Predicting Temperatures in a Li-ion Battery using a Model-based Prognostics

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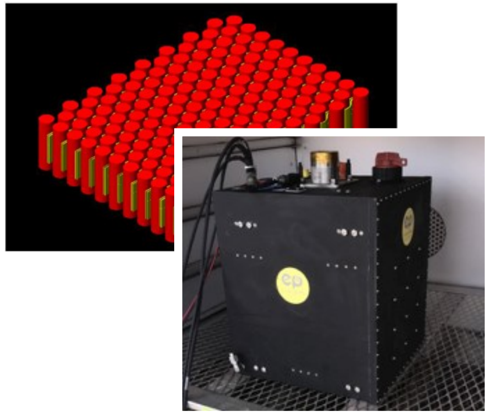
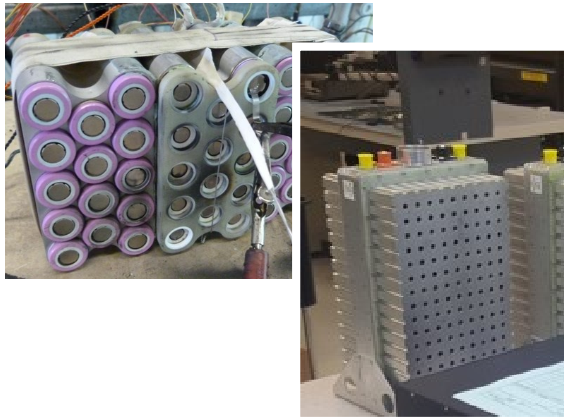
Outline

1. Project Overview
2. Li-ion Failure Introduction
3. Li-ion Failure Modeling and Simulation
4. Prognostics Overview
5. Li-ion Discharge Time and Temperature Estimation
6. Conclusion

Today's Bulky Pack Designs



Safety Testing -
Thermal Runaway



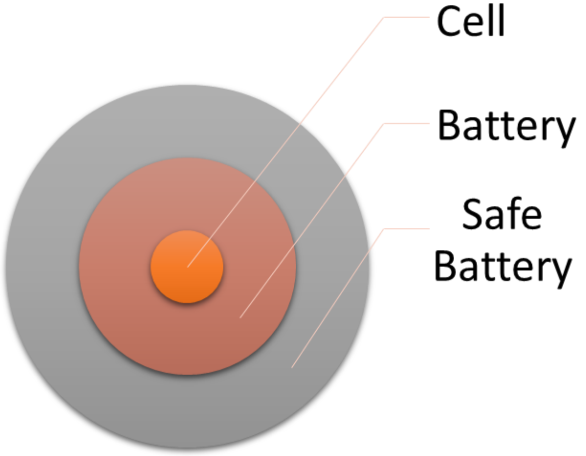
Pack penalty: 23% → **Safe pack penalty: 61%**

Additional mass for "safe" packs

Problem Formulation

Emerging Electric Aircraft need Better and Safer Batteries

SOA Battery Weight Penalty



Significant Weight Added!

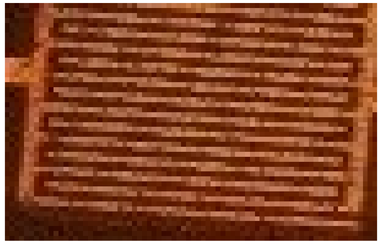
- **Current Monitored Battery Parameters**
  - Voltage
  - Current
  - Temperature
- **Consequence of Unmitigated Cell Thermal Runaway Events**
  - Fire
  - Explosion
  - Debris

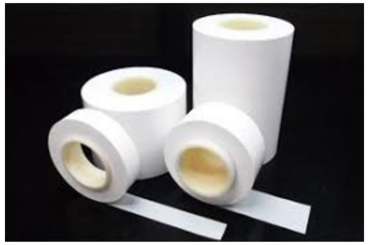
✓ **Internal** Monitoring
✓ Failure **prevention** via internal fault detection & mitigation

Project Overview

Different components

1. **Experimental**
   - Embedded Sensors





2. **Modeling**
   - Detect and Model Fault precursors
   - Develop state estimation and prognostic algorithms
   - Battery Management System (BMS) Capable of Fault Mitigation

Li-ion (an Overview)

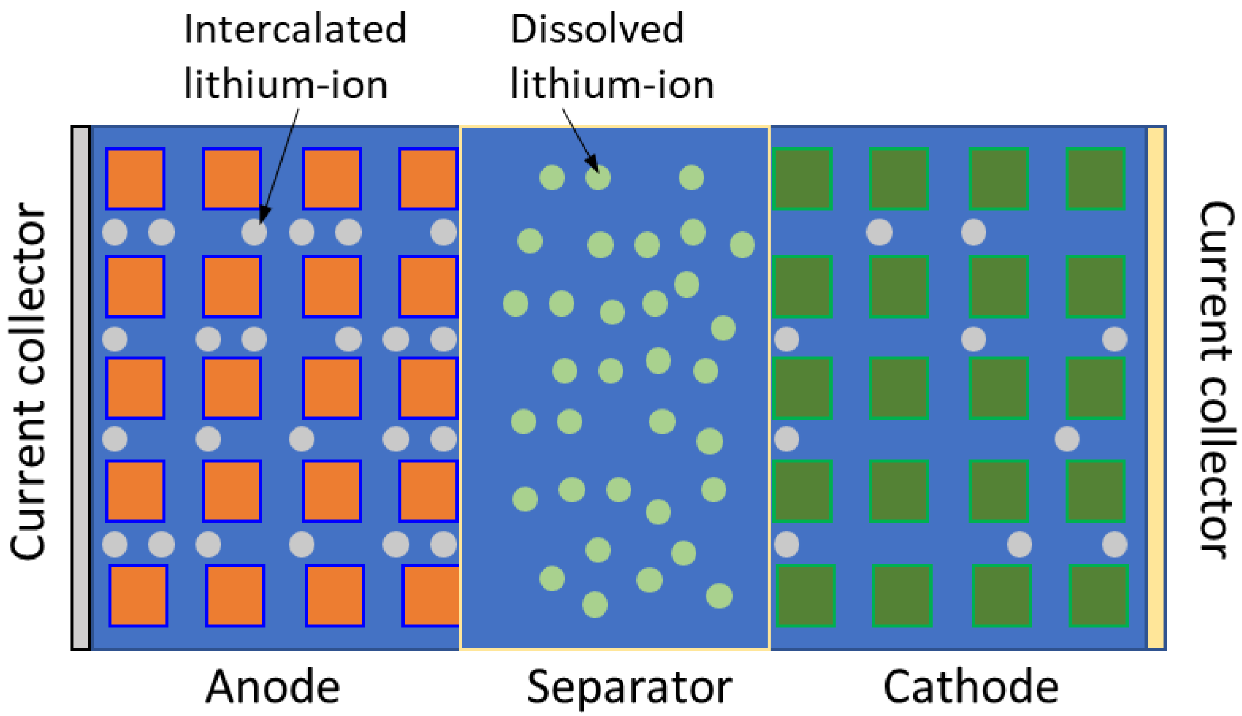
- Li-ion Chemistry
  - Cathode (LCO/NMC/LFP)
  - Anode (Graphite/Lithium)
  - Electrolyte ($LiCF_3SO_3$, $LiPF_6$ in EC/DMC)
  - Separator (PP/Al_2O_3)

Anode reaction

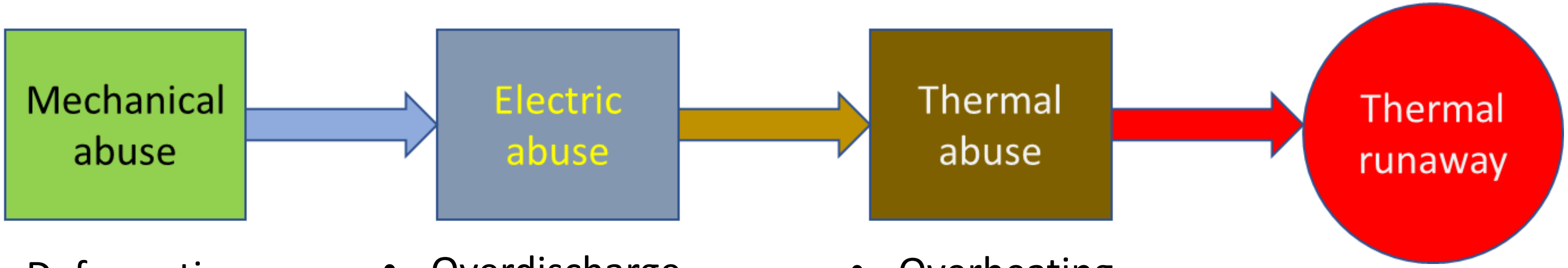
$$Li_xC \rightarrow C + xLi^+ + xe^-$$

Cathode reaction

$$Li_{1-x}CoO_2 + xLi^+ + xe^- \rightarrow LiCoO_2$$



Common Sources of Thermal Runaway



- Deformation
- Crash

- Overdischarge
- Overcharge
- Dendrite growth
- Internal short circuit

- Overheating
- High Temperature

Q. Wang, B. Mao, S.I. Stoliarov, J. Sun, A review of lithium ion battery failure mechanisms and fire prevention strategies, Progress in Energy and Combustion Science. 73 (2019) 95–131. DOI: 10.1016/j.pecs.2019.03.002.

A Cell's Path to Thermal Runaway

SEI decomposition	Anode/electrolyte reaction	separator melt	electrolyte decomposition	Electrolyte/cathode reaction
$69^{o}C$	$100^{o}C$	$130^{o}C$	$200^{o}C$	$300^{o}C$

Q. Wang, B. Mao, S.I. Stoliarov, J. Sun, A review of lithium ion battery failure mechanisms and fire prevention strategies, Progress in Energy and Combustion Science. 73 (2019) 95–131. DOI: 10.1016/j.pecs.2019.03.002.

Finite Element Failure Modeling

Inputs

- Materials
- Chemistry
- Geometry
- Cell Configuration
- Experimental Condition

→

Phenomena

- Thermal
- Lithium Plating
- Capacity Fade
- Dendrite Growth
- Chemical Decomposition
- Overcharge
- Shrinking Core Model

→

Outputs

- Cell Temperature
- Cell Potential
- Cell Capacity
- Discharge Time
- Cycle

A typical model for Li-ion

Electrolyte Transport

$$\frac{\partial \varepsilon_e c_e}{\partial t} - \nabla \cdot (D_e^{eff} \nabla c_e) - \frac{1 - t_+^0}{F} a_s j_n = 0$$

Electrolyte Potential

$$\nabla \cdot \left(\kappa_e^{eff} \nabla \phi_e - \frac{2RT\kappa_e^{eff}}{F}(1 - t_+^0)\left(1 + \frac{d \ln f_\pm}{d \ln c_e}\right) \nabla \ln c_e \right) + a_s j_n = 0$$

Electrode Potential

$$\nabla \cdot (\sigma_s \nabla \phi_s) - a_s j_n = 0$$

Reaction Kinetics

$$j_n = i_0\left(\exp\left(\frac{\alpha_a F}{RT}(\phi_s - \phi_e - U_{eq})\right) - \exp\left(-\frac{\alpha_c F}{RT}(\phi_s - \phi_e - U_{eq})\right)\right)$$

$$i_0 = k c_e^{\alpha_a}(c_{max} - c|_{r=R_s})^{\alpha_a} c|_{r=R_s}^{\alpha_c}$$

Particle Diffusion (Shrinking Core Model)

$$\frac{\partial c_\alpha}{\partial t} = \frac{1}{r^2}\left(D_\alpha r^2 \frac{\partial c_\alpha}{\partial r}\right)$$

Degradation Model

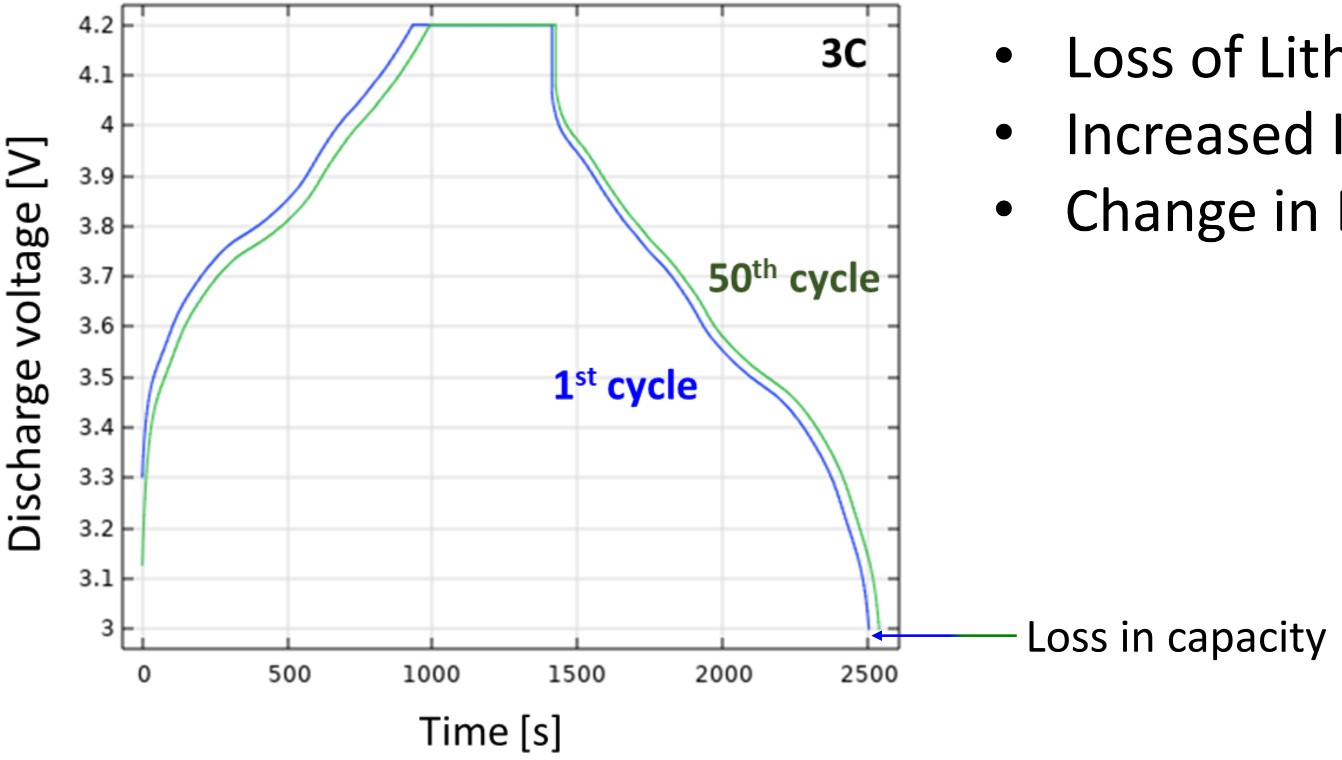
$$i_{loc, SEI} = -(1 + HK)\frac{J i_{loc, 1C, ref}}{\exp\left(\frac{\alpha \eta_{SEI} F}{RT}\right) + \frac{q_{SEI} f J}{i_{loc, 1C, ref}}}$$

Thermal Model

$$\rho C_p \frac{\partial T}{\partial t} = q_{rev} + q_{irr} + q_{ohm} + q_{chem} - q_{radiation} - q_{convection}$$

Finite Element Model Simulations

SEI formation and the loss of useable lithium

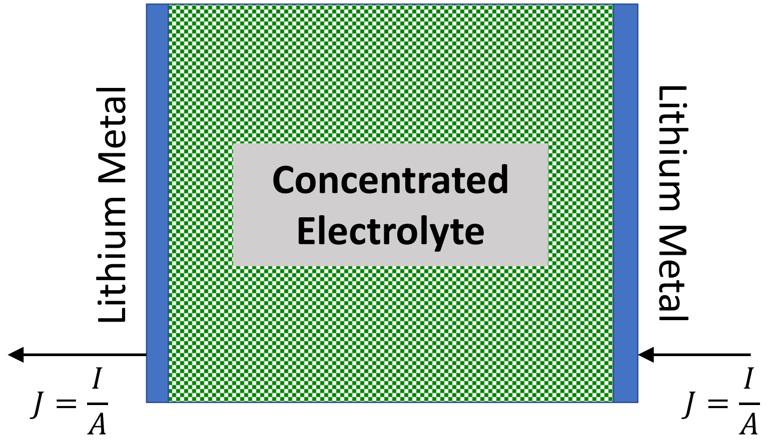


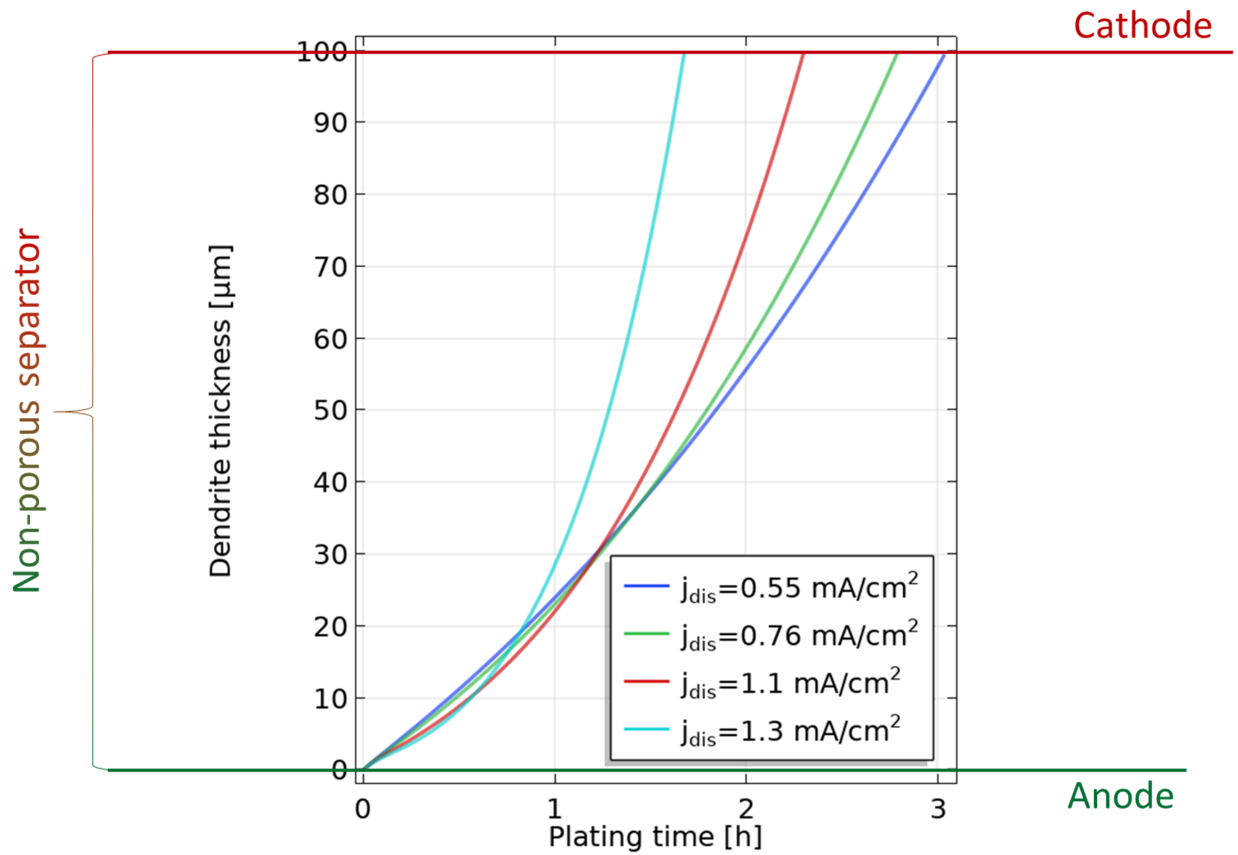
- Loss of Lithium
- Increased Impedance
- Change in Exothermic Profile

SEI not only affects Capacity but also the Internal Cell Temperature

FEM Simulations with Failure Model

Lithium Dendrite Growth on a Lithium Metal Anode



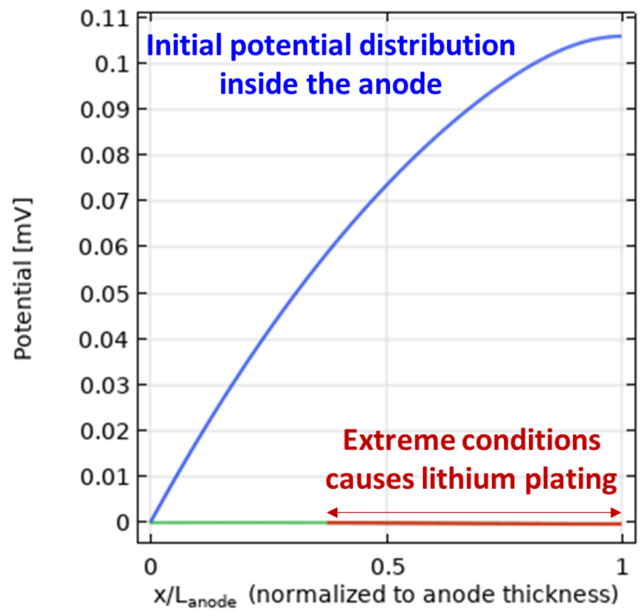


Internal Short Circuit by Lithium Dendrites can cause Thermal Runaway

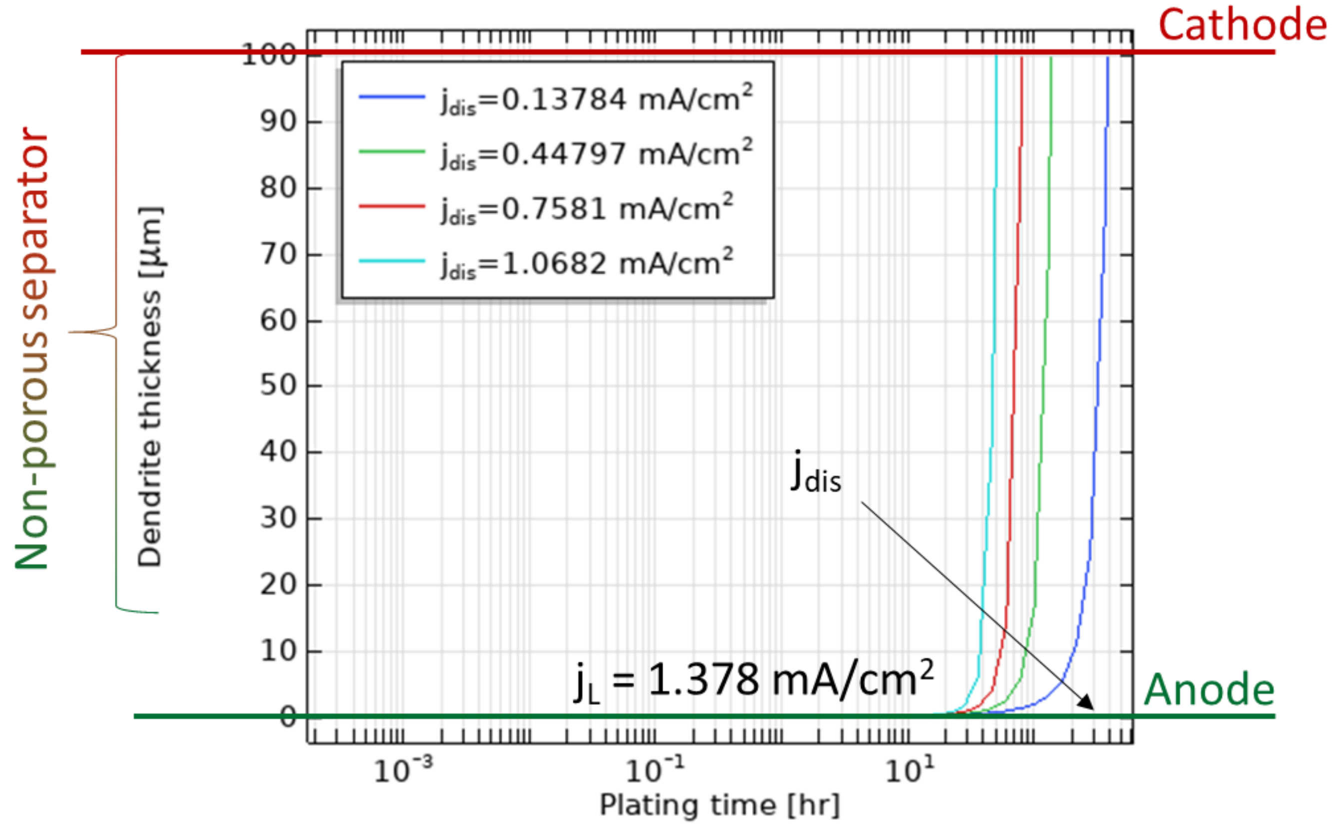
Monroe, C., & Newman J. *Journal of The Electrochemical Society* 150, no. 10 (October 1, 2003): A1377–84. DOI: 10.1149/1.1606686

Finite Element Model Simulations

Dendrite Growth in a Graphite anode



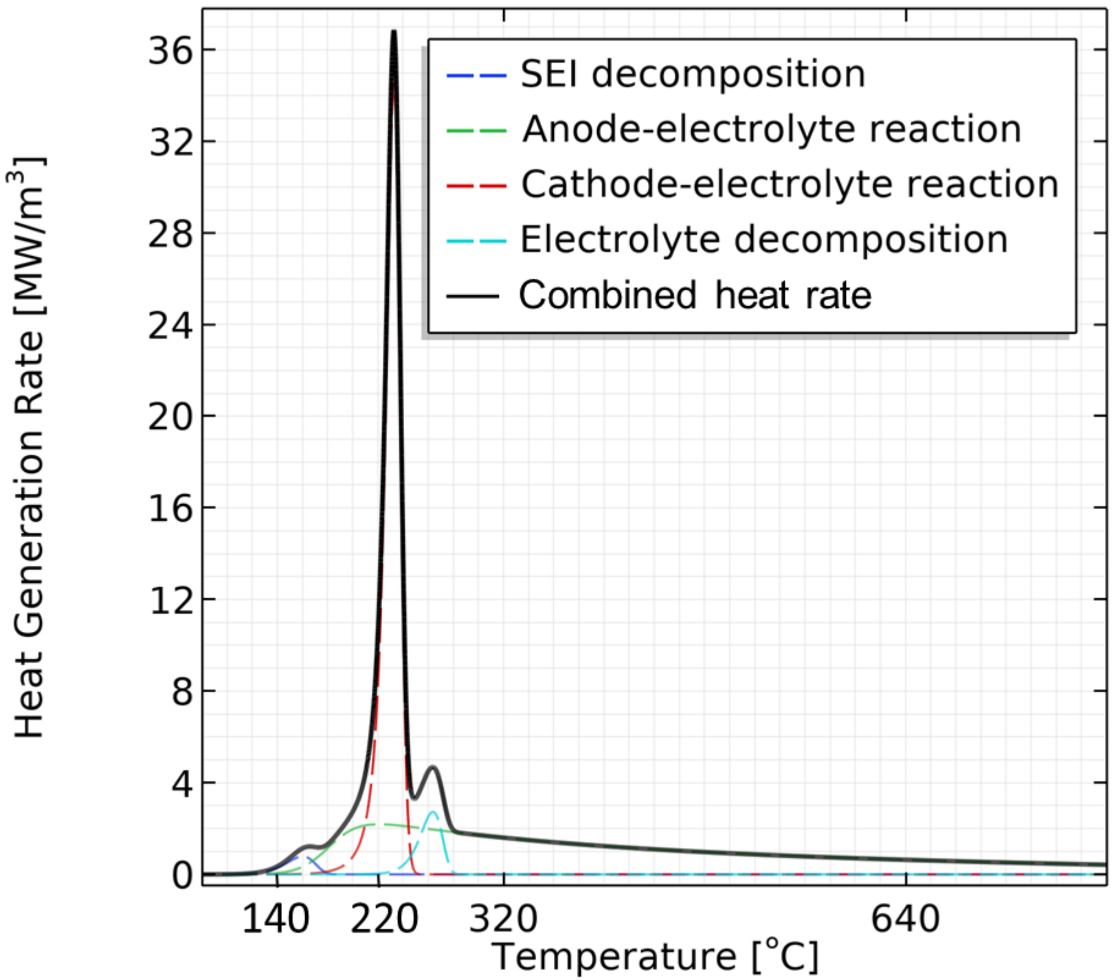
Lithium plating coupled with lithium dendrite growth represents internal short circuit



Abused Graphite Anodes could lead to Thermal Runaway

Failure Modeling (Chemical Decomposition)

- Chemical decomposition reaction are exothermic
- Peak heating rates are activated at different temperatures
- Temperature rise during short circuit is often followed by a chemical thermal runaway



Battery Materials are Exothermic and Sensitive to the Internal Cell Temperature

Failure Simulation (Chemical Decomposition)

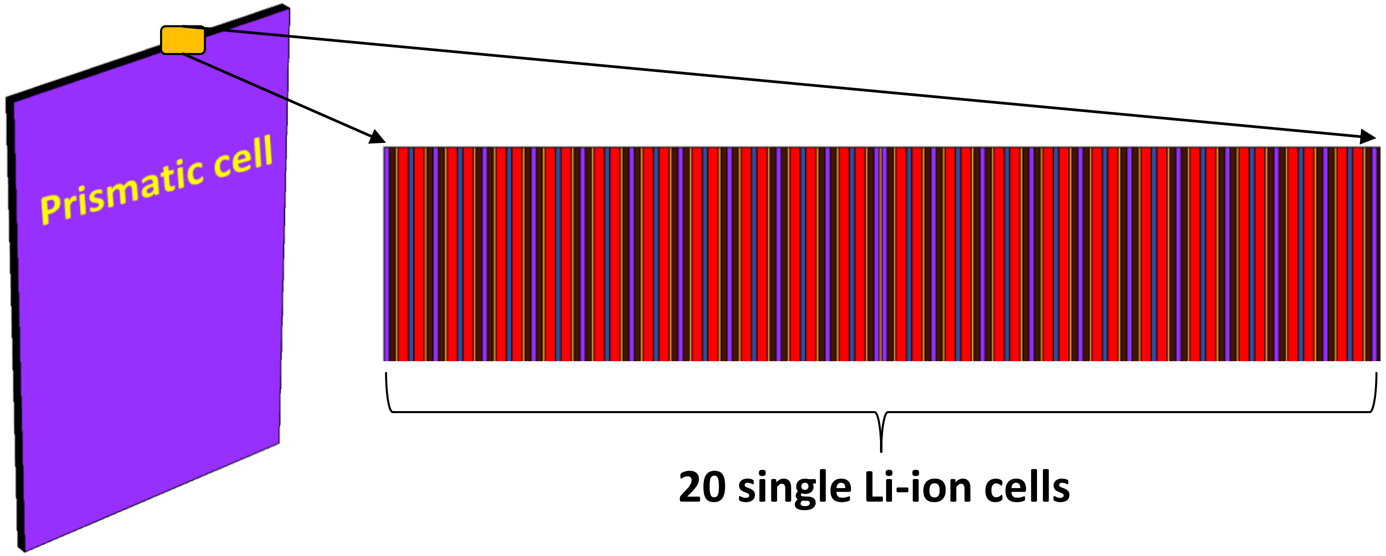
$$\rho C_p \frac{\partial T}{\partial t} = \lambda \nabla^2 T + q_{rev} + q_{irr} + q_{ohm} + q_{chem}$$

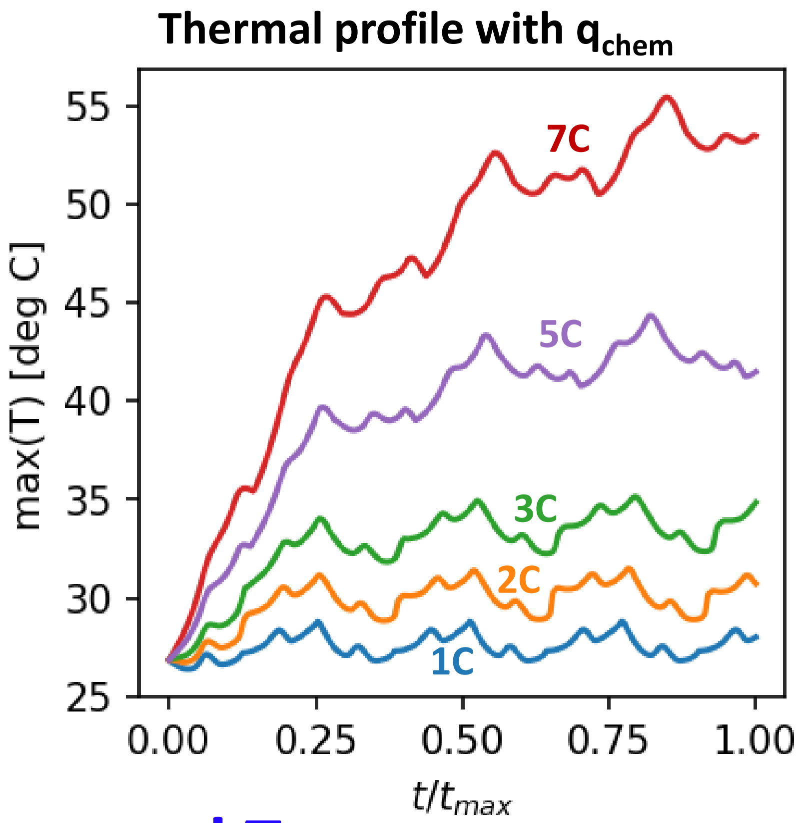
Electrochemical

Chemical decomposition

Thermodynamic

Ohmic and short-circuit





Effect of Chemical Decomposition on the Internal Temperature on a Nominal Li-ion Cell

Thermal Monitoring and Estimation

Estimating Temperature for Predicting Failure

- Finite Element simulations is used to identify important precursors
- Temperature is easy and cheaper to monitor
- A BMS with internal temperature monitoring and a physics-based estimation algorithm could be used for failure prediction

$$\frac{\partial T}{\partial t} = \frac{1}{\rho C_p}[q_{rev} + q_{irr} + q_{ohm} + q_{chem}]$$

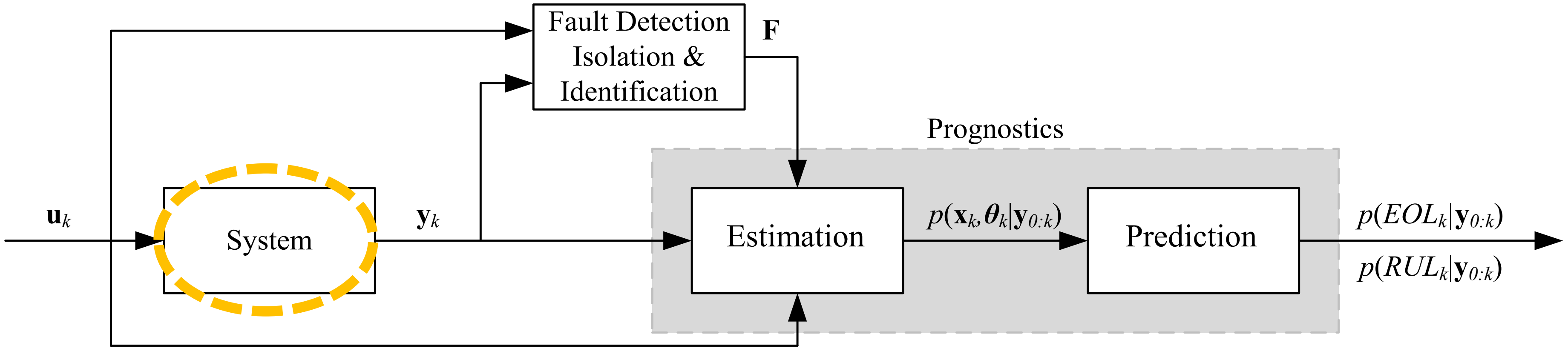
Thermodynamic (q_{rev}), Electrochemical (q_{irr}), Ohmic and short-circuit (q_{ohm}), Chemical decomposition (q_{chem})

Battery Prognostics

Model Based Architecture

1 System receives inputs, produces outputs

2 Identify active damage mechanisms

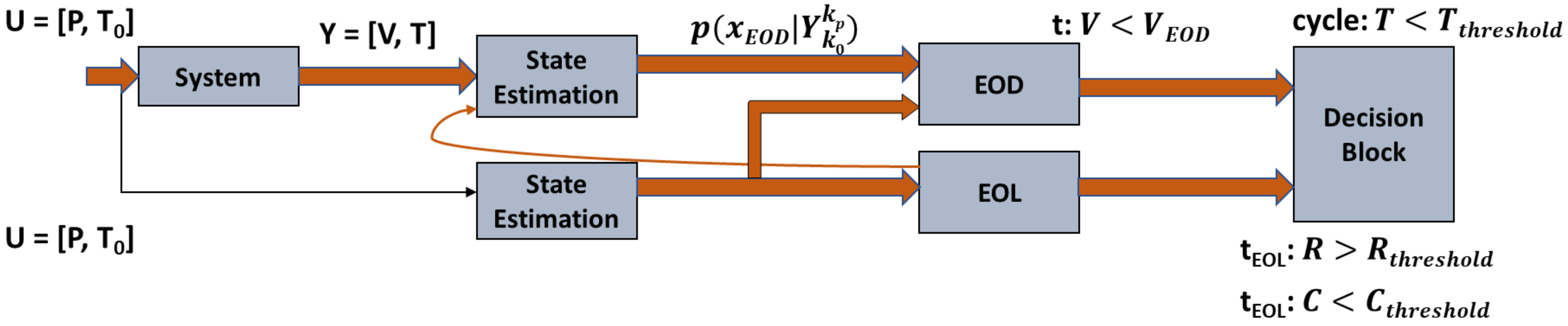


3 Estimate current state and parameter values

4 Predict EOL and RUL as probability distributions

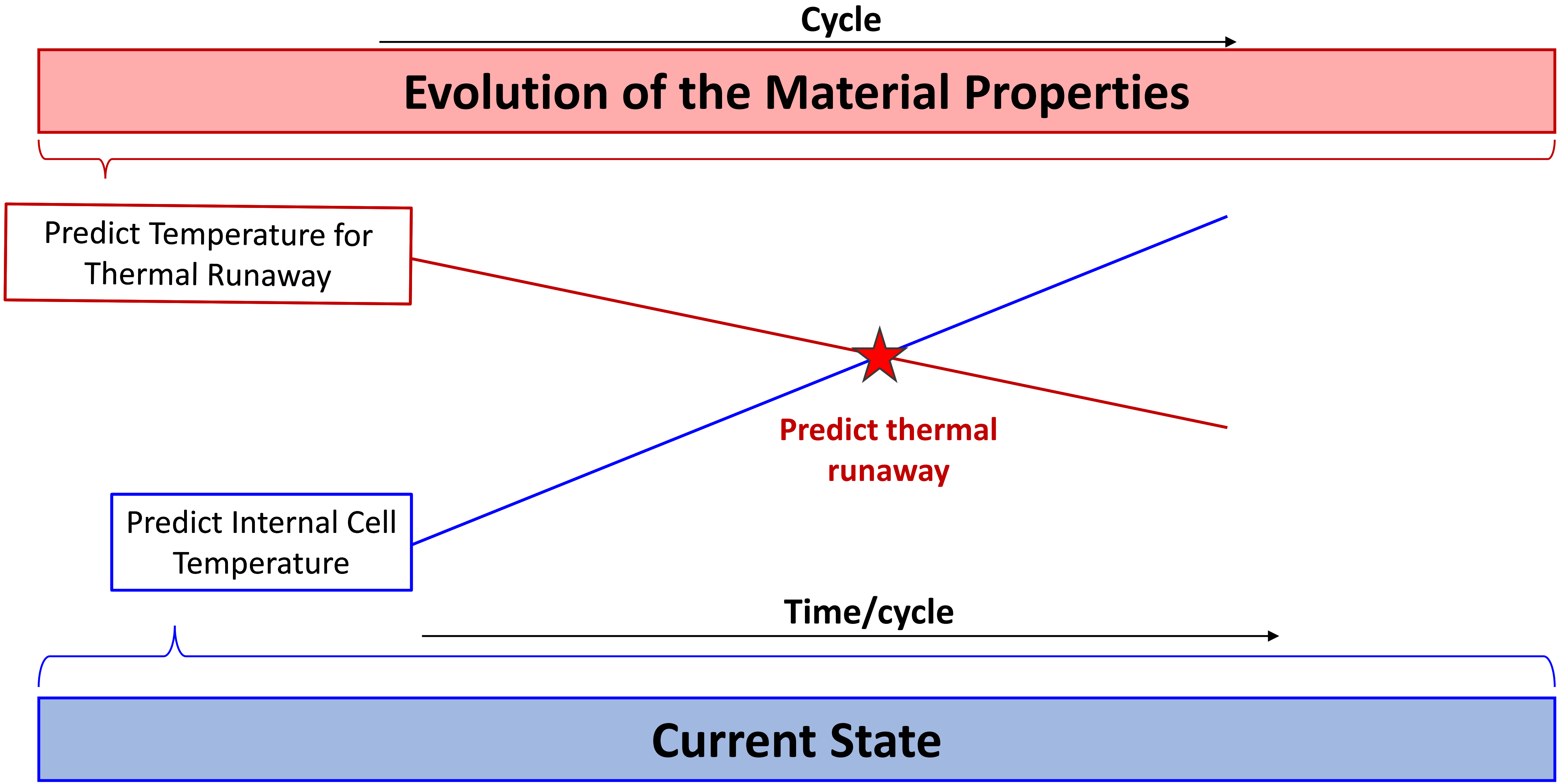
Battery Thermal Prognostics

Modifying the Model for Temperature

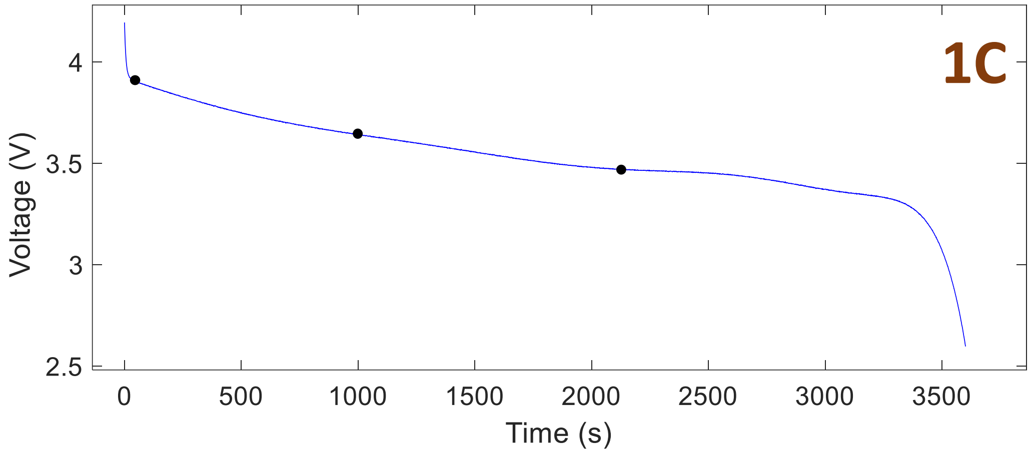


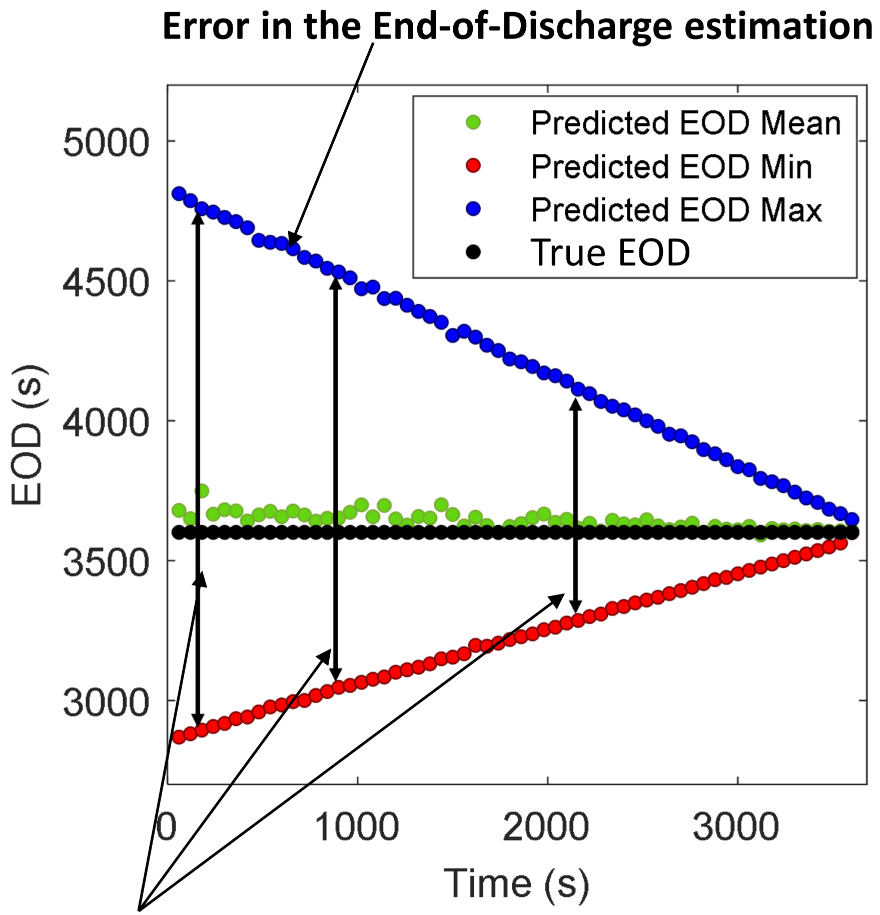
Two State Estimation Blocks can estimate Cell Voltage, Discharge Time, Cycle Life, and Temperature Thresholds

Current Goal for Prognostics



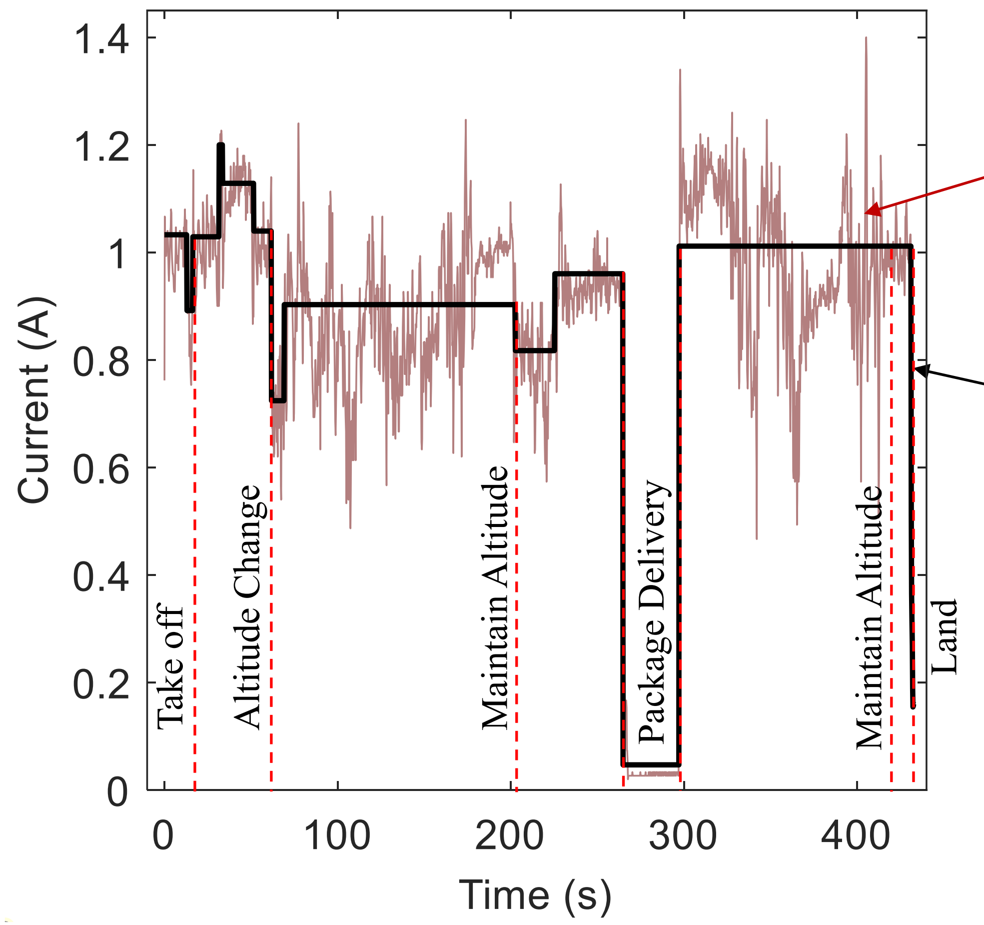
Results From the Prognostics Algorithm





The estimation error reduces as the discharge time increases

Data from a Short Test Flight



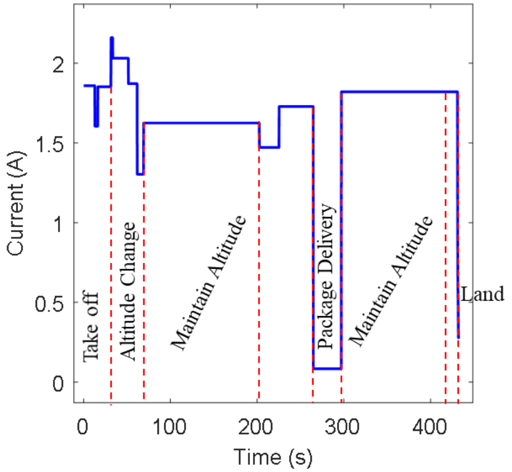
“Noisy” sensor data

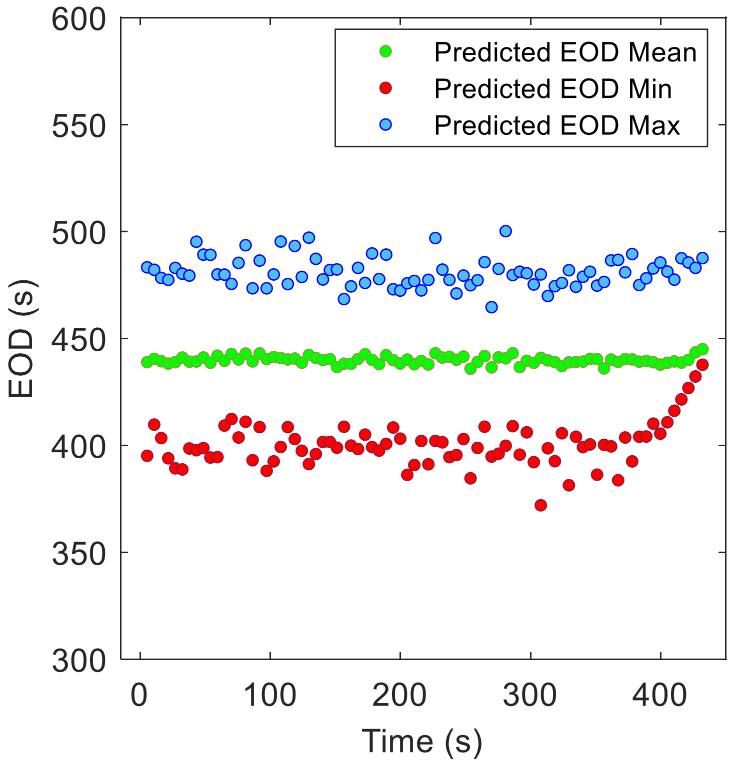
Smoothed data used for prognostics

Data pre-processing is needed for accurate estimation

Preliminary Results for EOD Estimation

Applying Prognostics Algorithm on a Short Test Flight Profile

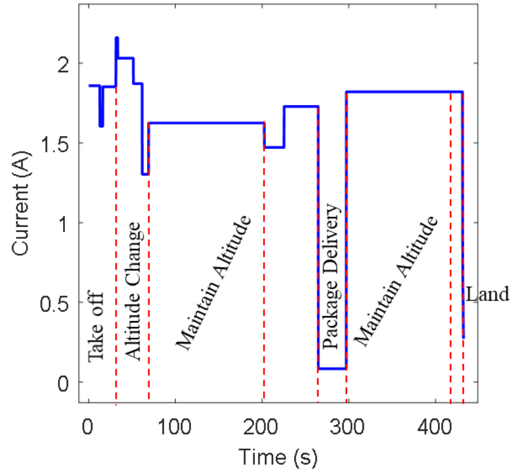


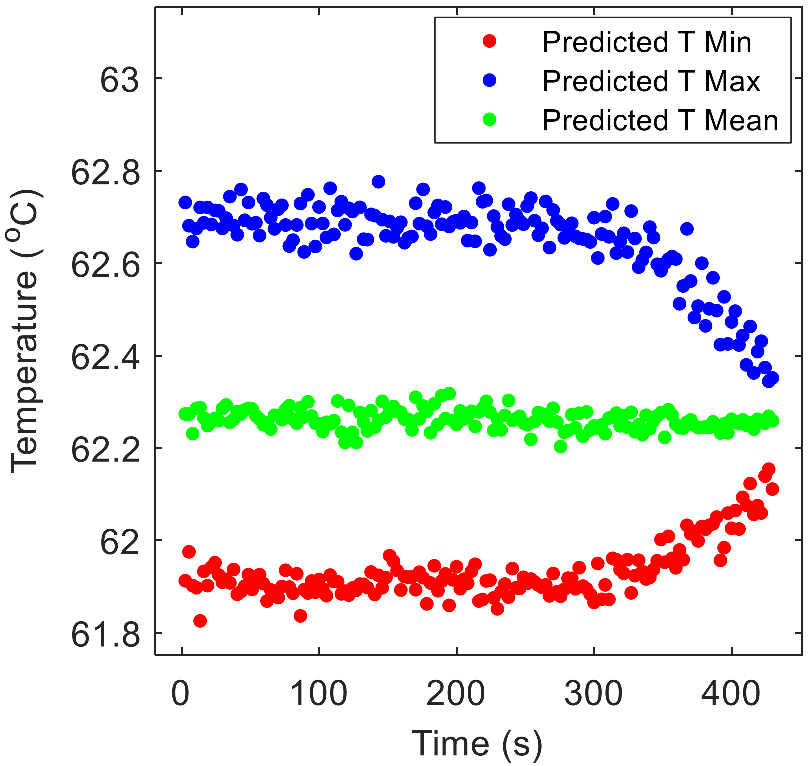


The Distribution of the End-of-Discharge Estimation shows that the Algorithm is working correctly.

Preliminary Results for Temperature Estimation

Applying Prognostics Algorithm on a Short Test Flight Profile





Temperature variation on a nominal and fresh cell is not significant

Summary

- Failure modes identification
- Finite Element Modeling of Failure modes
- Identification of temperature as a failure precursor
- Coupled a thermal model with battery prognostics algorithm
- Voltage and temperature estimation for a single cycle

Next Steps

- Estimating temperature over cycle life
- Estimating temperature for off-nominal behavior