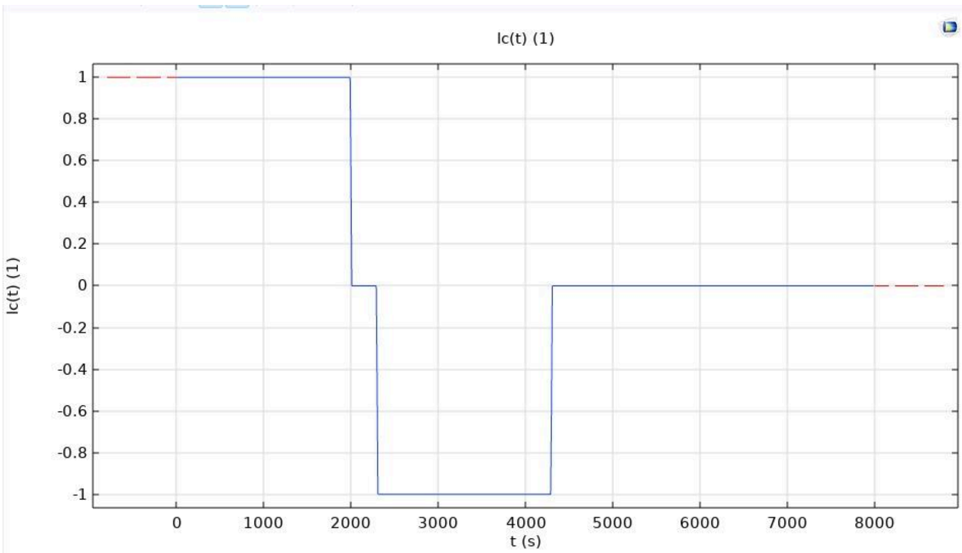
4. Reaction Current:



Piecewise Function:

The simulation cycle consists of the following sequence:

- Discharge Phase: 2000 seconds at nominal current density
- Rest Phase: 300 seconds under open-circuit conditions
- Charge Phase: 2000 seconds at nominal current density
- Final Rest Phase: Open-circuit conditions



Conclusion:

The project successfully modeled a 1D isothermal sodium-ion battery using COMSOL Multiphysics 6.3, focusing on fundamental electrochemical behaviors. Key variables such as solid and liquid phase current densities, overpotential, and reaction current were extracted for a single load cycle to understand the internal dynamics of the battery. Additionally, a charge-discharge cycle was implemented using a piecewise function to simulate realistic operational conditions. This work provides a strong basis for extending the model to more complex load profiles and for further studies in battery performance analysis and optimization.