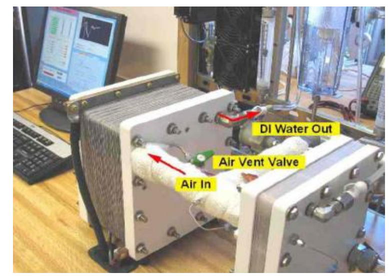
Research on High Power Battery for power system



Auburn University
Mechanical engineering

Advanced Propulsion Research Lab.
Director: Song-Yul (Ben) Choe

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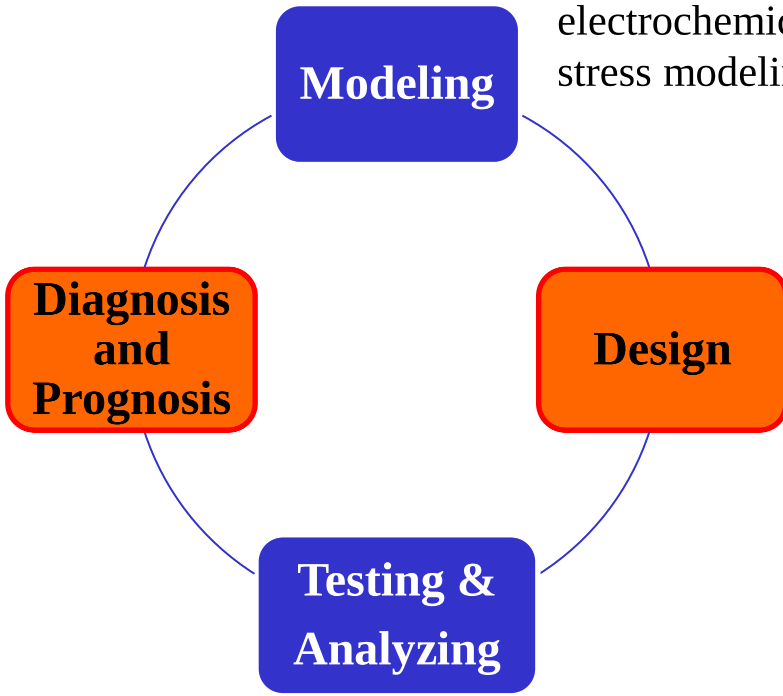
Research Areas for Lead-acid, LiPB and others

<u>Research Objectives</u>: 1) understanding physical principles, 2) solving the most important power system complex problems associated in realizing a robust, reliable, fast and high efficient charging and discharging methodology :

Multiscale and high resolution electrochemical, thermal and mechanical stress modeling

Diagnotic and prognostic methodologies using the model developed and advanced controls



1) Prototype of module and pack
2) Cooling systems with controls
3) Fast charging and discharging methodologies

Testing: 1) Terminal current and voltage profiles produced by connected generators or chargers and loads like electric machines, 2) Cell, modue and pack testing: from -30 ^{0}C to 50^{0}C temperature range under thermal cyclings, and vibrations, 3) Modul and vehicle testing, 4) XEM , SEM, XRD and others to analyze material properties.

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Model Development for LiPB:
Multi-physics and Multi-scale modeling and Validation of -
High Power Battery

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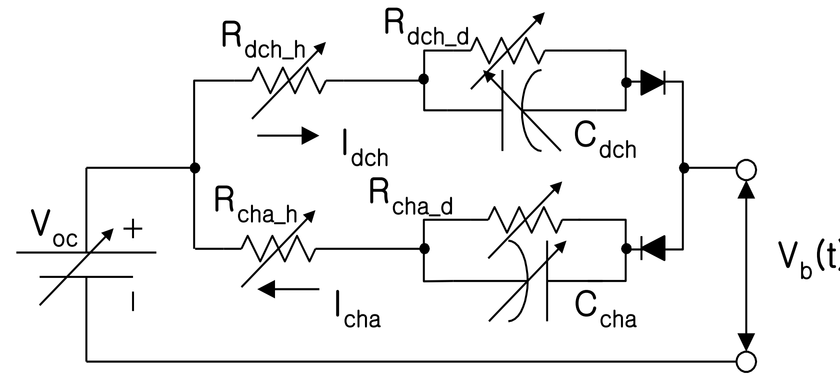
Background

- Equivalent electrical circuit
  - Statics: resistors in series to a voltage source
  - Dynamics: a capacitor connected in parallel to a resistor



Ignored effects :

1. Electrical behavior of the terminal as a function of SOC , T and material degradation, and OCV as a function of hysteresis and SOC.
2. Battery calendar life as a function of cycles and load profile
3. Heat generation as a function of SOC , change of entropy and I (charge and discharge), heat transfer
4. Various temperature effects caused by gradients of ion concentrations and side reactions

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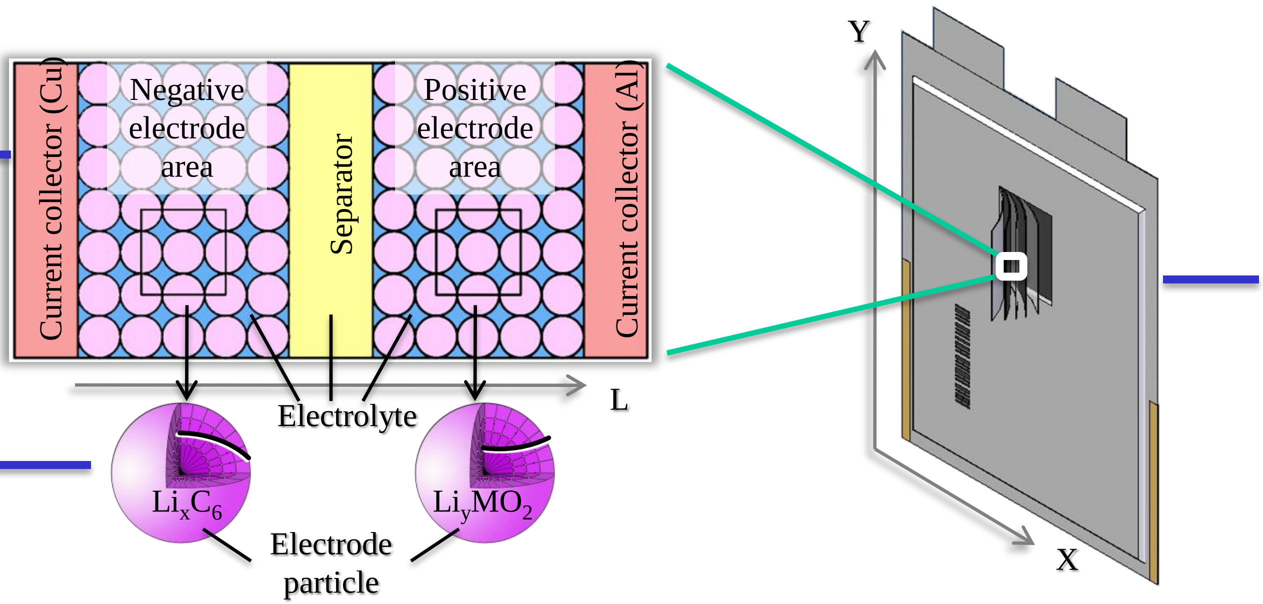
Scalable Model setup for a pouch type cell

- c_e
- Φ_e
- Φ_s
- η_{SEI}
- c_s



- T

• A pouch type cell is assumed to consist of microcells that have multiple layers in the L direction, so that the microcell is simplified with one dimensinal model.

• Once the rate of heat generation in the micro cell is calculated, the value is transferred to a two dimensional cell model, where temperature distribution is obtained. At the same time, the temperature resulted from the single cell is back transferred to the 1D microcell model and coupled with physical equations used.

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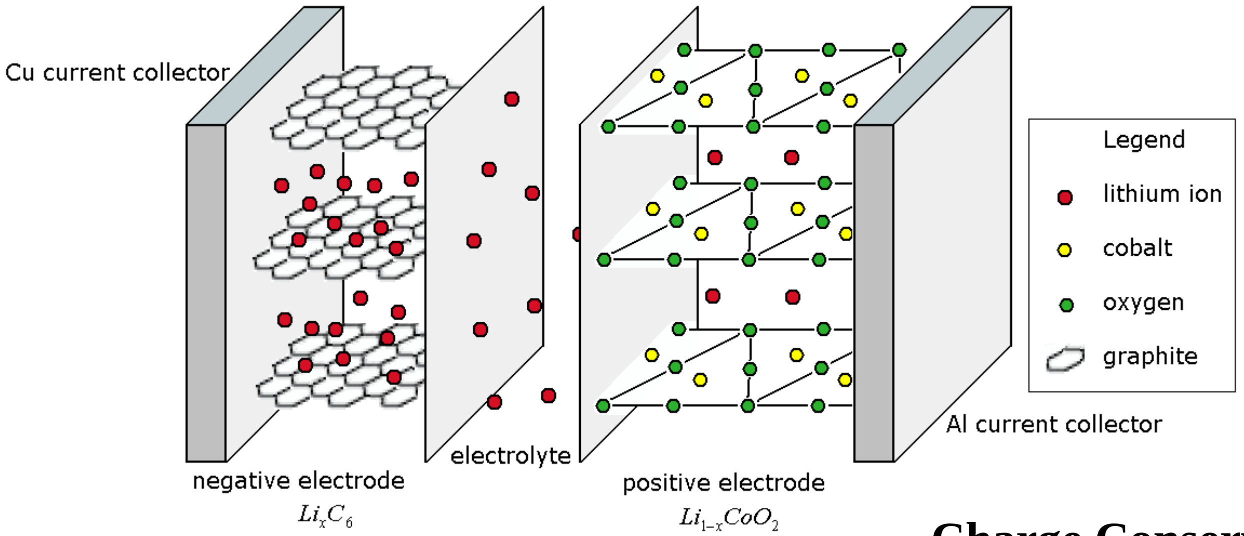
Governing equations for micro cell

Chemical Kinetics

$$j^{Li} = a_s i_0 \left\{ \exp\left[\frac{\alpha_a F}{RT}(\eta - \eta_{SEI}) \right] - \exp\left[-\frac{\alpha_c F}{RT}(\eta - \eta_{SEI}) \right] \right\}$$

$$i_0 = (c_e)^{\alpha_a} (c_{s,\max} - c_{s,e})^{\alpha_a} (c_{s,e})^{\alpha_c}$$

$$\eta = \phi_s - \phi_e - U$$



Mass Transport

$$\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial c_s}{\partial r} \right)$$

$$\frac{\partial(\varepsilon_e c_e)}{\partial t} = \frac{\partial}{\partial x}\left(D_e^{eff} \frac{\partial}{\partial x} c_e \right) + \frac{1 - t_+^0}{F} j^{Li}$$

Charge Conservation

$$\frac{\partial}{\partial x}\left(\kappa^{eff} \frac{\partial}{\partial x} \phi_e \right) + \frac{\partial}{\partial x}\left(\kappa_D^{eff} \frac{\partial}{\partial x} \ln c_e \right) + j^{Li} = 0$$

$$\frac{\partial}{\partial x}\left(\sigma^{eff} \frac{\partial}{\partial x} \phi_s \right) - j^{Li} = 0$$

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Heat transport

Heat transfer: $$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial}{\partial x} T\right) + q$$

Total sum of the heat sources: $$q = q_{rev} + q_{irr}$$

Reversible heat sources. $$q_{rev} = j^{Li} \cdot T \cdot \frac{\partial E}{\partial T}$$

Irreversible hear sources

I. The heat geneated in electrode + heat generated in electrolyte + heat generated by overpotential

$$q_{irr.1} = \sigma^{eff}\left(\frac{\partial \phi_s}{\partial x}\right)^2 + \kappa^{eff}\left(\frac{\partial \phi_e}{\partial x}\right)^2 + \kappa_D^{eff} \frac{\partial \ln c_e}{\partial x}\frac{\partial \phi_e}{\partial x} + j^{Li}\eta$$

II. Joule heating in current collector $$q_{irr.2} = I^2 \cdot R$$

III. Heat of mixing: $$q_{irr.3.} = \frac{1}{L}\int_L (\Delta U_{equ}^{+} \cdot i(r,l) - \Delta U_{equ}^{-} \cdot i(r,l))dl$$

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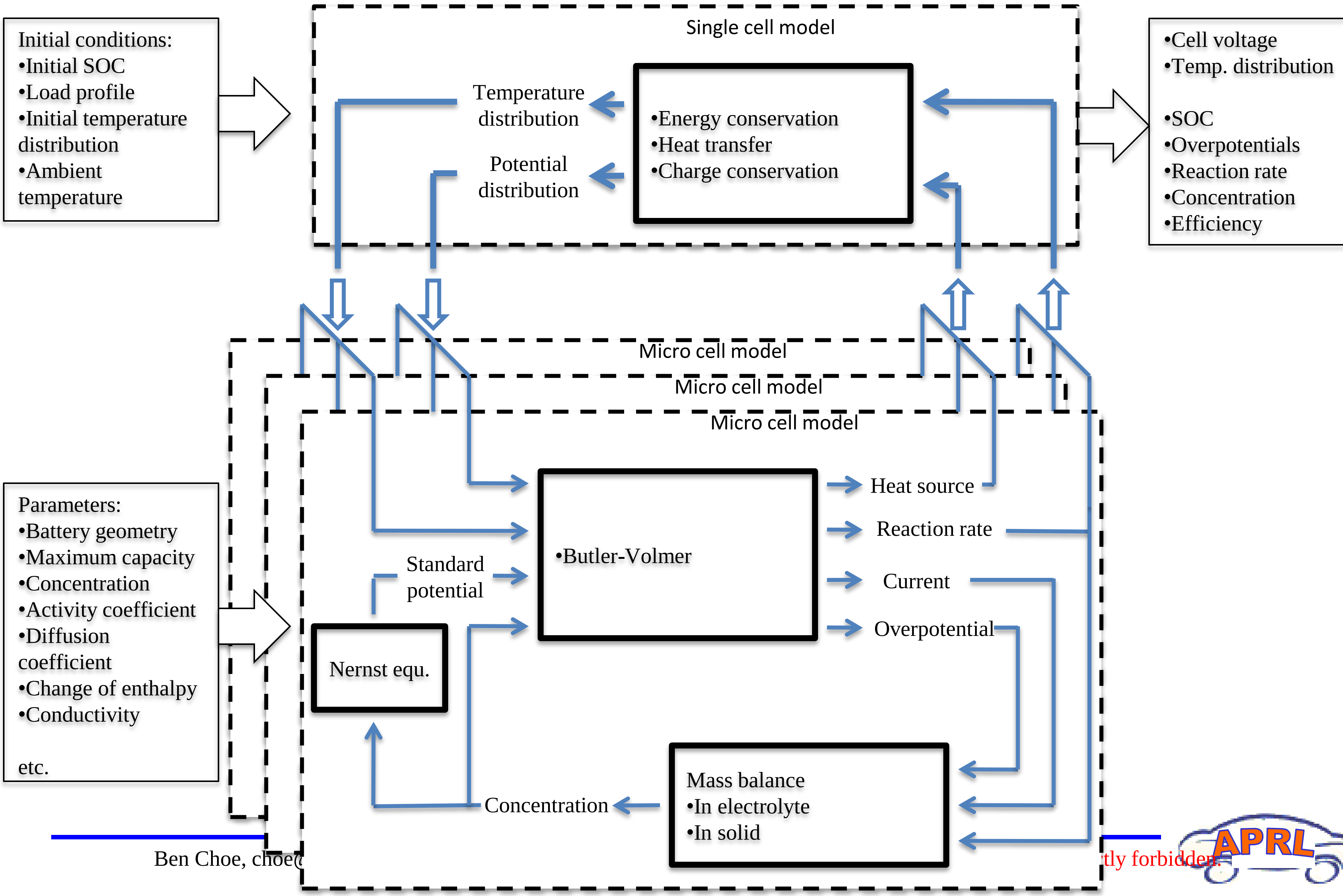
Overview of dynamic model



Modeling for a Pouch cell

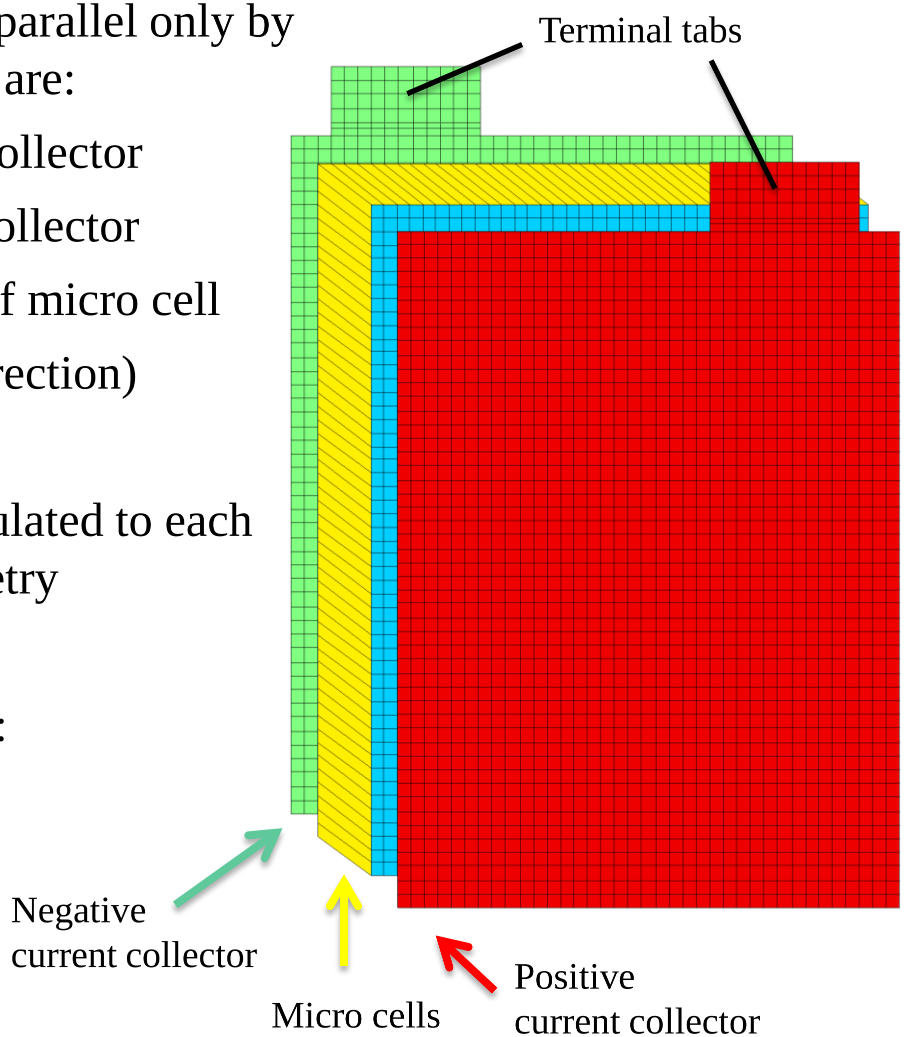
- Every grid is a micro cell, they are connected parallel only by current collectors. Variables for each micro cell are:
  - $\varphi_{cc-}(x,y)$, potential on negative current collector
  - $\varphi_{cc+}(x,y)$, potential on positive current collector
  - $V_{micro}(x,y)=\varphi_{cc+}(x,y)-\varphi_{cc-}(x,y)$, voltage of micro cell
  - $I_{micro}(x,y)$, current of micro cell (on z direction)

- All of the layers at same position (x,y) are insulated to each other but have the same state because of symmetry

- Ohm's law for potentials on current collectors:

$$\sigma_{cc-}\left(\frac{\partial^2\phi_{cc-}}{\partial x^2}+\frac{\partial^2\phi_{cc-}}{\partial y^2}\right)-\frac{I_{micro}}{l_{cc-}}=0$$

$$\sigma_{cc+}\left(\frac{\partial^2\phi_{cc+}}{\partial x^2}+\frac{\partial^2\phi_{cc+}}{\partial y^2}\right)+\frac{I_{micro}}{l_{cc+}}=0$$



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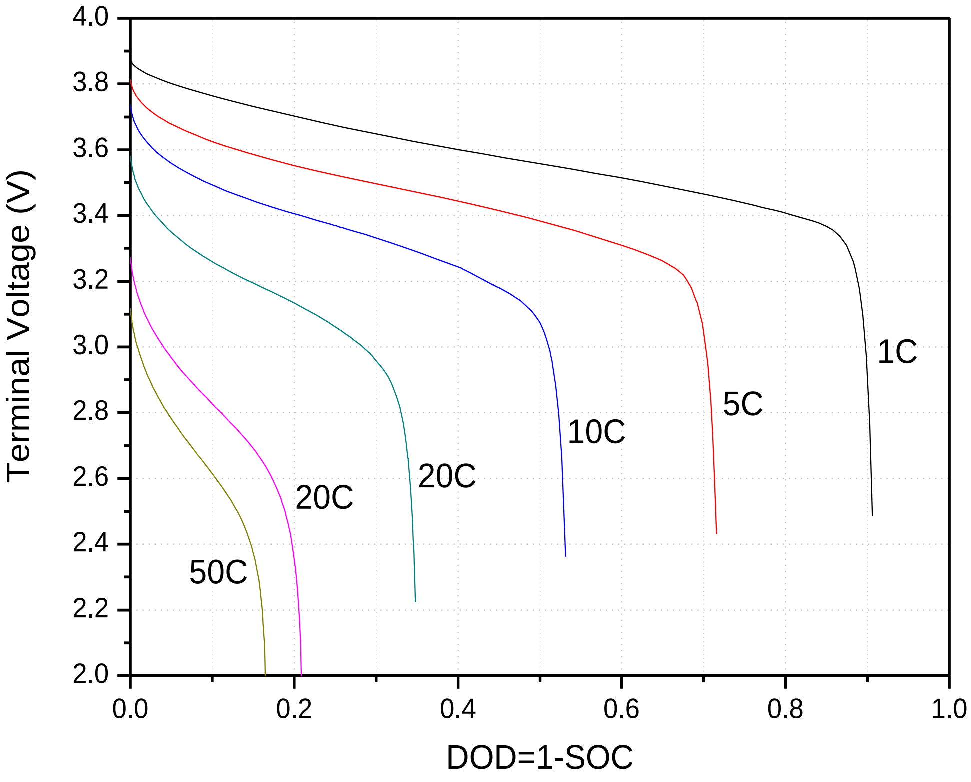
Discharge characteristics at different current

Discharge characteristics at different current rates using variable step calculation (T=300K and SOC=100%)



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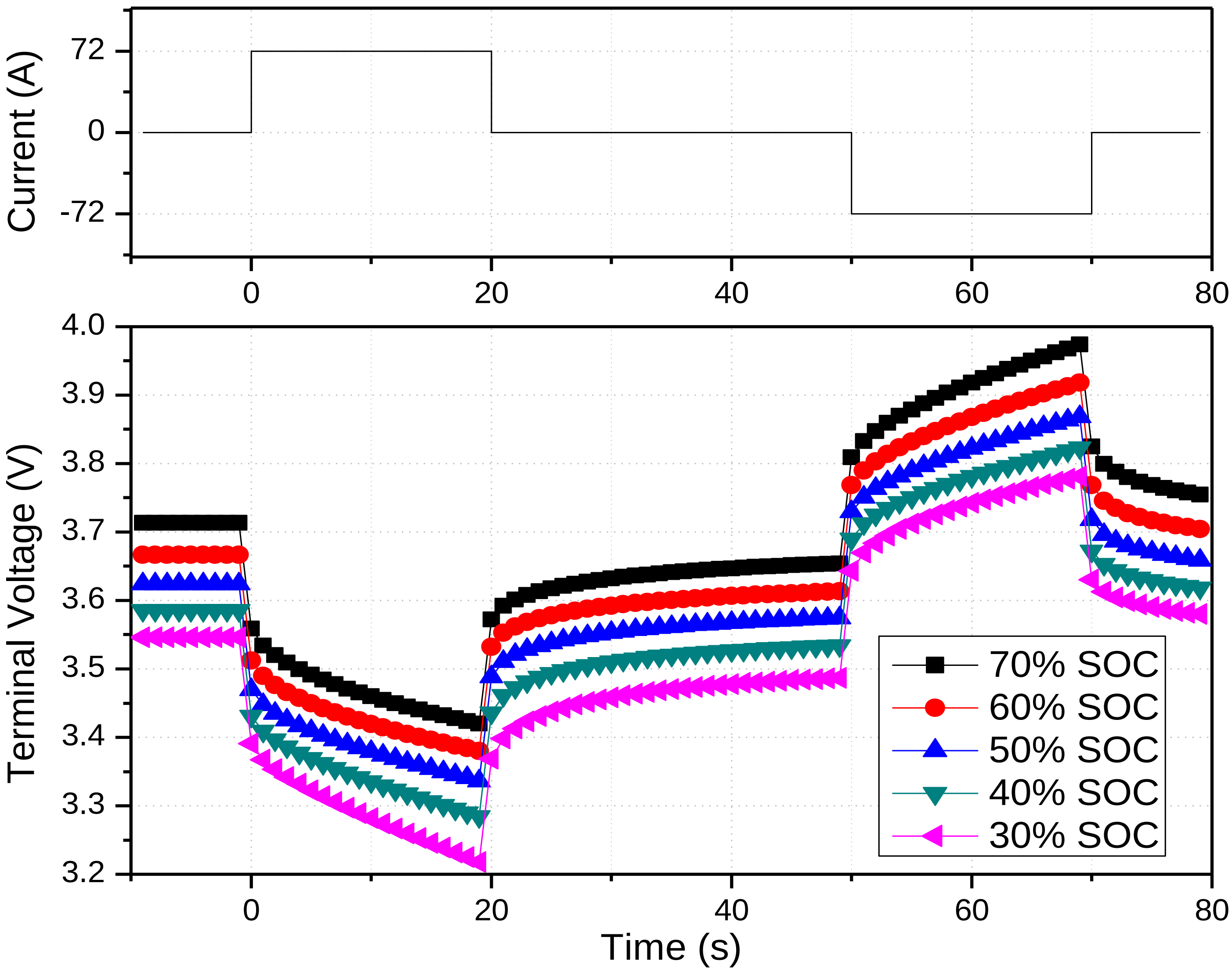
Terminal voltages at charging and discharging current



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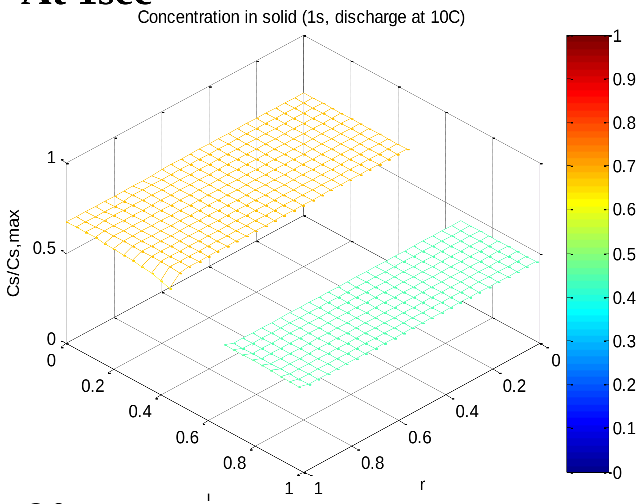
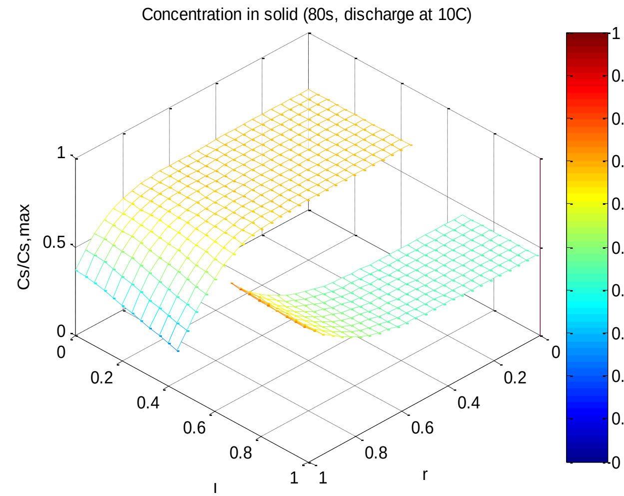
Discharging behavior at a step current of 10C

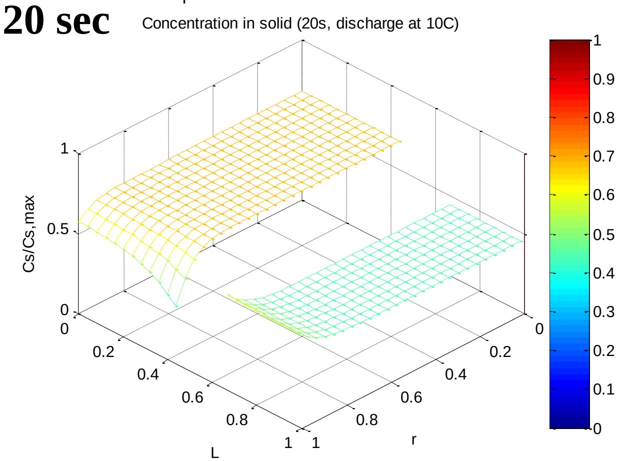
At 1sec



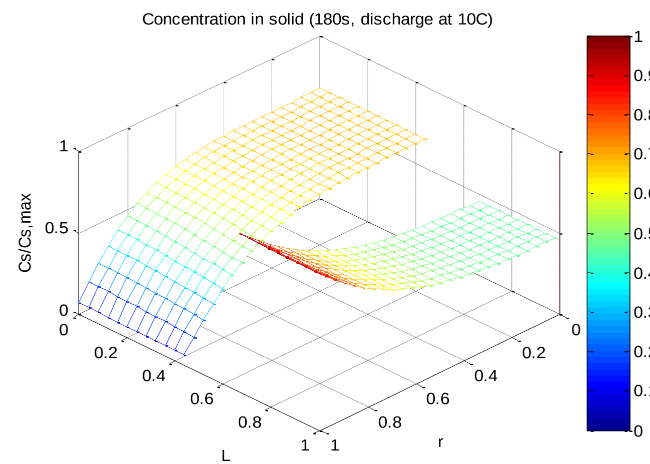
At 80 sec



At 20 sec



At 180 sec



As lithium ion leaves from negative electrode and deposited in positive electrode, concentration at the interface of the negative electrode drops rapidly when compared with that of inners, while opposite phenomena occurs in the positive electrode.

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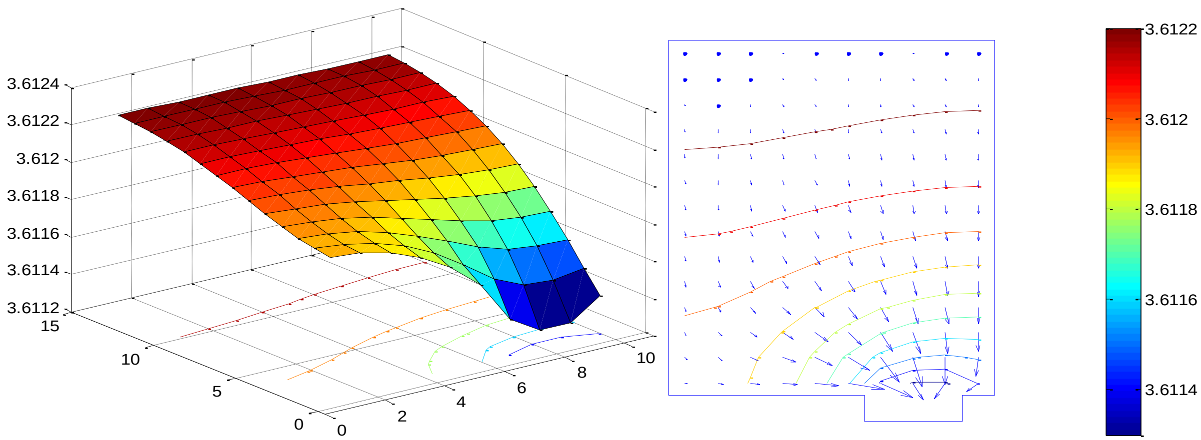
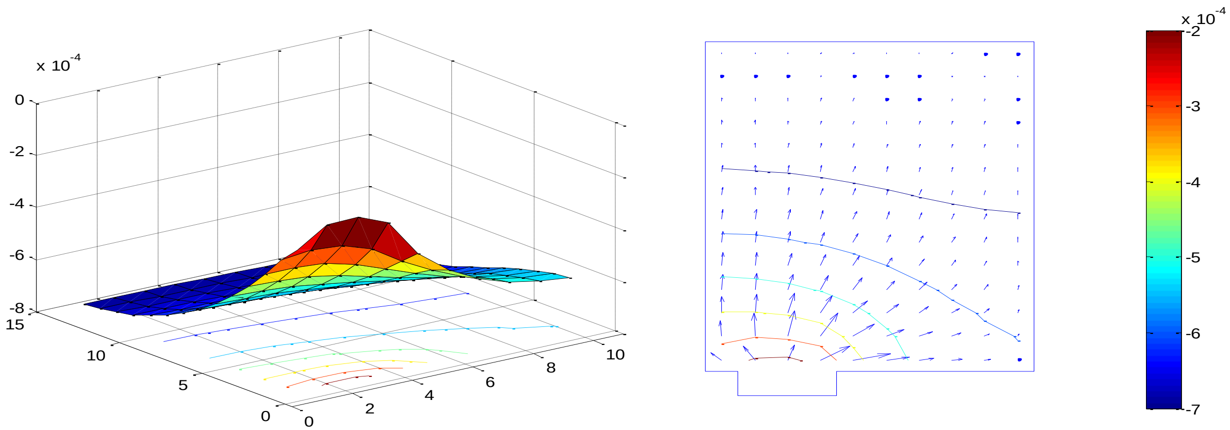
Potentials at positive and negative current collector





- Potential difference between to current collectors near tab is lower when the battery is discharging and higher when charging
- The reaction rate near tabs is higher
- In this case the reaction rate near positive tab is highest, 3% larger than the lowest point

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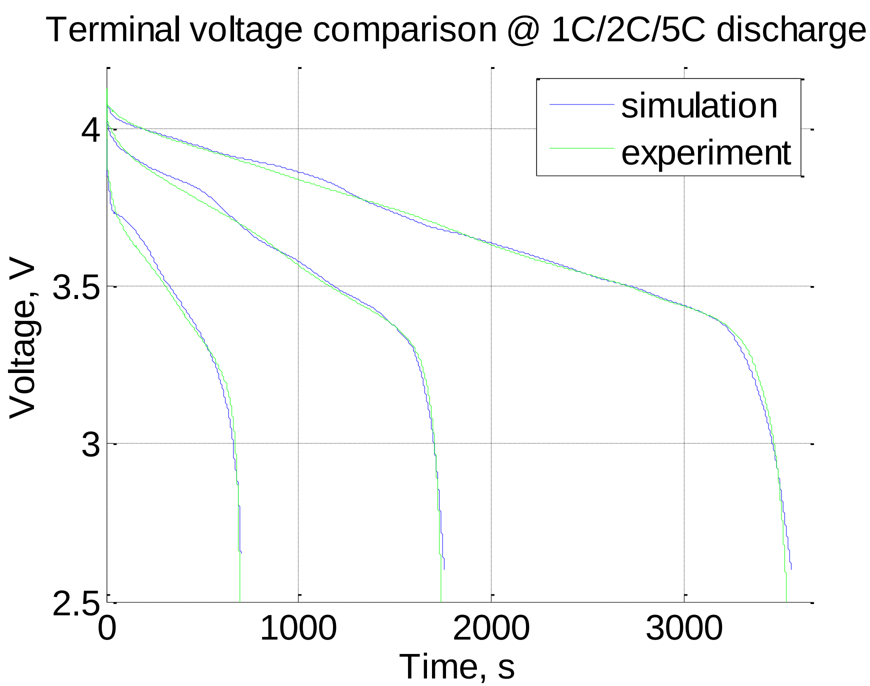
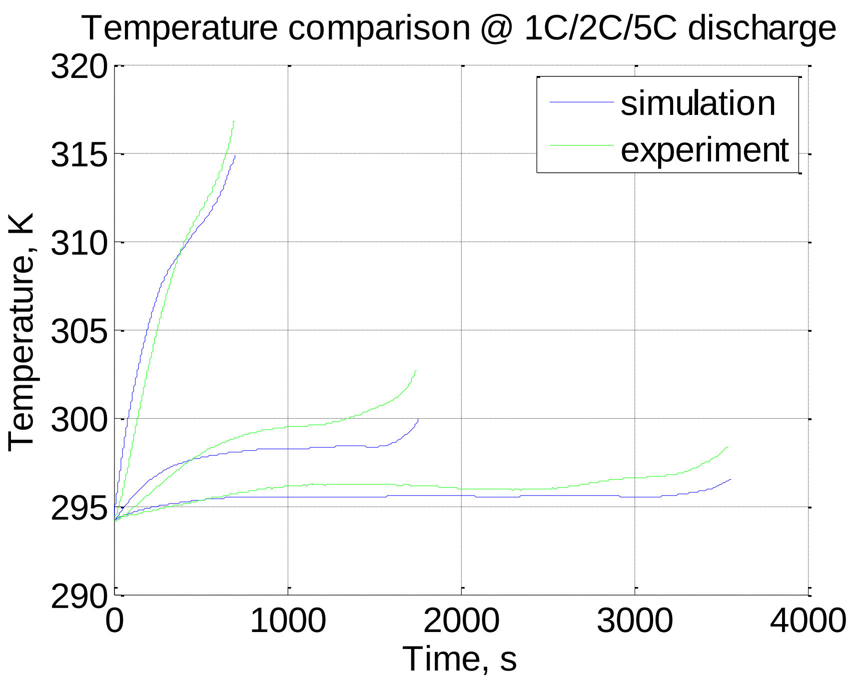
Validation of a single pouch cell at 1C/2C/5C discharge





Auburn's modeling capability is unique in accurately (validated) in predicting battery behavior.

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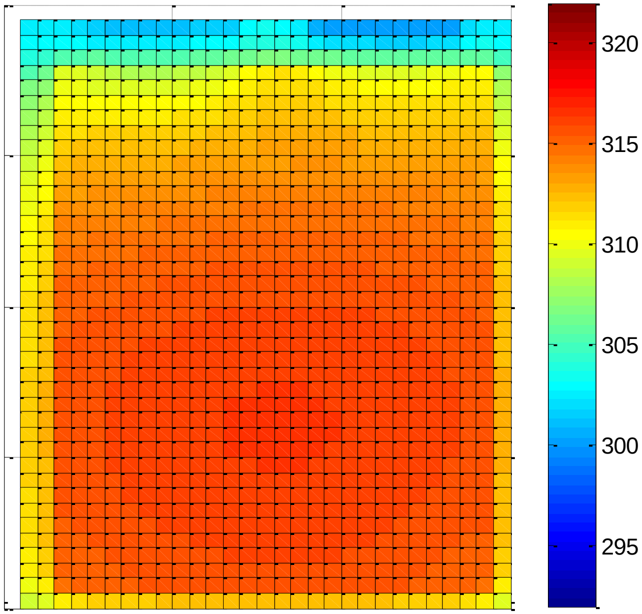
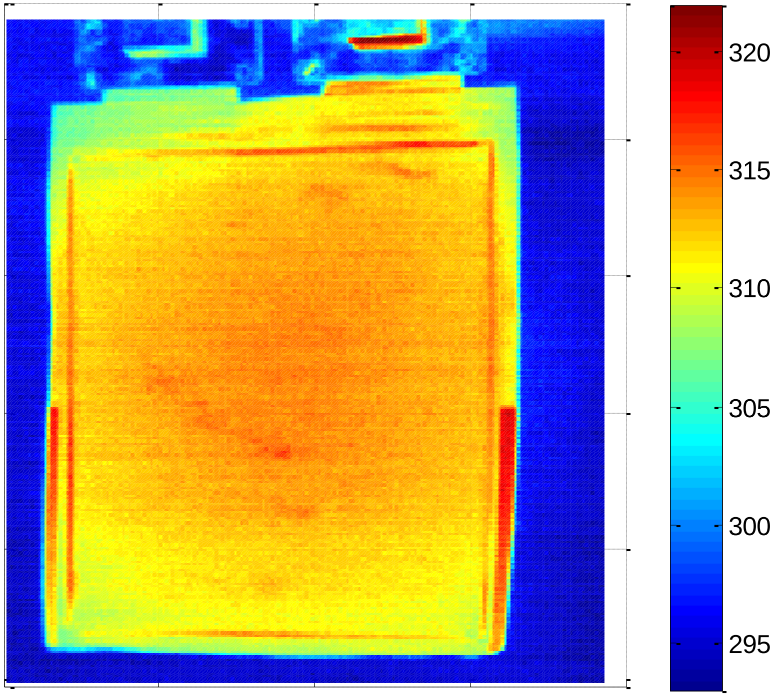
Validation of temperature distribution of a single pouch cell

Simulation



Experiment



5C discharge, 700s

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Mechanical Stress Generation and Dimension Changes

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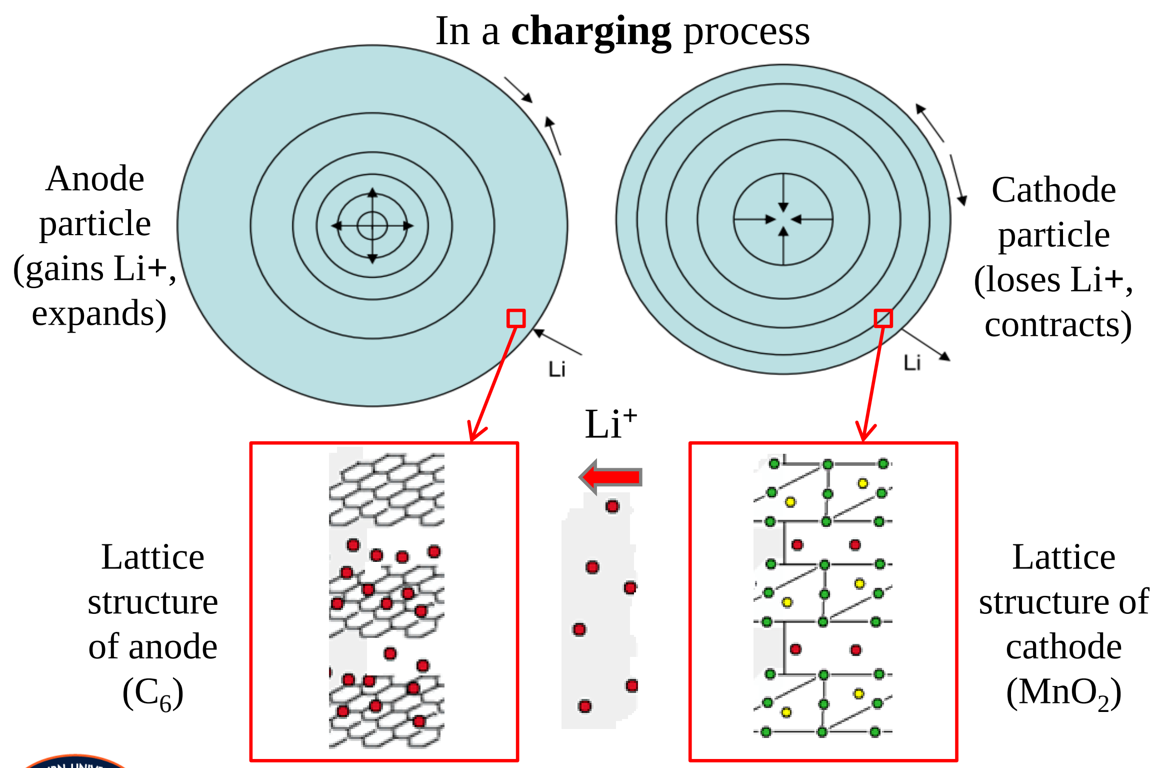
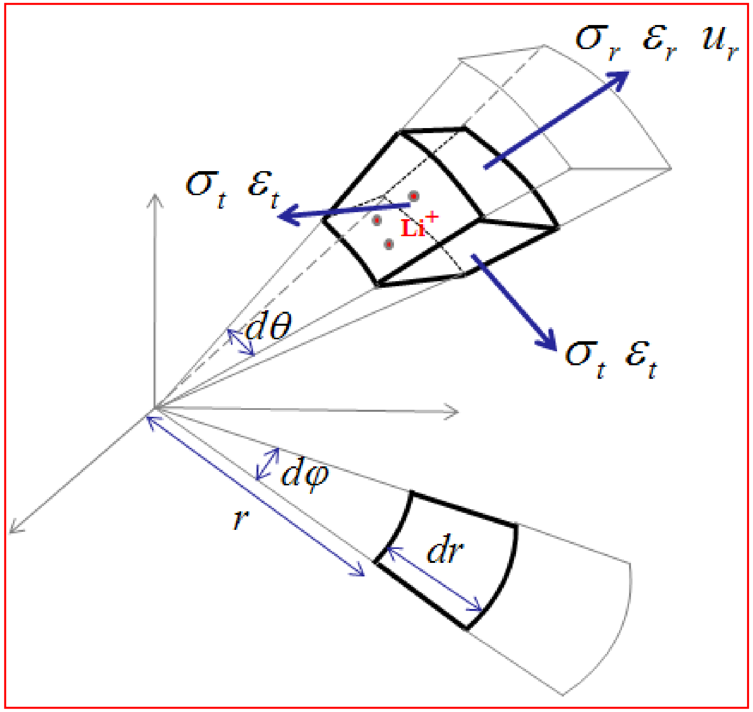
Physical Principle

- In certain region of a electrode particle, the inclusion of Li^+ results in localized volume expansion.
- The inhomogeneous distribution of Li^+ inside the particle causes inhomogeneous localized volume changes, which induces stress.





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Governing Equations

Governing equations	Principles in details
Calculation of radial, tangential and hydrostatic stress $\sigma_r = \frac{2\Omega E}{3(1-\nu)}\left(\frac{1}{r_0^3}\int_0^{r_0}\tilde{c}r^2dr - \frac{1}{r^3}\int_0^{r}\tilde{c}r^2dr\right)$ $\sigma_t = \frac{\Omega E}{3(1-\nu)}\left(\frac{2}{r_0^3}\int_0^{r_0}\tilde{c}r^2dr + \frac{1}{r^3}\int_0^{r}\tilde{c}r^2dr - \tilde{c}\right)$ $\sigma_h = \frac{1}{3}(\sigma_r + \sigma_t + \sigma_t)$	• Dimensionless volume change caused by concentration where Ω is the partial molar volume of Li+ (cm^3/mol). $\varepsilon_r' + \varepsilon_t' + \varepsilon_t' = c\Omega$ • The strain-stress relation=Hook's law + an extra term induced by concentration: $\varepsilon_r = \frac{1}{E}[\sigma_r - \nu(\sigma_t + \sigma_t)] + \frac{1}{3}c\Omega \quad \varepsilon_t = \frac{1}{E}[\sigma_t - \nu(\sigma_t + \sigma_r)] + \frac{1}{3}c\Omega$
Effect of stress on diffusion in electrodes $\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_s}{\partial r}\right)$ $-\frac{D_s\Omega}{RT}\left[\frac{\partial c}{\partial r}\frac{\partial \sigma_h}{\partial r} - c\left(\frac{\partial^2\sigma_h}{\partial r^2} + \frac{2}{r}\frac{\partial \sigma_h}{\partial r}\right)\right]$	• Calculation of chemical potentials using the Gibbs equation and substitution with stress and concentration $dU = TdS - PdV + \mu dn$ $\mu = \mu_0 + RT\ln c - \Omega\sigma_h$ • Fick's law: $J = -\frac{D}{RT}c\nabla\mu = -D\left(\nabla c - \frac{\Omega c}{RT}\nabla\sigma_h\right)$

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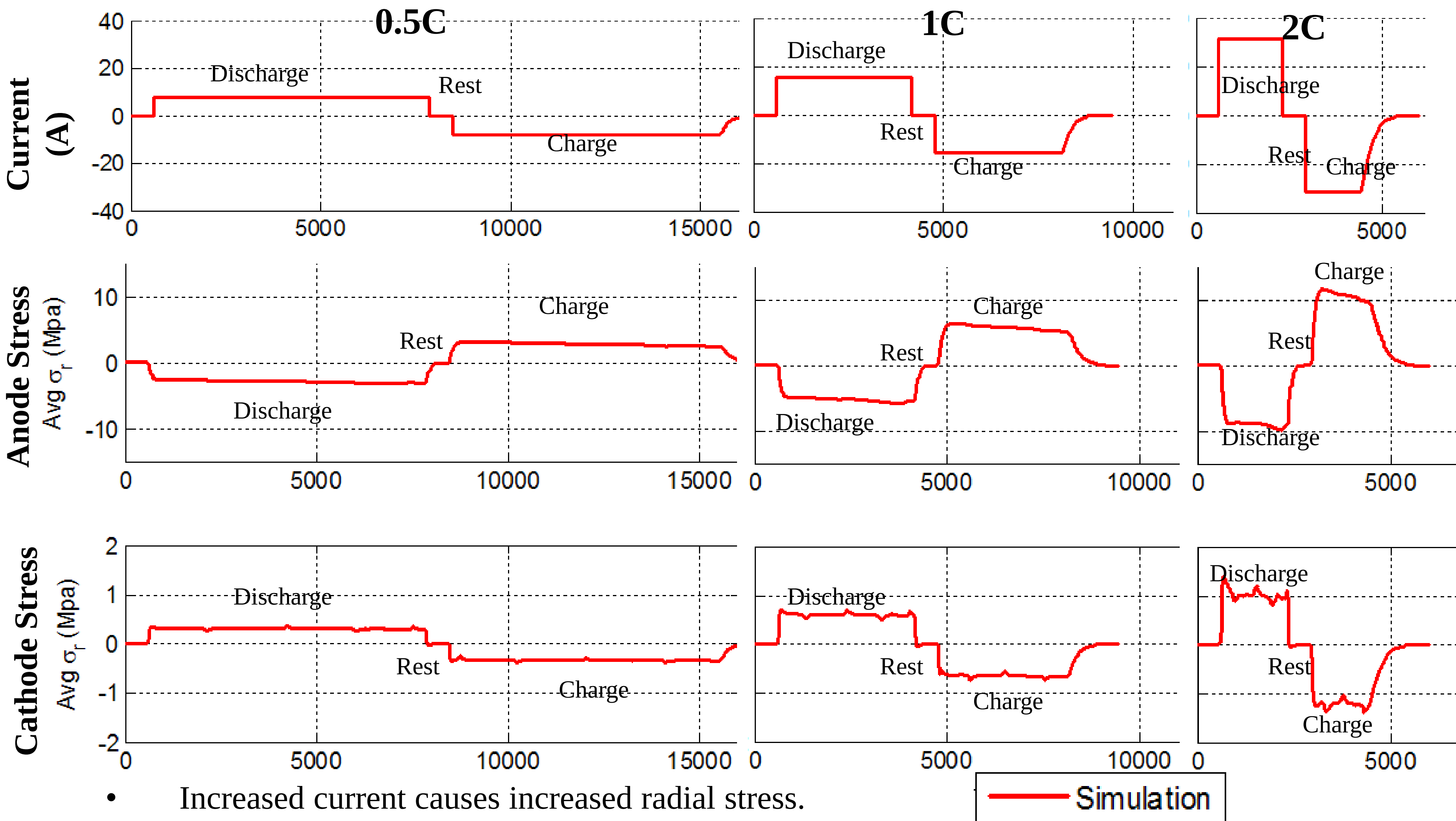
Averaged Radial Stress in 0.5C, 1C and 2C Cycling



- Increased current causes increased radial stress.
- The radial stress in anode is larger than cathode.

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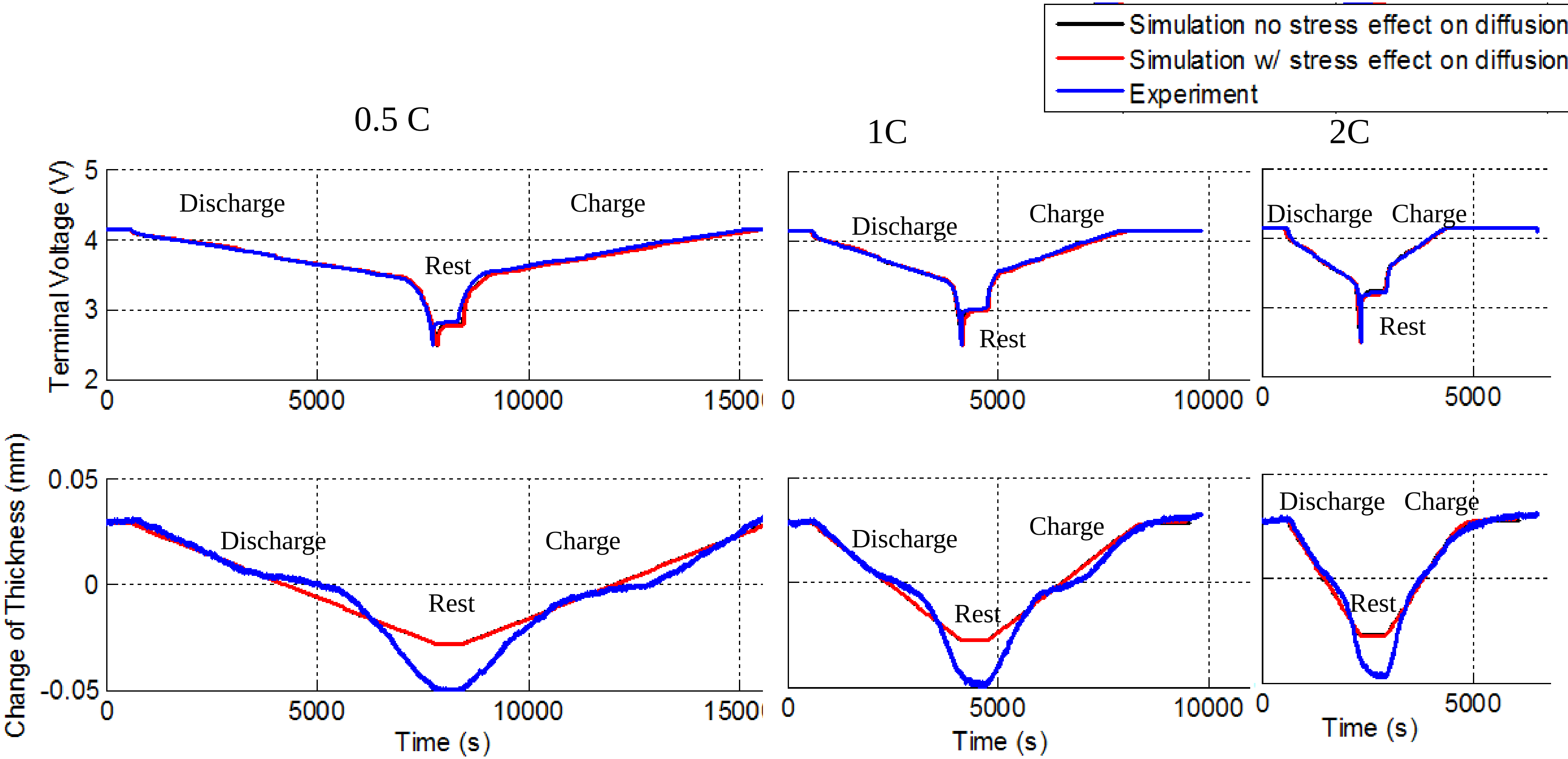
Voltage and Thickness in 0.5C, 1C and 2C Cycling



- Voltage curves match.
- Mismatch of thickness in low SOC region.

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Reduced Order Model (ROM)

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Reduction methods

- Electrolyte
(State space approach)

The m*th* order model:

$$\hat{\mathbf{A}} = diag\left[\lambda_1\ \lambda_2 \cdots \lambda_m\right]$$
$$\hat{\mathbf{B}} = \left[11\cdots1\right]^T$$
$$\hat{\mathbf{C}} = \left[\mathbf{r}_1\lambda_1\ \mathbf{r}_2\lambda_2 \cdots \mathbf{r}_m\lambda_m\right]$$
$$\hat{\mathbf{D}} = \left[\mathbf{Z} + \sum_{k=1}^{m}\mathbf{r}_k\right] = \mathbf{D}$$

truncation → grouping

The n*th* order model:

$$\mathbf{A}^* = diag\left[\bar{\lambda}_1\ \bar{\lambda}_2 \cdots \bar{\lambda}_n\right]$$
$$\mathbf{B}^* = \left[11\cdots1\right]^T$$
$$\mathbf{C}^* = \left[\bar{\mathbf{r}}_1\bar{\lambda}_1\ \bar{\mathbf{r}}_2\bar{\lambda}_2 \cdots \bar{\mathbf{r}}_n\bar{\lambda}_n\right]$$
$$\mathbf{D}^* = \left[\mathbf{Z} + \sum_{f=1}^{n}\bar{\mathbf{r}}_f\right]$$

- Electrodes
(Polynomial approach)

$$C_{s,ave} = \int_{r=0}^{R_s}\frac{3r^2}{R_s^{\,3}}C_s(r,t)dr$$
$$q_{ave} = \int_{r=0}^{R_s}\frac{3r^2}{R_s^{\,3}}\left(\frac{\partial}{\partial r}C_s(r,t)\right)dr$$
$$C_{s,surf}(r\ ,t) = a(t) + b(t)\left(\frac{R_s^{\,2}}{R_s^2}\right) + d(t)\left(\frac{R_s^{\,4}}{R_s^4}\right)$$

→

$$C_{s,ave} = \frac{3}{7}d(t) + \frac{3}{5}b(t) + a(t)$$
$$q_{ave} = \frac{3b(t)}{2R_s} + \frac{2d(t)}{R_s}$$
$$C_{s,surf} = a(t) + b(t) + d(t)$$

- BV, ion transport and potentials
(Parameters simplification)

$$j^{Li} = a_s i_0\left\{\exp\left[\frac{\alpha_a F}{RT}\eta\right] - \exp\left[-\frac{\alpha_c F}{RT}\eta\right]\right\}$$
$$\frac{\partial}{\partial x}\left(k^{eff}\frac{\partial}{\partial x}\phi_e\right) + \frac{\partial}{\partial x}\left(k_D^{eff}\frac{\partial}{\partial x}\ln c_e\right) + j^{Li} = 0$$
$$\frac{\partial}{\partial x}\left(\sigma^{eff}\frac{\partial}{\partial x}\phi_s\right) - j^{Li} = 0,\ \ \eta = \phi_s - \phi_e - U$$

→

$$\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}\phi_{s-e}\right) = j^{Li}\left(\frac{1}{\sigma^{eff}} + \frac{1}{k^{eff}}\right)$$
$$j^{Li} = \frac{a_s i_0 F}{RT}\left(\phi_{s-e} - U\right)$$

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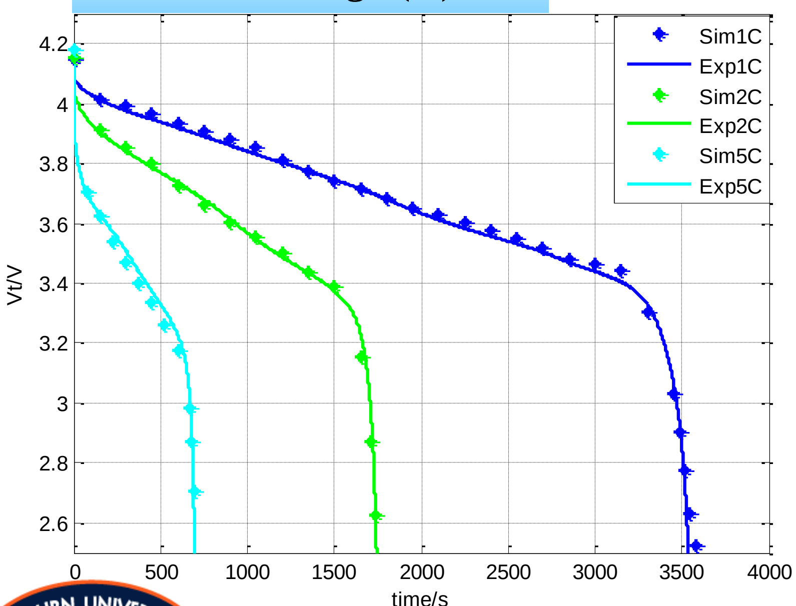
Comparison of simulation results and experimental results: Discharging

Test condition:
Temperature=25°C
Initial V_t= 4.15V
Discharge current: 1C/2C/5C rate

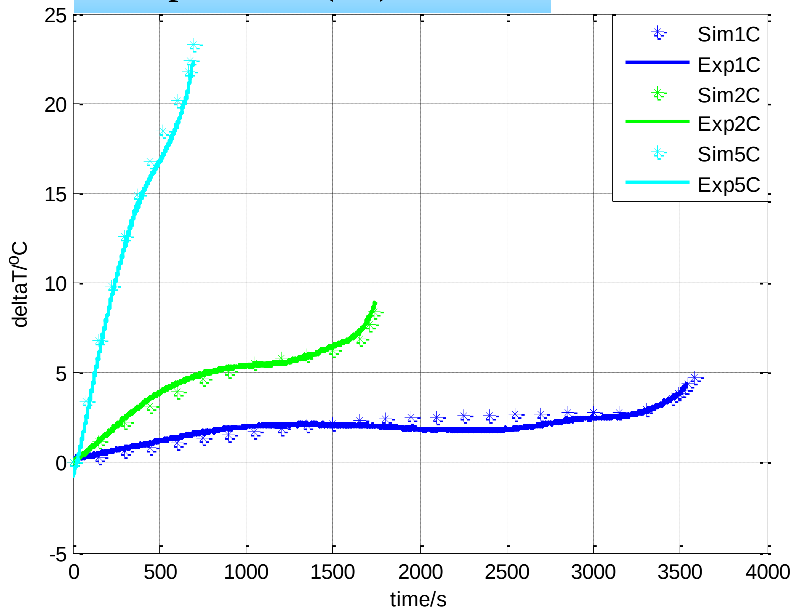
Computational time (s)

Model	Full discharge@1C	Full discharge@2C	Full discharge@5C	Time step (sec)
Full order model	79	45	26	1
Reduced order model	8.7	3.9	2.7	1

Terminal Voltage (V)



Temperature (°C)



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SOC estimation using ROM

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Definition of SOC

- SOC: ratio of releasable charge to maximum charge capacity
  - $$SOC = \frac{Q_{releasable}}{Q_{\max}} \times 100\%$$
    - $Q_{releasable}$: releasable charge capacity from current SOC to 0% SOC (Ah)
    - Q_{max}: releasable charge capacity from 100% SOC to 0% SOC (Ah)
  - Values are based on a standard T_{amb}=25°C and I=1C

- Formal definition considers SOC to be a ratio of the average concentration of lithium ions to the maximum concentration in the negative electrode
  - $$SOC = \frac{1}{\delta^-} \int_0^{\delta^-} \frac{\left(c_{s,ave} - c_{s,\max} \cdot S_0\right)}{c_{s,\max} \cdot (S_{100} - S_0)} dx$$
    - δ^-: width of anode (cm)
    - $c_{s,ave}$: volume-averaged solid phase concentration (mol·cm^{-3})
    - $c_{s,max}$: maximum solid phase concentration (mol·cm^{-3})
    - S_0: lithium stoichiometry value at 0% SOC
    - S_{100}: lithium stoichiometry value at 100% SOC

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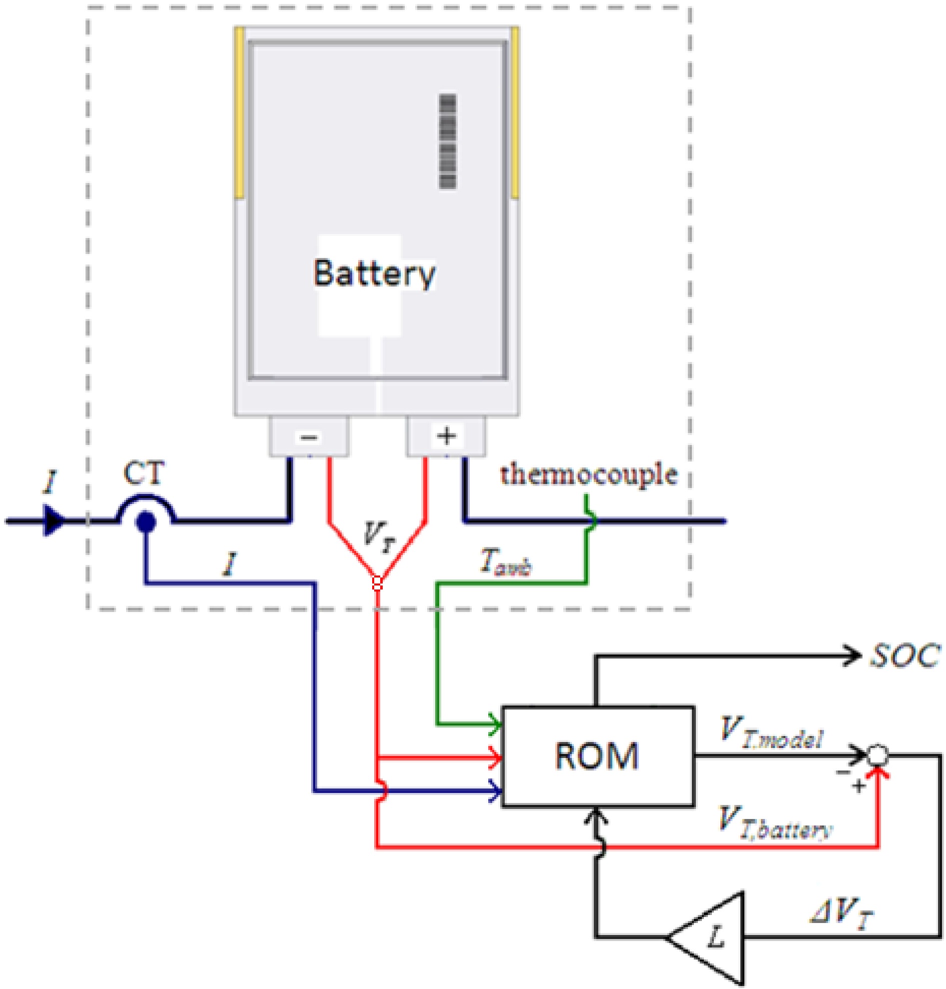
SOC estimation with a Feedback – Concept



- Typical observer takes form of

$$S^{k+1} = A \cdot S^{k} + Bu + L \cdot \Delta V_T$$
$$V_T^{k+1} = C \cdot S^{k+1} + Du$$

S: stoichiometry number

- $SOC = \dfrac{S - S_0}{S_{100} - S_0}$ where $S = \dfrac{\overline{c_{s,ave}}}{c_{s,\max}}$
  - $c_{s,ave}$ averaged through electrode thickness

$$S^{k+1} = S^{k} - \frac{1}{c_{s,\max}} \frac{3 \cdot I}{R_s a_s F A \delta} \cdot \Delta t + L \cdot \Delta V_T \cdot \Delta t$$

$$V_T^{k+1} = C \cdot S^{k+1} + Du$$

$$L = \begin{bmatrix} \left.\begin{matrix} -36.4 \times 10^{-4} \cdot 0.5 \\ \vdots \\ -36.4 \times 10^{-4} \cdot 0.5 \end{matrix}\right\} anode \\ \left.\begin{matrix} 0 \\ \vdots \\ 0 \end{matrix}\right\} separator \\ \left.\begin{matrix} 50 \times 10^{-4} \cdot 0.58 \\ \vdots \\ 50 \times 10^{-4} \cdot 0.58 \end{matrix}\right\} cathode \end{bmatrix} \cdot \ell$$

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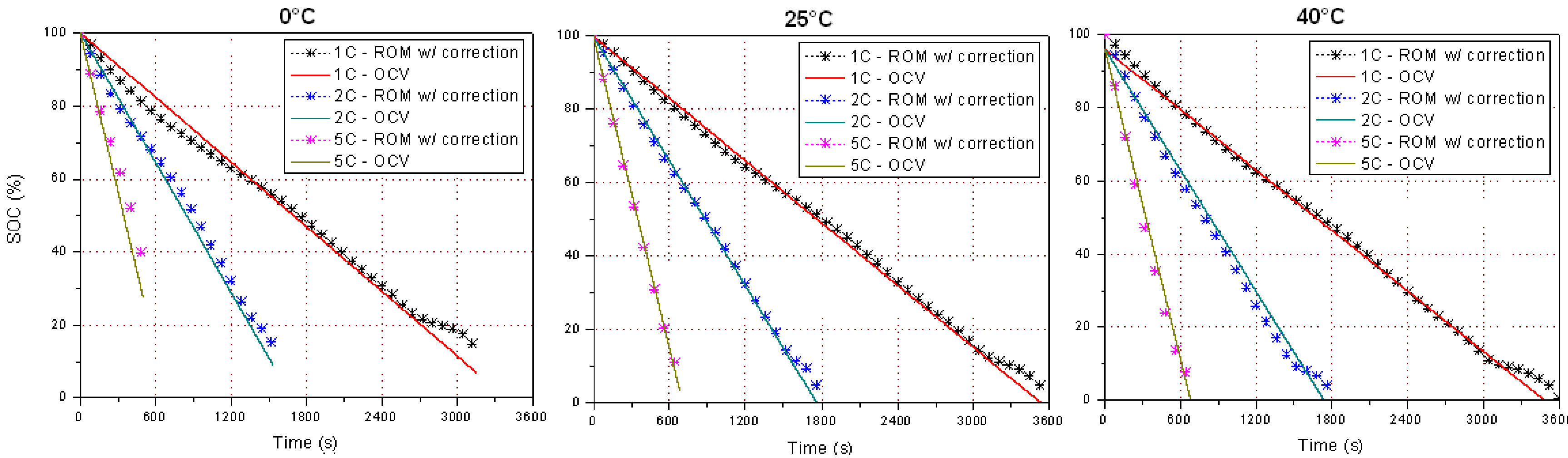
SOC estimation with a Feedback – Results



- Maximum error
  - Full discharge: 3.58% (5C, 40°C)
  - Single cycle: 1.51% (1C, 0°C)
  - HPPC test: 4.95% (5C, 0°C)
  - 5 cycles: 3.15% (5C, 0°C)

<u>Synopsis</u>

Proposed method meets ≥ 95% SOC accuracy for every case investigated

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Experimental Capability
: Test Stations and Characterization of Cells

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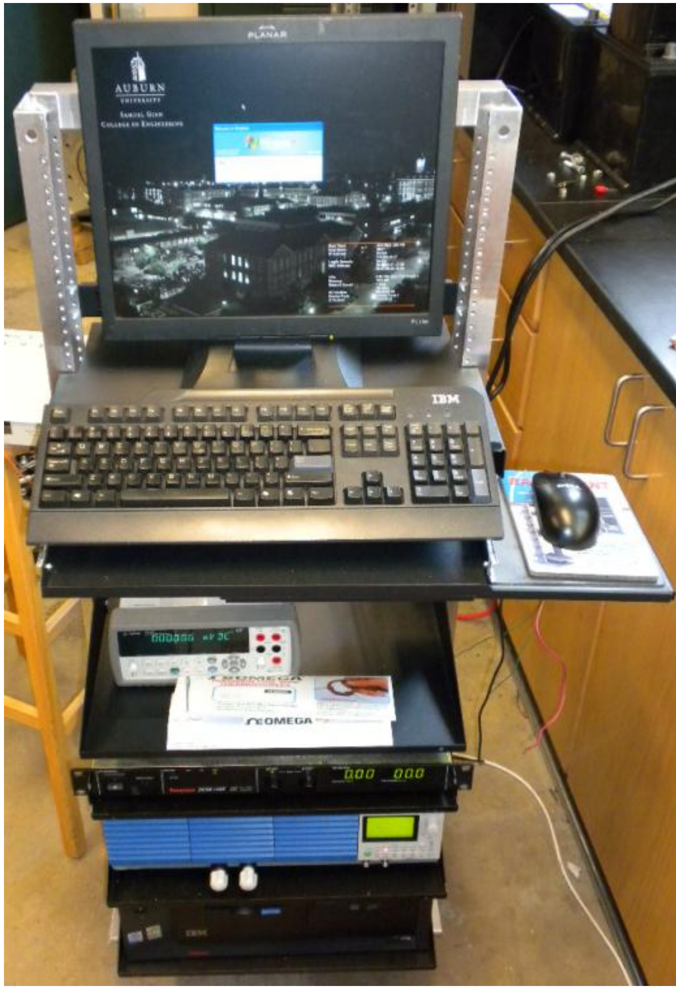
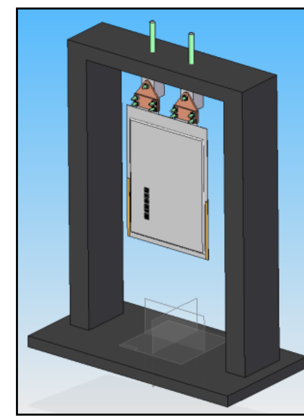
Test Station Equipment



Type	Model	Rated Voltage (V)	Rated Current (A)
Power Supply	Sorensen DCS 8-125E	0-8	0-125
	Sorensen DCS 8-125E	0-8	0-125
	Sorensen DCS 20-50E	0-20	0-50
Electronic Load	Kikusui PLZ1004W	1.5-150	0-200
	Dynaload DLVP-50-300-3000A	0-50	0-300
	Dynaload DLF100-50-250	0-100	0-50
Bipolar Power Supply	Kikusui PBZ20-20	±20	±20
	Kepco BOP20-20	±20	±20

- Six test stations
  - Fast charging
  - Current ripples
  - Material degradation
  - Cycling
  - EIS
  - Charging/discharging for formation
- Charge/discharge profile is programmed in LabVIEW
  - Time, temperature, voltage, and current data is recorded at sample rates up to 10Hz
  - Programmable relays allow for quick switching
    - CT accuracy of 0.0044%
    - Cell held vertically in fixture
  - Specially designed terminal clamps made of Cu/Al



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AU Equipment

- JEOL 7000 Field Emission Scanning Electron Microscope (SEM) with energy dispersive (EDS) and wavelength dispersive (WDS) X-ray detectors
  - Electrode morphology and composition gradients
  - 3.0nm resolution
- Two Bruker D8 X-Ray Diffractometers (XRD) with line and area detectors, low angle capabilities, hot/cold stage
  - Crystalline phases and transformations
- JEOL 5200 Scanning Tunneling Microscopy (STM) / Atomic Force Microscopy (AFM)
  - Electrode morphology
- JEM–2010 200 kV Transmission Electron Microscope (TEM) with EDS
  - Local / high magnification electrode morphology, composition, and crystalline phase

FE-SEM

TEM

STM/AFM

XRD

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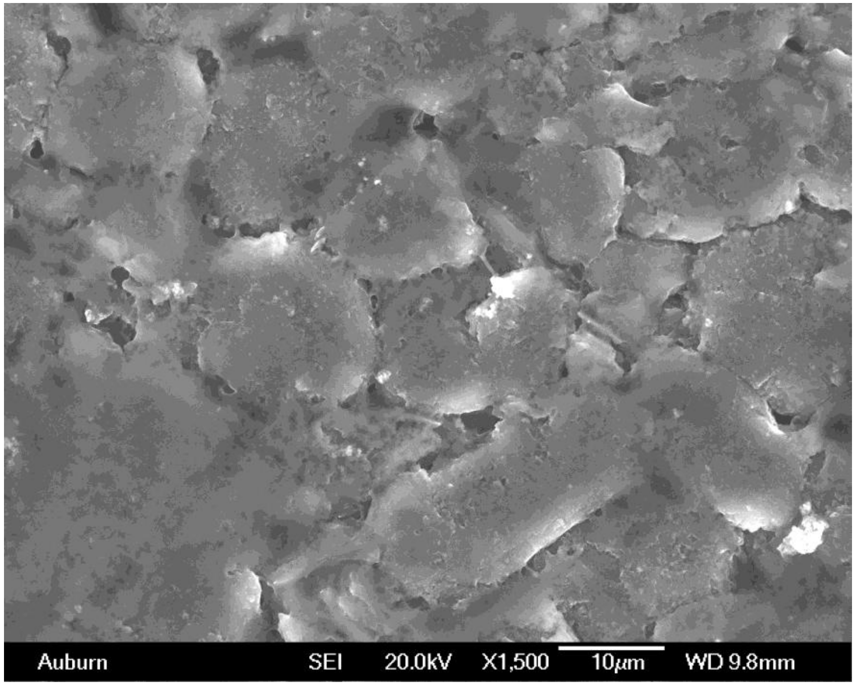
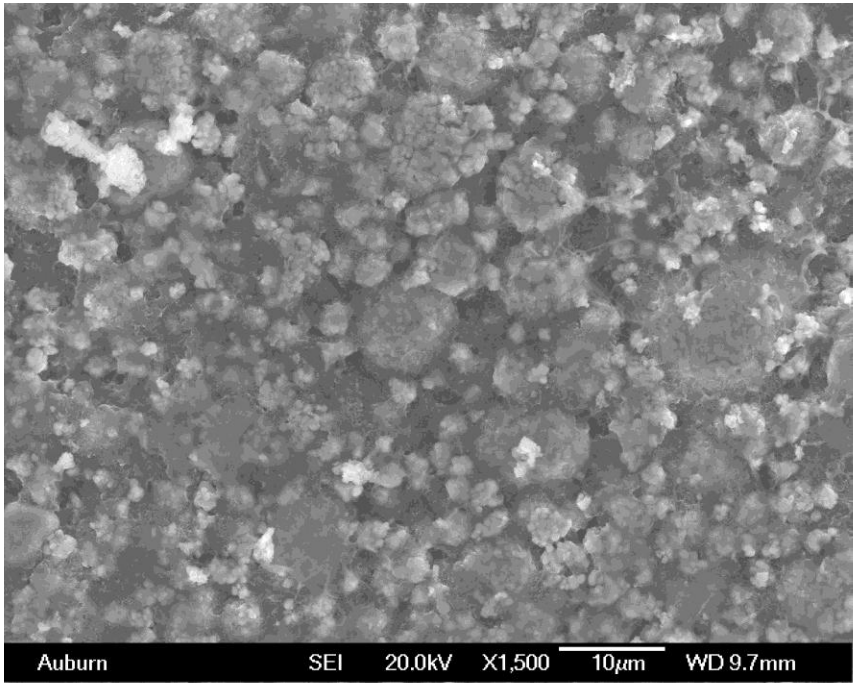
Sample Images

- Anode



- Cathode



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AU Testing Facilities for Vehicles

Auburn not only has modeling capability but the ability to validate and test components and systems for HEV/EV in conjunction with vehicle performance.

- On-Road
  - NCAT Test Track
    - 1.7 mile oval
    - Well Surveyed
      - Level
      - 2% Crowns
      - 15% Banked Turns
- Off-Road
  - AU College of Agriculture Extension Centers
  - USDA-ARS National Soil ("Tillage") Lab

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Major research topics

1. **Modeling** :
   a. Multi-physics and Multi scale modeling
   b. One dimensional microcell
   c. Quasi-three dimensional single cell
   d. Model Reduction for real time applications

2. **Applications**:

   - SOC Estimation for active and passive cell balancing
   - Controls for fast or rapid charging
   - Design of heating and cooling systems and associated controls
   - Prognoses and diagnoses: SOH

3. **Testing and analysis of cells and packs**
   - Cells
     - Electric effects
     - Thermal effects
     - Mechanical, thermal, electrochemical and material properties
   - Vehicles: Test track

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Summary

The research team in Auburn University has established a research capability of theoretically and experiementally solving complex problems and developing new methodologies for different types of battery.;

- Modeling and simulations,
- Design of pack and module with associated controls,
- Analysis of material structure and properties,
- Health monitorings.

We welcome the opportunity to solve your important problems. As a first step, I presented current research to show how to leverage our modeling and testing capabilities.

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