Development of Thermal Runaway Risk Database

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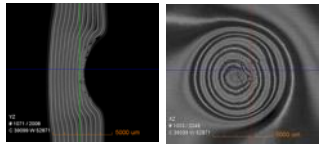
Sandia National Laboratory

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

Battery Pack

Battery Modules

Battery Cells



XCT: Indented Battery

Project Overview

- To develop a Li-ion battery thermal runaway risk database for energy storage systems
- It is important to understand and manage the safety risks of Li-ion batteries in energy storage systems, especially for thermal runaway
- This work fits specifically into OE efforts to ensure a resilient, reliable, and flexible electricity system

Ultimate Goal: Select a Li-ion cell with unknown safety risk; perform a single indentation test; use the database and machine learning prediction tools to rank/predict the cell thermal runaway risk

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Thermal Runaway Risk Database Development

- **Project Period:** FY18-FY20 (actual start in June 2018)
- **Annual Budget:** $300K (ORNL)
- **Project Team:** Collaboration with Sandia National Laboratory (J. Lamb, J. Stanley and L. Torres-Castro)
- **Project Milestones:**
  - Complete 33 Ah and 26 Ah cells testing at ORNL and Sandia
  - Data Analysis: Rank the cells in terms of thermal runaway score
  - Expand database covers wide ranges of cells, capacities, chemistries
  - Data analyzed using machine learning tools: Basic and advanced

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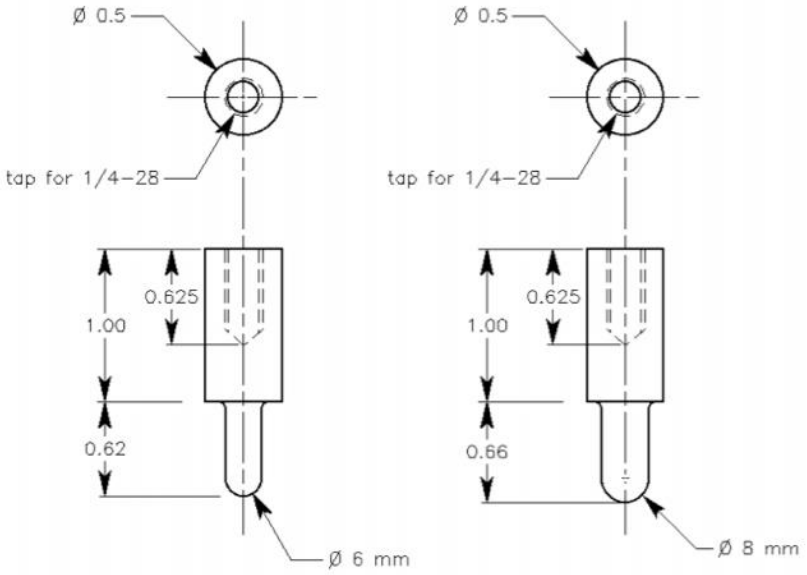
ORNL-Sandia Test Procedures and Standards

Internal Short-ciruit Induced Thermal Runaway

- **Mechanical abuse (indentation)**
- **Thermal abuse**
- **Electrical abuse**

<u>Final Test Protocols:</u>

- **Cycle cell 5 times at C/2 between 3.0-4.2V to determine SOC and discharge to test SOC**
- **Hydraulic or servo-motor driven load frame**
- **6 mm punch (most sensitive, small contact)**
- **0.05 inch per minute loading**
- **100 mV Voc drop**
- **Hold the punch after short circuit**



Punches for Battery Testing		
ELC-2019.03.001		Scale: 1.5:1
Dimensions: inches (unless otherwise specified)		Material: stainless steel
Make four (4) pieces of each		
Edgar Lara-Curzio	ORNL	March 2019

Select the most sensitive test to allow safety risk ranking

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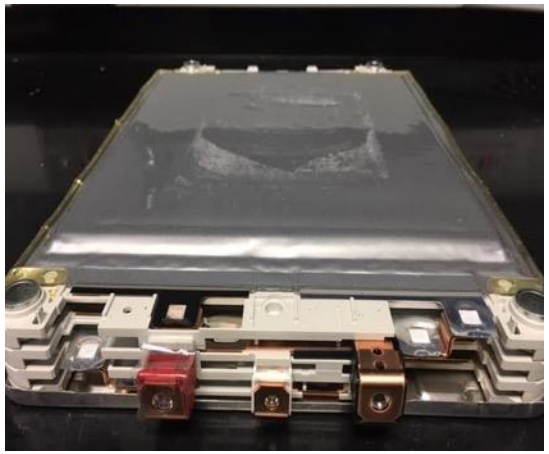
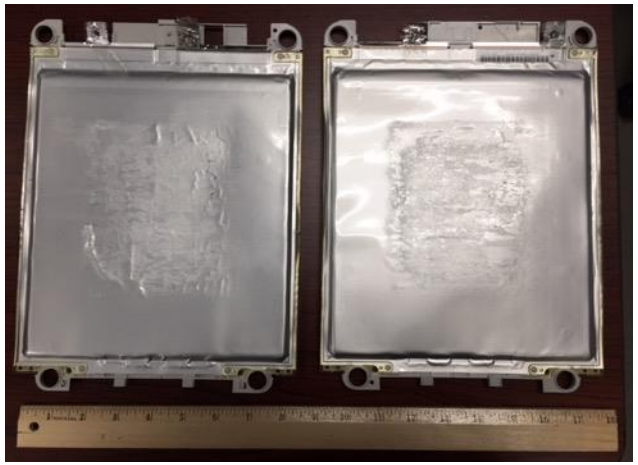
Challenge: Source of Li-ion Cells with No Strings Attached

Energy Storage System

Large Format Cells Tested at ORNL and Sandia



Disassembled Module



Individual Cells (32 Ah)

Commercial NMC Cells (10 Ah)

Disassembled Module

Individual Cells (26 Ah)

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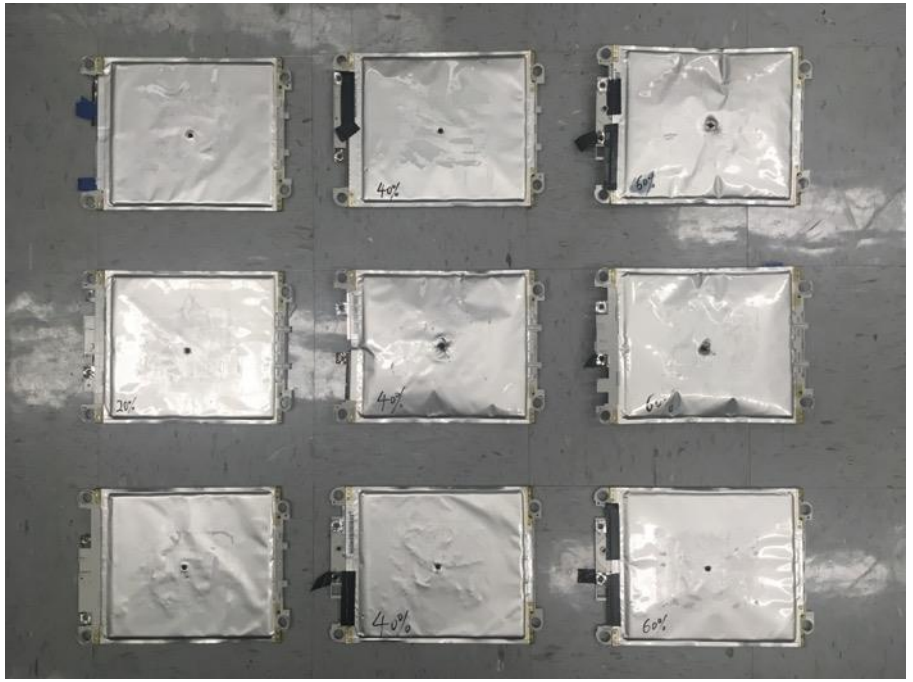
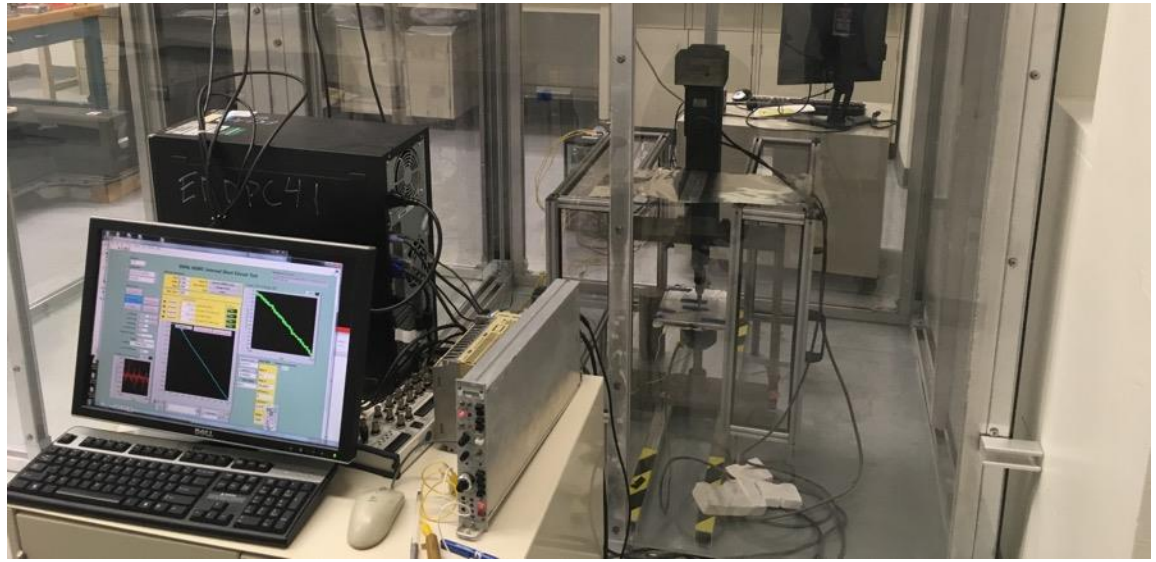
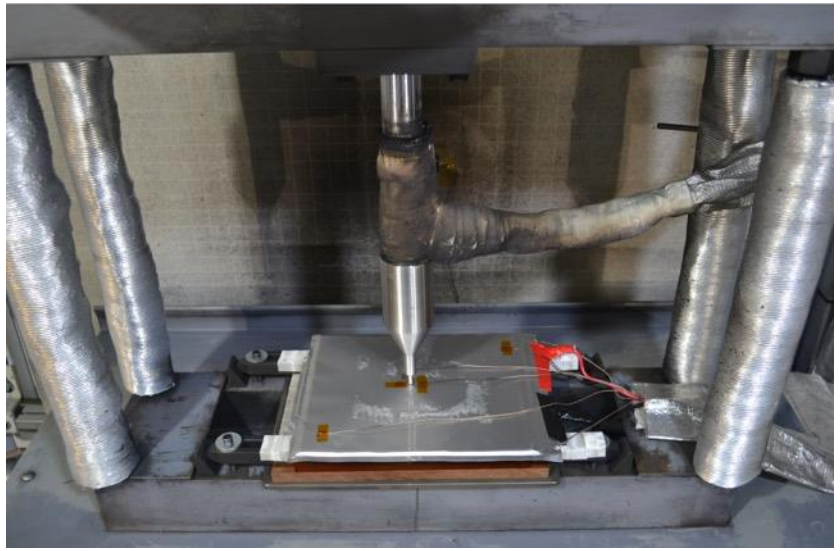
ORNL Testing Facility: Large Format Cells



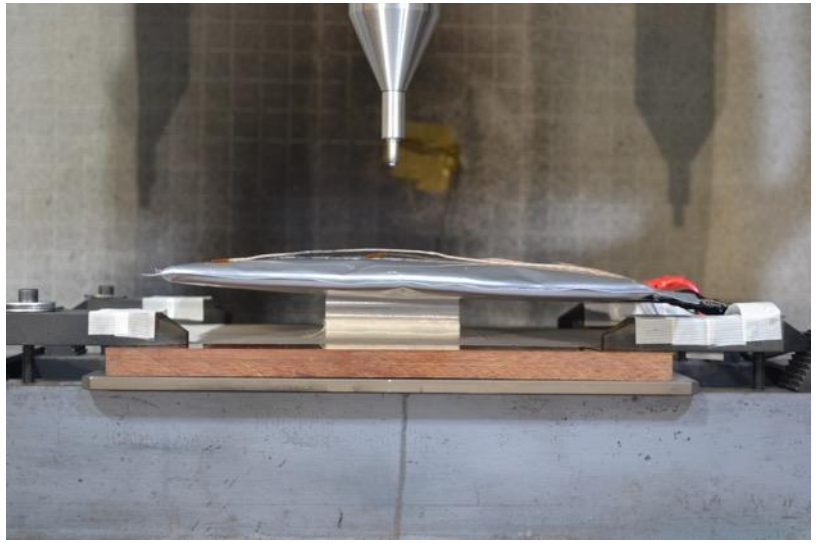


Sandia Efforts: Large Format Cells Testing, Data Analysis

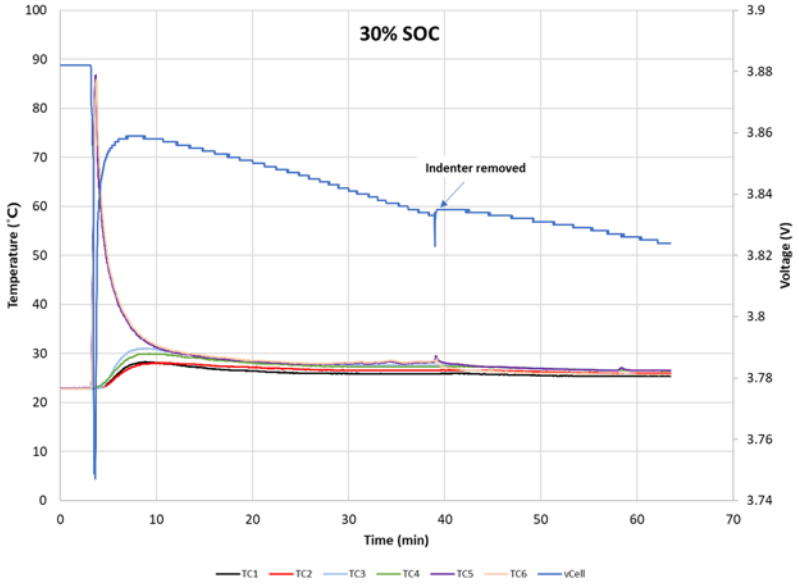
Nissan Leaf Cell in Sandia Test Chamber

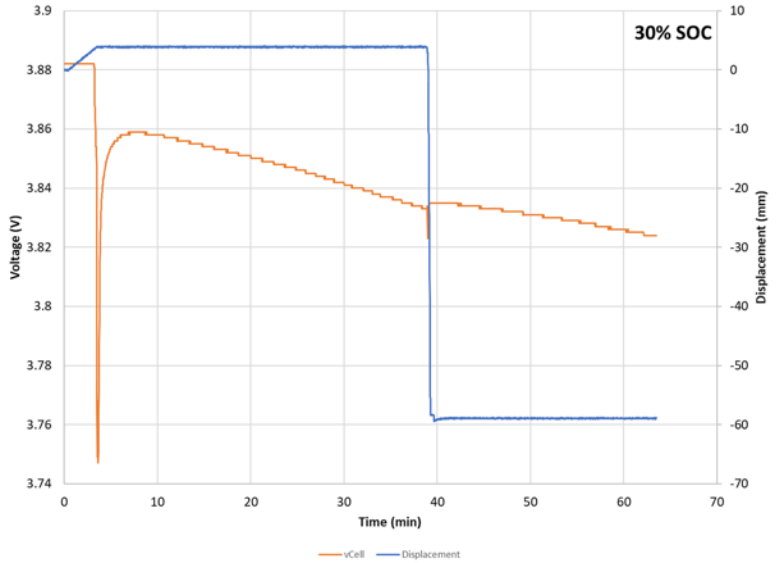


Nissan Leaf Cell After Indentation



Voltage and Temperature





Voltage and Displacement

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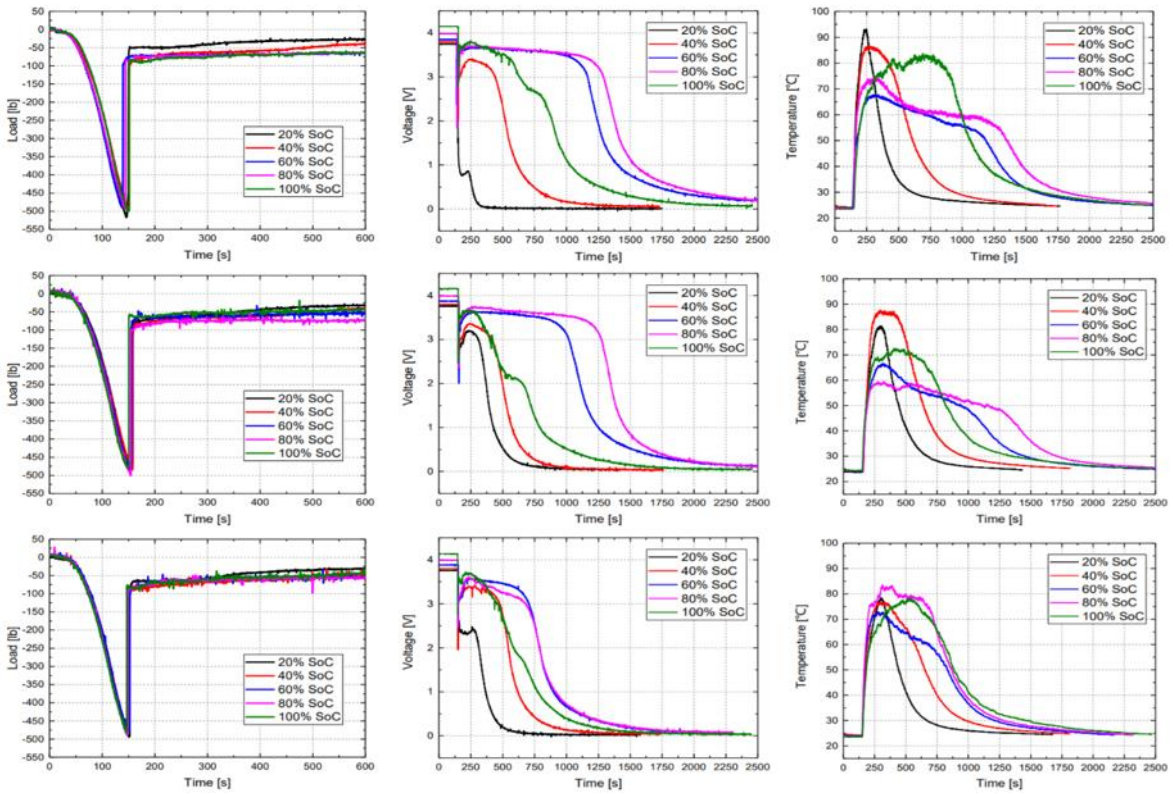
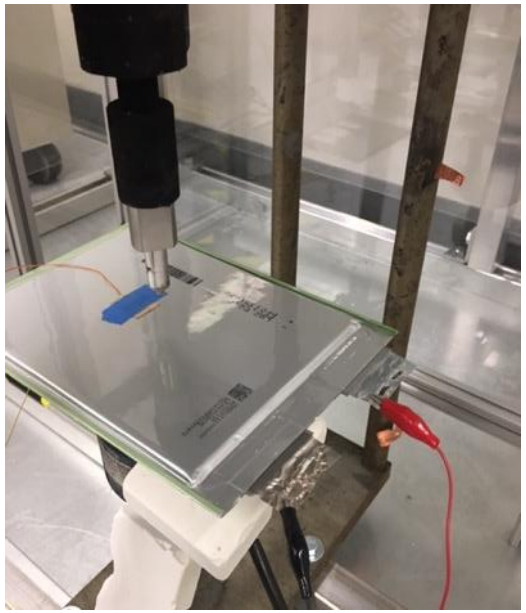
Thermal Runaway Risks for Li-ion Batteries (ORNL-Sandia)

Load **Voltage** **Temperature**





Test Data and Cell Information:

- Cell Capacity
- Loading curve: before & after short
- Cell Voltage: drop and response
- Cell Temperature vs. Time
- Open cell voltage
- Anode thickness
- Cathode thickness
- Separator thickness
- C/2 Charge curve
- 1C discharge curve

Example of Traditional Data Analysis

Cell Capacity (mAh)	500	500	500	500	500
SOC %	20%	40%	60%	80%	100%
Test Cell Capacity (mAh)	100	200	300	400	500
Voc (V)	3.75	3.784	3.861	3.991	4.147
V drop Initial (V)	0.25	2.284	0.351	3.581	3.955
V at 300 sec (V)	0.0183	0.095	0.407	0.15595	0.033569
Sumof V*Δt (V-Sec)	120.63	110.47	220.09	77.176	29.462
Load at failure (lb)	-338	-337.52	-345.7	-355.16	-353.82
Load during hold (lb)	-81.79	-88	-131.6	-170.04	-147.09
Temp Max	79.83	78.055	82.93	81.913	86.655
Sum of ΔT*Δt (K-Sec)	6685.3	8093.482	10168.27	14668.71	17089.57
Time to reach Tmax (sec)	62.57	33.6	61.2	60.8	57.8

Small Cells Testing at ORNL:
SOC: 20%, 40%,60% 80%,100%
Capacity at 500, 1500, 200 mAhr
Number of Cells: 4 cells/condition

ESS Batteries at Various SOCs:
Sandia: 30%, 50%, 75%, 100%
ORNL: 20%, 40%,60% 80%,100%

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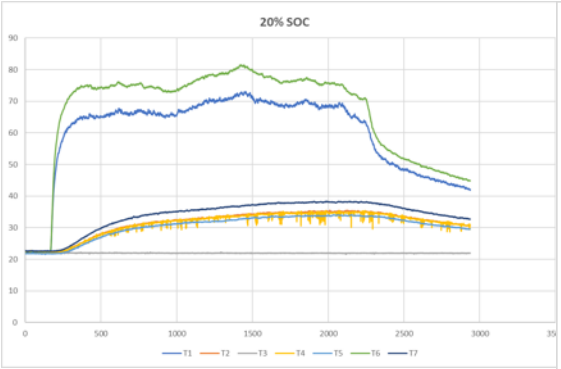
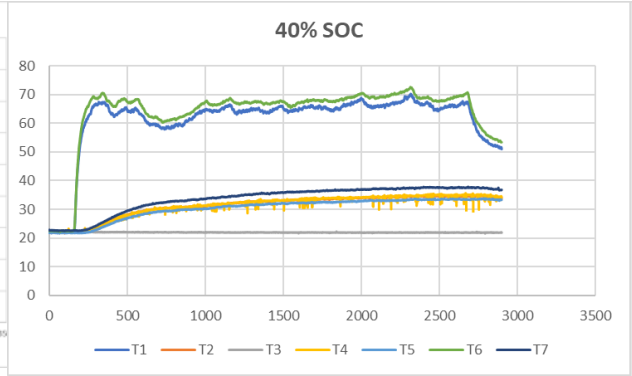
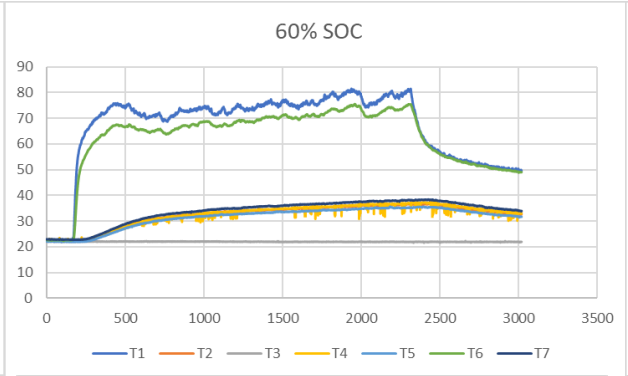
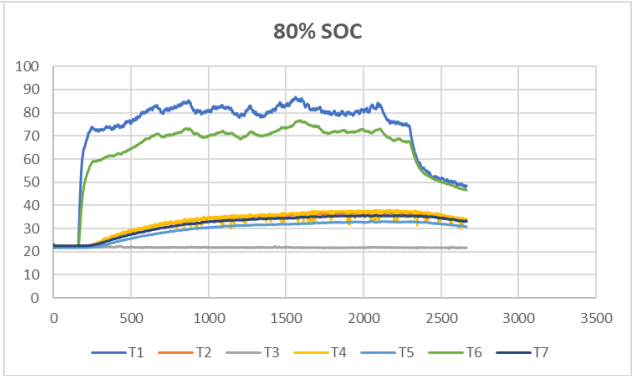
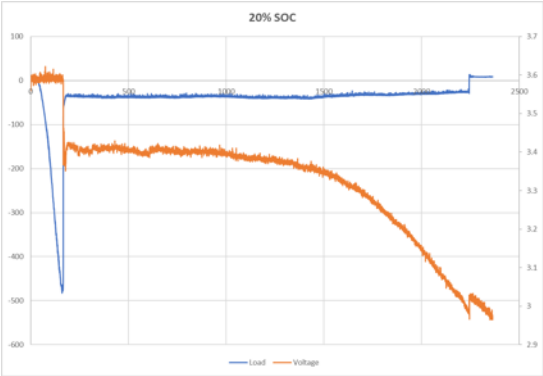
Chevy VOLT Test Data and Nissan Leaf Test Data

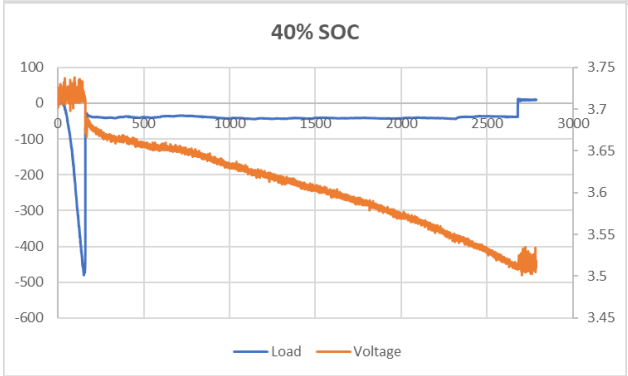


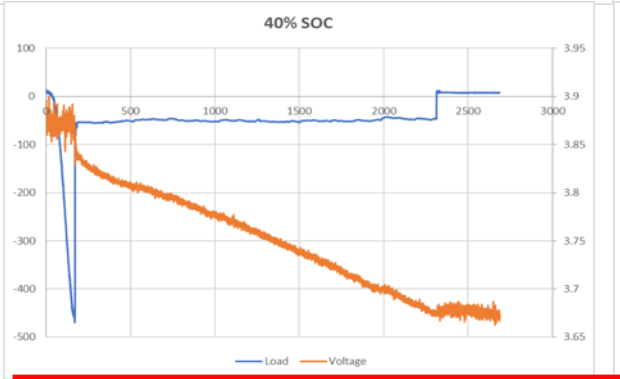


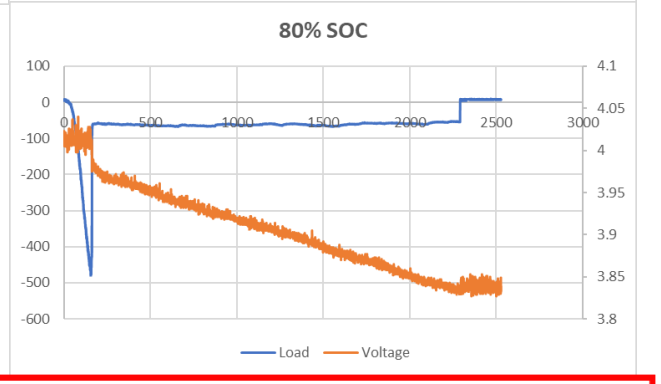


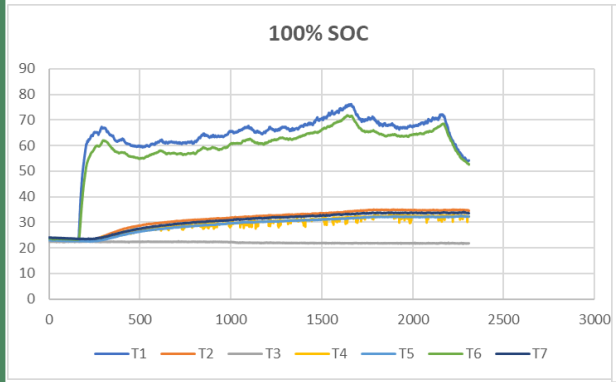


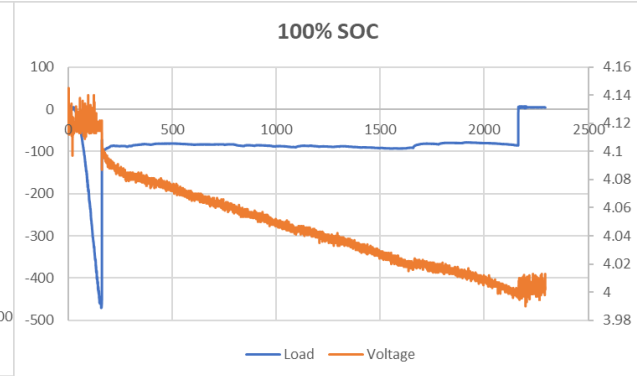


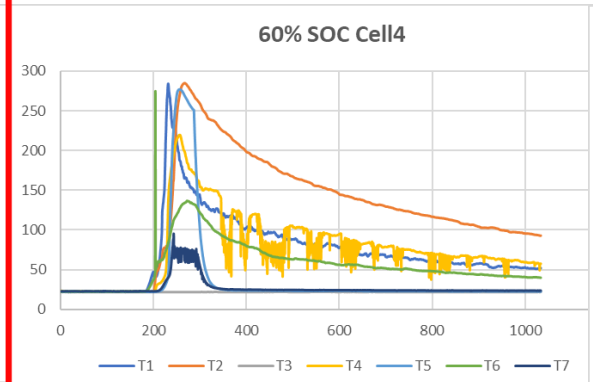


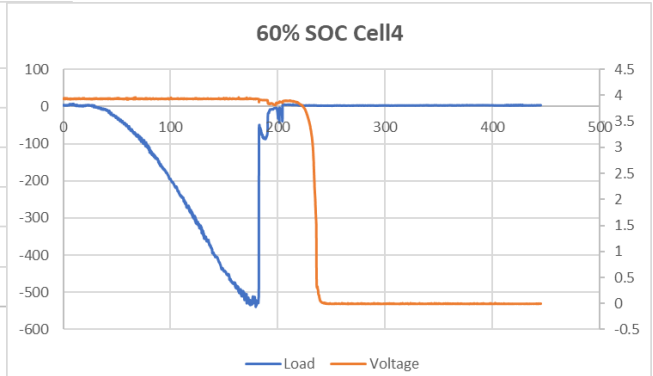










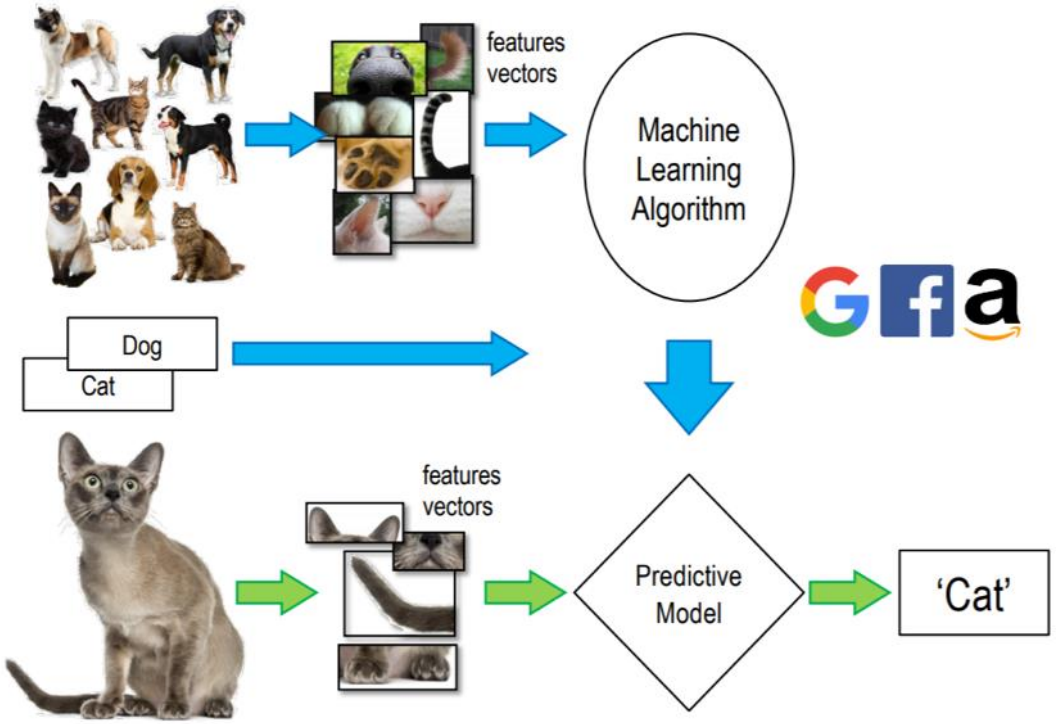


Thermal Runaway

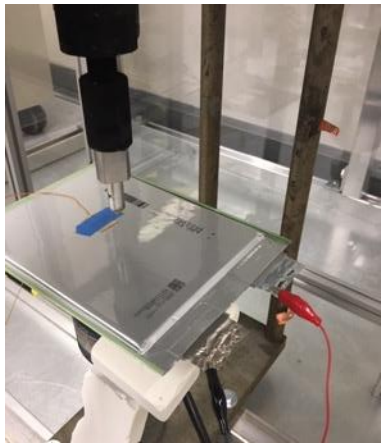
Using Machine Leaning Tools for Battery Safety

How machine learning works?

- Simple superficial features (e.g., ear, nose, paw, tail)
- **Huge** training dataset is usually required to develop predictive models with high accuracy



This Project:
One battery
One Indentation



ML Model

Thermal Runaway Risk Score

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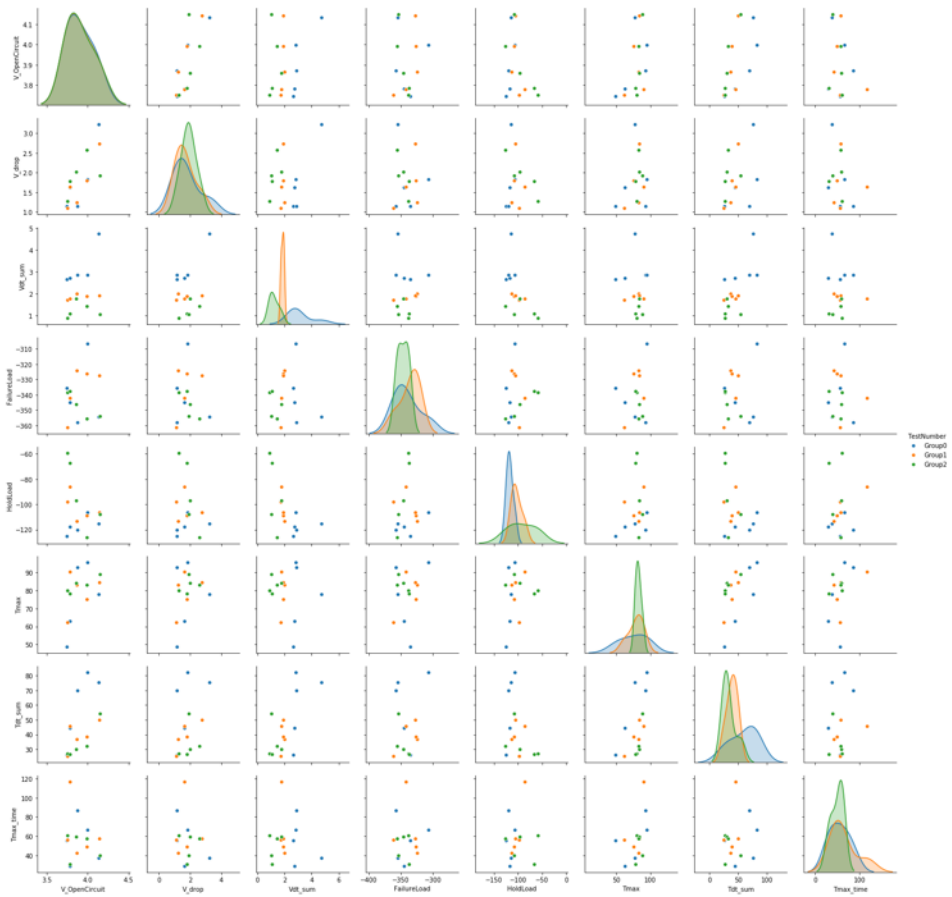
New Approach: Machine Learning Data Analysis

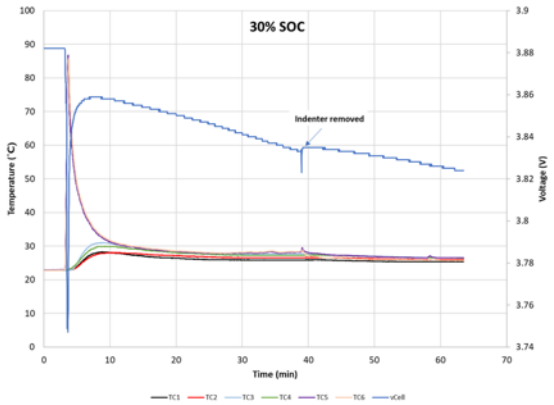
Project Goals:

- Rank cells in terms of thermal runaway risk via comprehensive testing at ORNL and Sandia
- Predict thermal runaway risk of new cells using the database information
- Predict thermal runaway risk unknown cells by limited testing and use ML for prediction



Example: ML Analysis Open Source Software

Voltage and Displacement vs. Time



ML Data Analysis Features:

- Analyze parameters correlation
- Identify sensitive parameters
- Training data sets: test data
- Prediction and ranking

SOC	TestedCapacity	V_OpenCircuit	V_drop	Vdt_sum	FailureLoad	HoldLoad	Tmax	Tdt_sum	Tmax_time
20	100	3.745728	1.147461	2.648559	-335.571680	-125.267985	48.749	26.3770	55.7
40	200	3.781433	1.621094	2.716705	-345.080566	-117.699707	63.111	44.5640	28.9
60	300	3.872986	1.150818	2.863648	-358.065820	-120.303061	92.944	69.6976	86.7
80	400	3.998108	1.834412	2.842712	-306.482666	-106.499088	95.381	82.2172	66.9
100	500	4.132080	3.233032	4.733307	-354.538330	-115.336545	77.753	75.3942	37.3
20	100	3.750610	1.092529	1.729156	-361.388818	-97.893185	62.223	25.2136	56.5
40	200	3.781128	1.636047	1.777618	-342.013184	-85.957838	90.343	45.6836	116.6
60	300	3.866882	1.236877	1.992035	-324.120117	-113.315894	83.152	36.9226	42.6
80	400	3.991394	1.799622	1.891968	-326.318408	-108.862092	75.258	38.3880	49.0
100	500	4.143677	2.741394	1.926453	-327.443115	-106.135606	84.331	50.1312	57.5
20	100	3.750916	1.278687	0.893341	-338.378906	-59.318439	79.900	27.0004	61.0
40	200	3.784485	1.784668	1.079346	-337.524414	-66.991820	78.071	26.6582	30.7
60	300	3.860779	2.014160	1.760529	-346.252441	-97.149743	83.985	30.2422	59.7
80	400	3.991089	2.581177	1.420196	-355.773926	-125.970826	82.976	32.0020	57.5
100	500	4.147034	1.920471	1.046448	-353.820801	-107.910288	88.944	54.2370	39.8

3 Sets of ORNL Test Data

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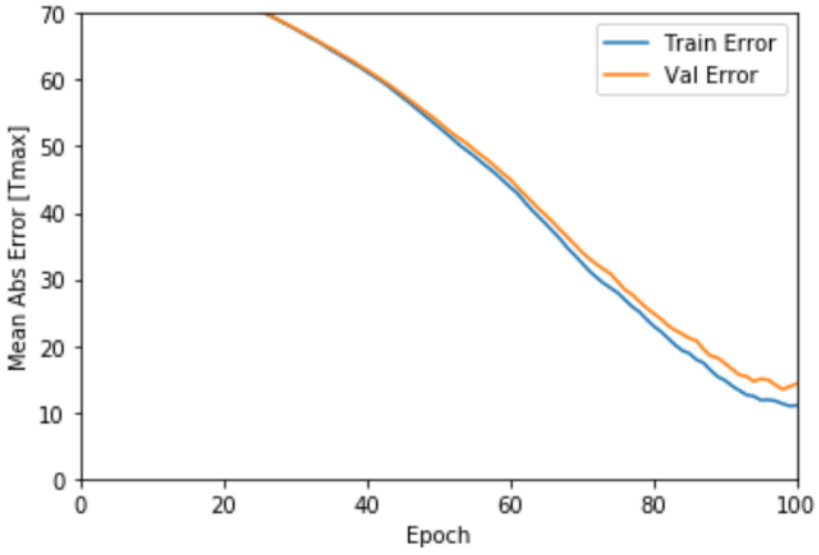
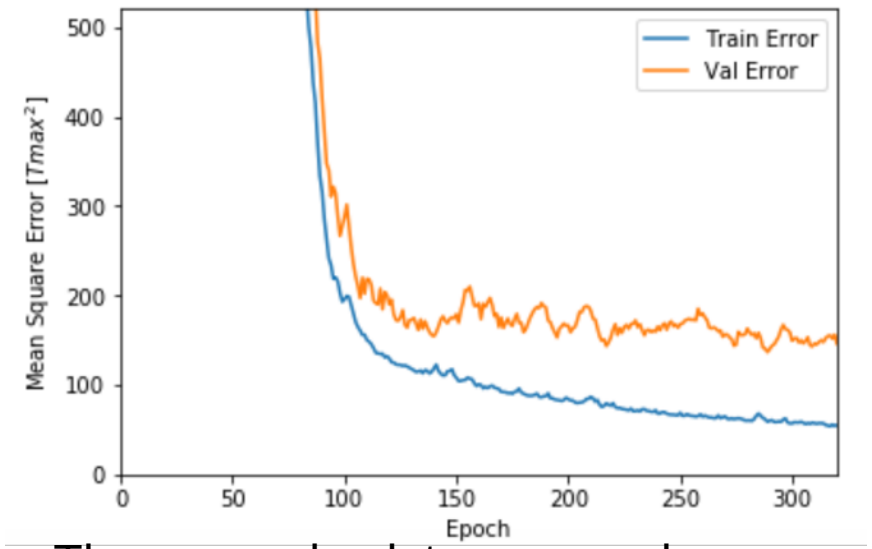
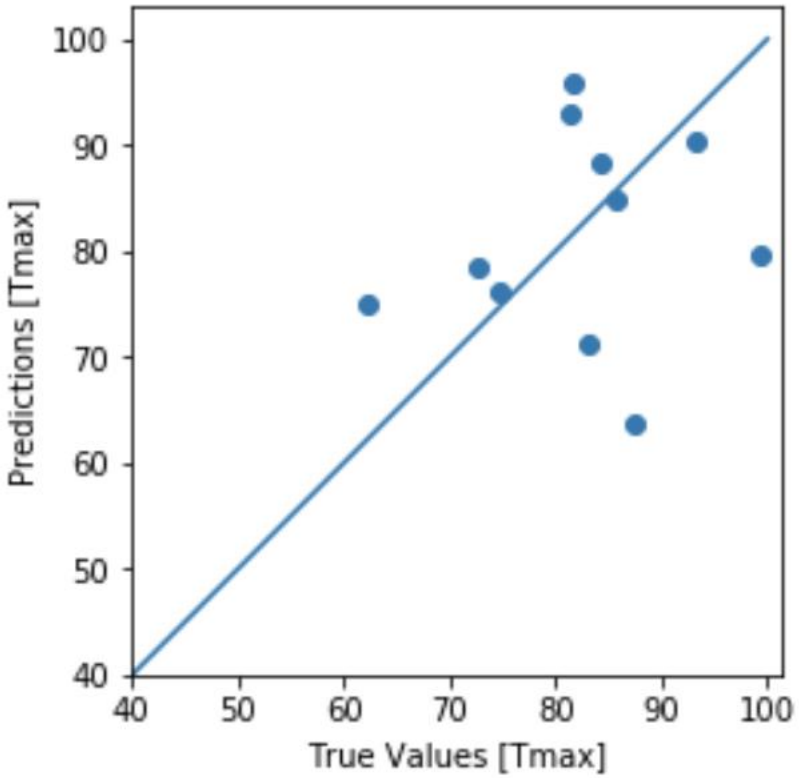
Machining Learning Tools and Predictions





The mean absolute error and mean square error of the network over trained data set shows good neural network fit.



A simple neural network predicts the maximum temperature of the test data set with error of less than 10 degrees

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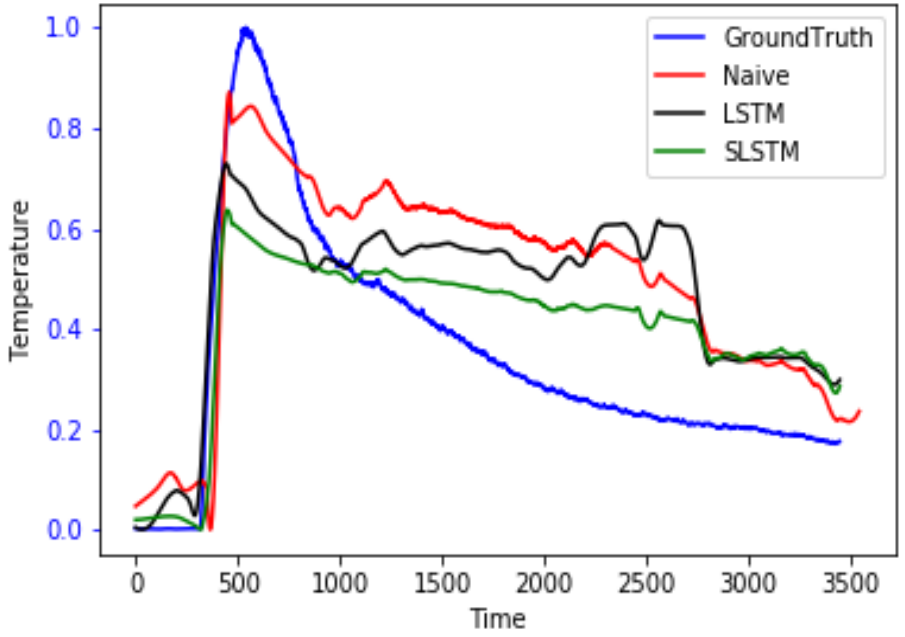
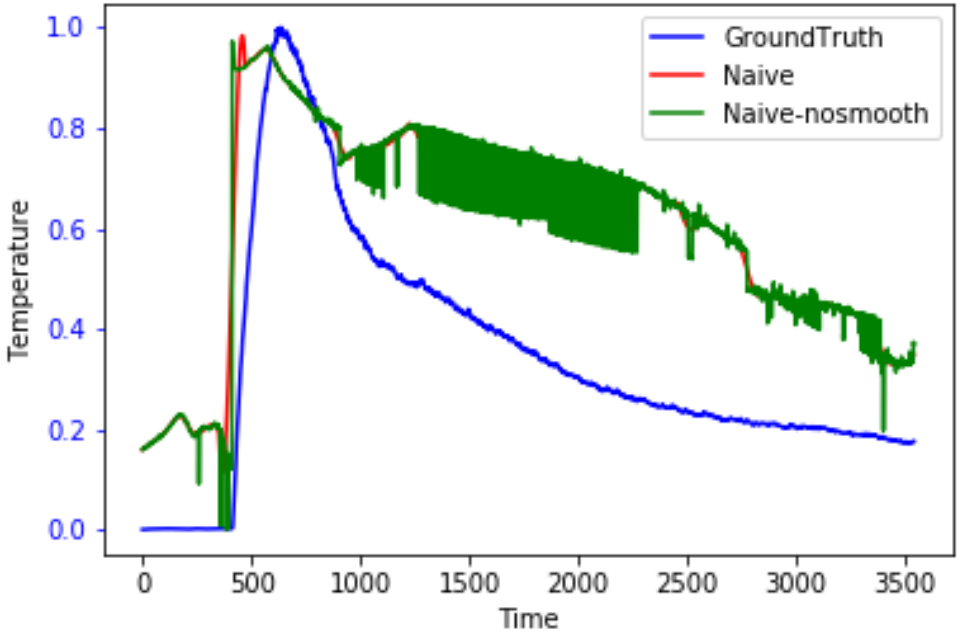
Performance of ML models based on the training of initial dataset





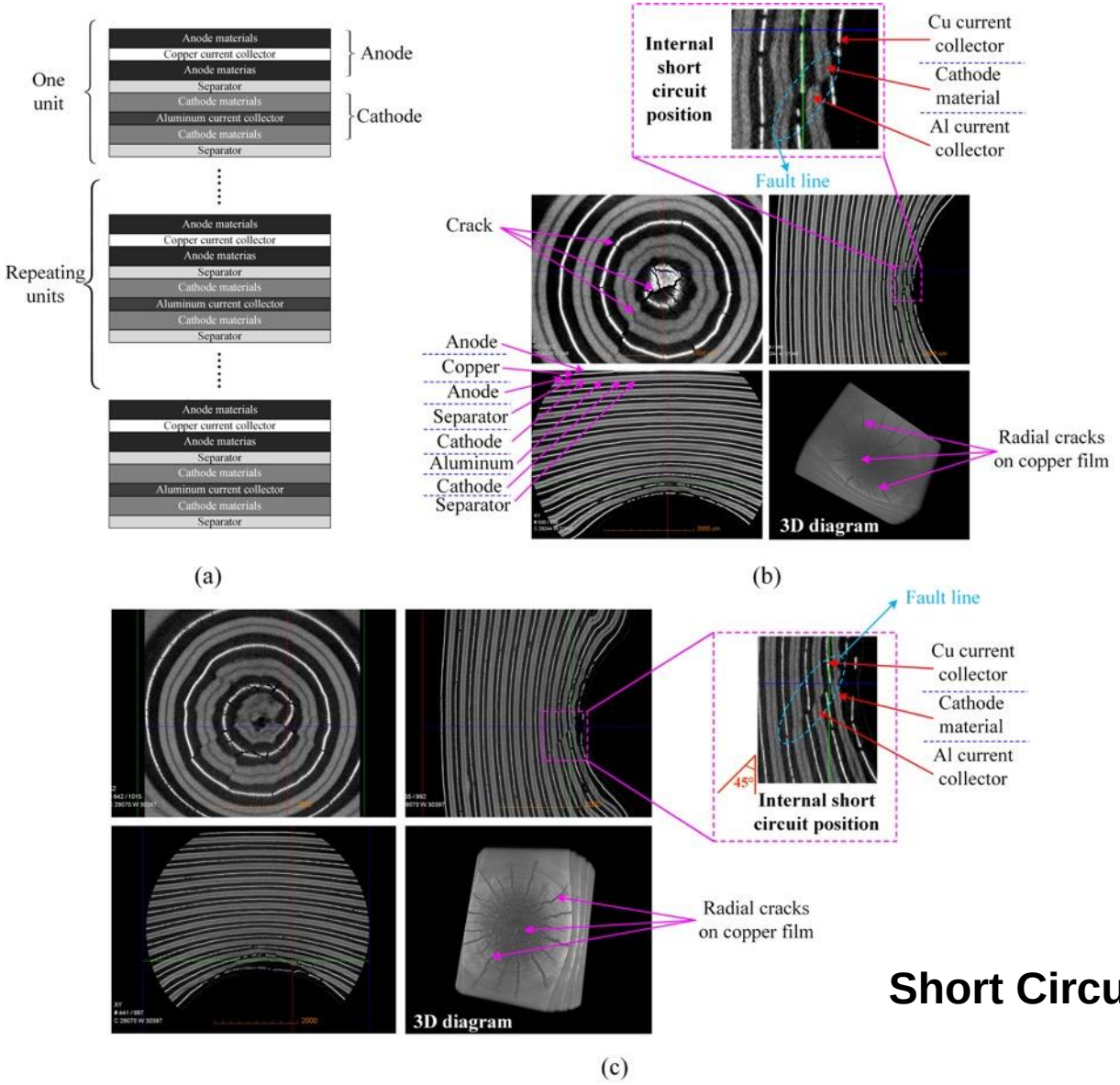
- A mini-batch training of size 13 and three layers of LSTM was chosen. Since there were 39 training points, a batch size of 13 gave sufficient randomization without replacement.

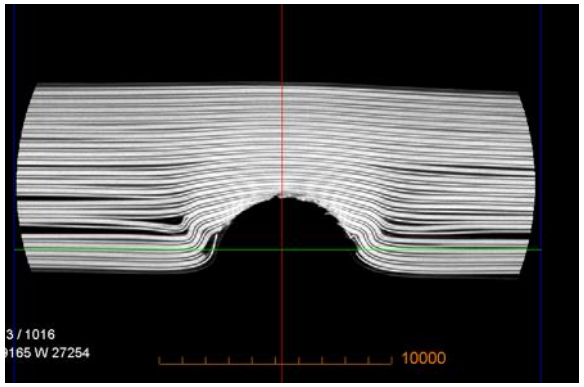
- We are using Mean Square Error $\frac{1}{n}\sum_{i=0}^{n}\sum_{t}(y_t - \hat{y}_t)^2$ to represent the closeness of the ground truth temperature with the predicted temperature.

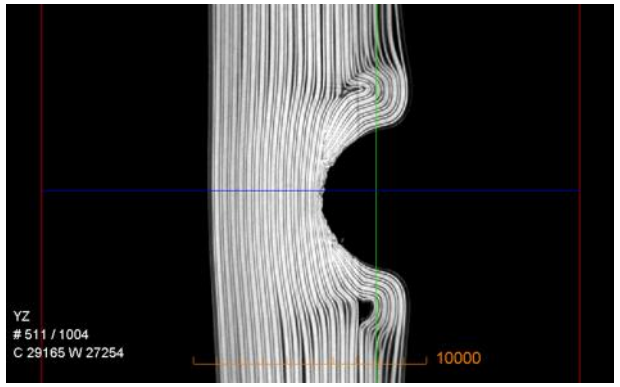
- We plot the temperature curves across the different variants *naïve, LSTM* and *SLSTM*. All the three variants were good in capturing the thermal run away. But, were differing in the max temperature and the decaying temperature

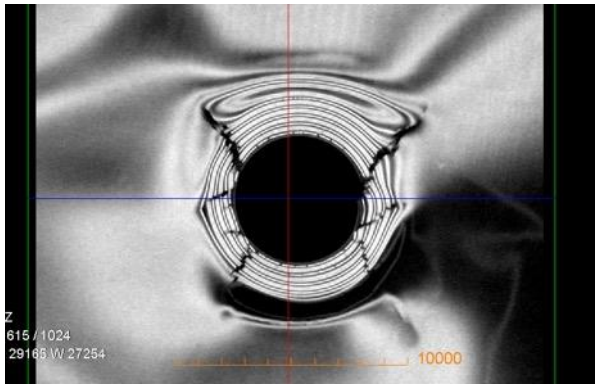
Long Short-Term Memory: LSTM

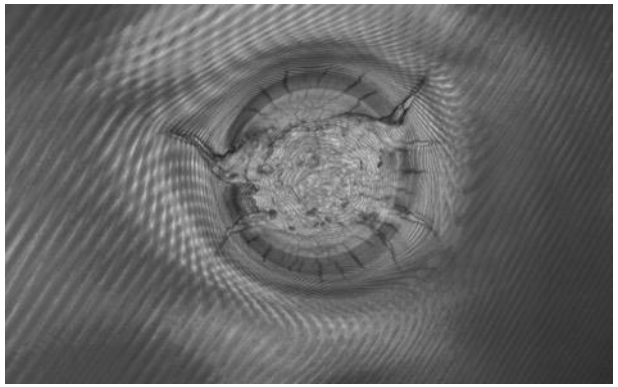
X-ray Computed Tomography (XCT) Scans of Indented Chevy Volt Cell











Short Circuit Induced on a Chevy Volt Cell Discharged to 2.80 V

National Laboratory

Summary and Future Plan

FY2020:

- Covid-19 slowed down large cell testing
  - ✓ Completed large format cells testing at ORNL and Sandia
  - ✓ Small cells test results published
  - ✓ 1Ahr NMC(811) tested
  - ✓ 10 Ahr NMC purchased/started
- Optimized machine learning functions of the database
- Other accomplishments/publications:
  - ✓ Capacity fade via indentation (published)
  - ✓ Internal short circuit method (published)
  - ✓ Large format cell testing (Sandia)
  - ✓ Machine learning analysis (ORNL)

FY 2021 Plan:

- Continue working with Sandia on database development and refinement of test procedures
- Include more cell testing data
  - More cell capacities
  - More cell chemistry: LFP, NMC
- ML/AI tool development
- Sandia web interface for database
- Standardization: UL and ESS test code
- Education: Communicate with ESS and cell manufacturers on test method and results

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Acknowledgement

Support of DOE Office of Electricity (Dr. Imre Gyuk)

ORNL Program Management: Tom King and Michael Starke

Publications:

1. Xiaoqing Zhu, Hsin Wang, Srikanth Allu, Yanfei Gao, Ercan Cakmak, Emma J Hopkins, Gabriel M Veith, Zhenpo Wang, "nvestigation on capacity loss mechanisms of lithium-ion pouch cells under mechanical indentation conditions", ***Journal of Power Sources***, Volume 465, 228314, July 2020,

2. Xiaoqing Zhu, Hsin Wang, Xue Wang, Yanfei Gao, Srikanth Allu, Ercan Cakmak, Zhenpo Wang, "Internal short circuit and failure mechanisms of lithium-ion pouch cells under mechanical indentation abuse conditions: An experimental study", ***Journal of Power Sources***, Volume 455, 15 227939, April 2020,

3. Zhenpo Wang, Jing Yuan, Xiaoqing Zhu, Hsin Wang, Lvwei Huang, Yituo Wang, Shiqi Xu,"Overcharge-to-thermal-runaway behavior and safety assessment of commercial lithium-ion cells with different cathode materials: A comparison study", ***Journal of Energy Chemistry***, Volume 55, April 2021, Pages 484-498 https://doi.org/10.1016/j.jechem.2020.07.028