

# Battery Lifetime Prediction and Management along with Safety and the Transition

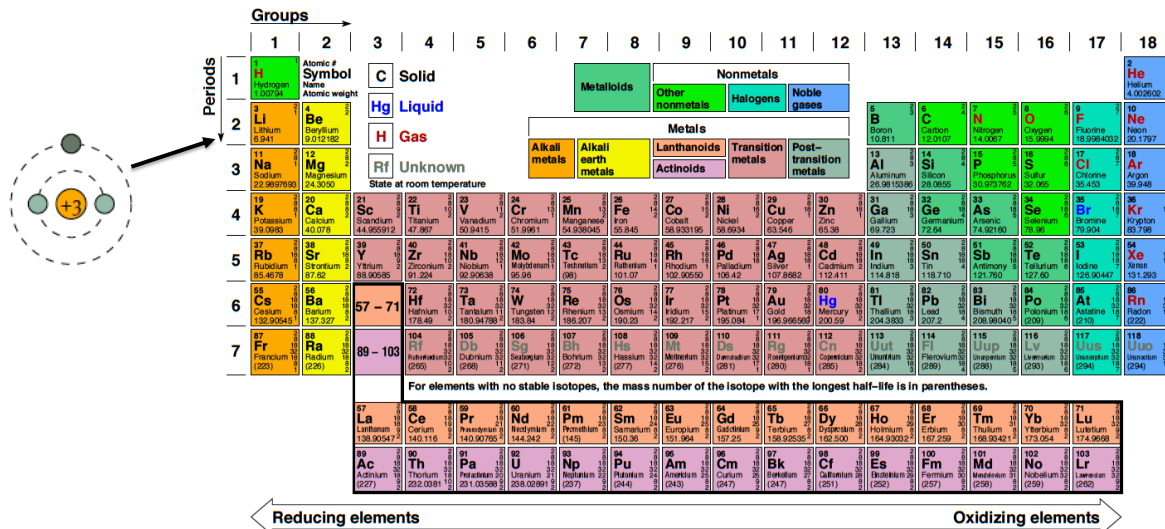
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Thanks to  
DOE (ARPA-E), U.S. ARMY (TARDEC), NSF, NIST  
A123, Amphenol, Daimler, Ford, GE, GM, LG, and Samsung



## Lithium-Ion Battery 101

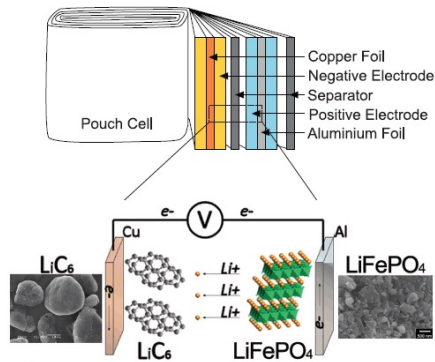


G. Plett, Battery Management Systems, Vol I, Battery Modeling, Artech House Publishers

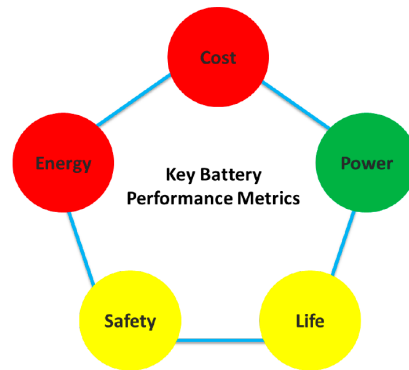


# Li-ion Battery Operation

## Five Layers



## Five Metrics

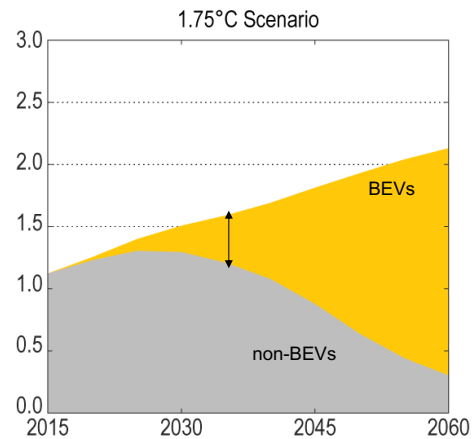
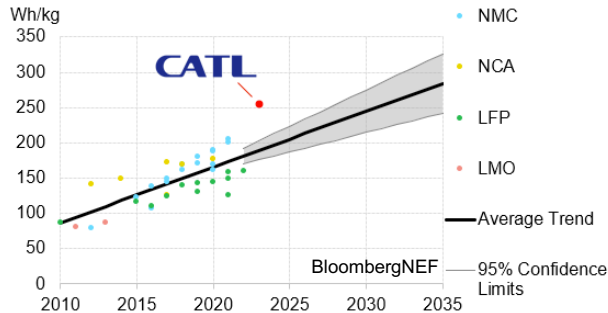


# Batteries Bonanza

US Goal: 50% of LDV sales by 2035  
 (10,000,000 EV/year)  
 → produce 2000 prismatic cells per min

IEA has projected that  
**500M BEVs are needed globally by 2035**  
 to maintain global warming at 1.75 degrees

Battery pack energy density



## Batteries Galore



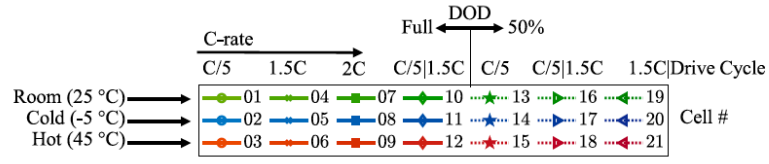
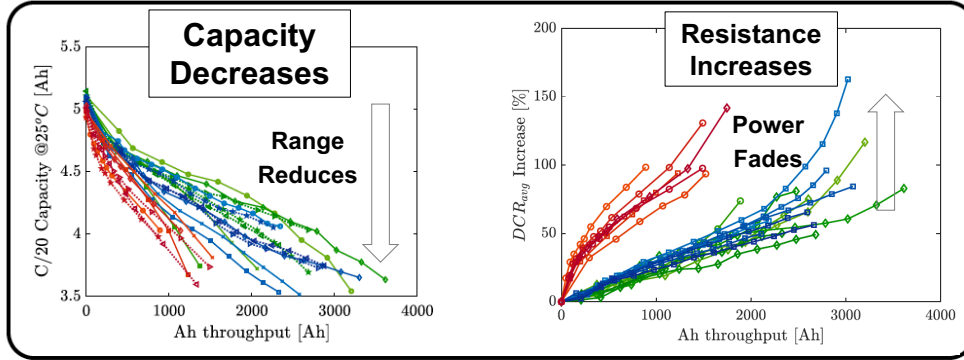
## Batteries are like Humans

- Hate to be overworked
- Fussy about external pressure
- Dislike extremes in temperature
- Diverse in chemistry, size, and shape
- Statistically faulty
- All cells must die, sometime



GM Brownstown Battery Assembly Plant Worker Tina Oaks attaches a wiring harness on a Spark EV battery pack Tu May 13, 2014; J.F. Martin for GM, appeared in Detroit Free Press Dec 18, 2018

# Cell-level Degradation

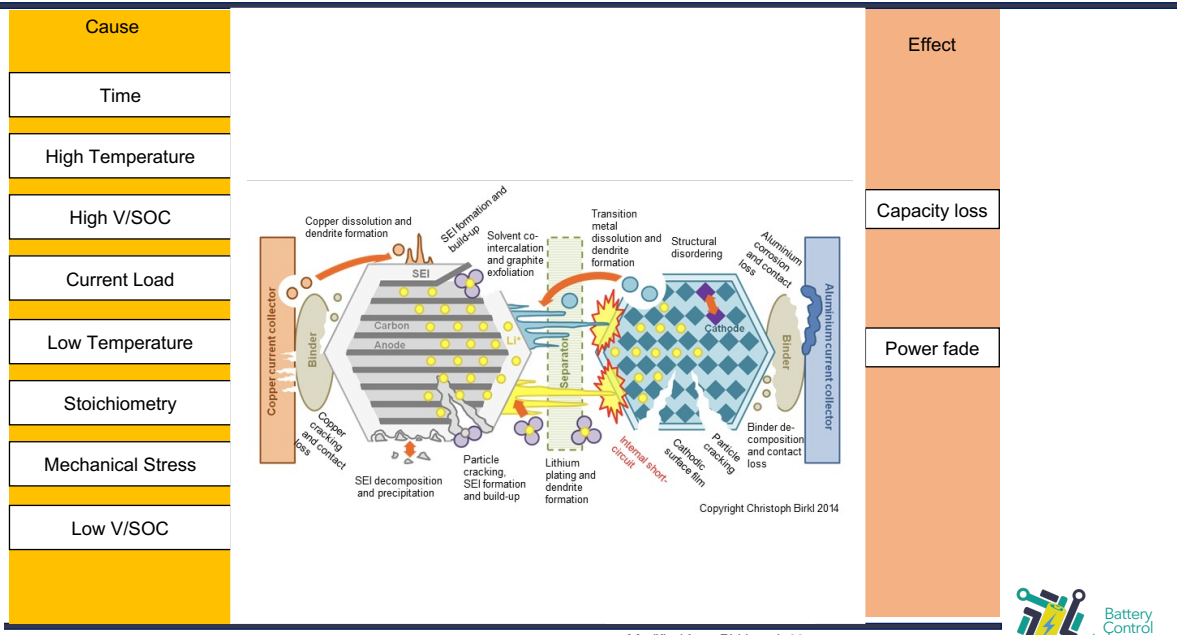


Montat et al., JECS 2021  
Mebtat et al., JPS 2021



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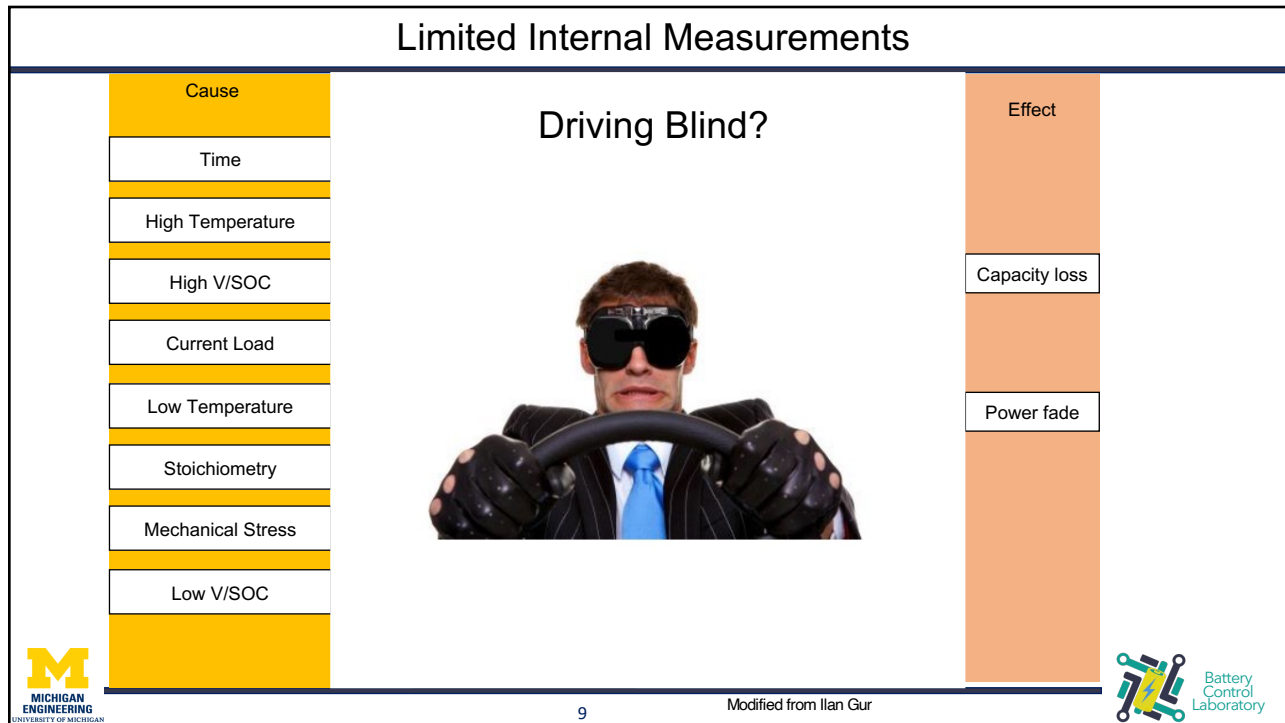
# Causes → → Degradation Mechanisms → → Effects



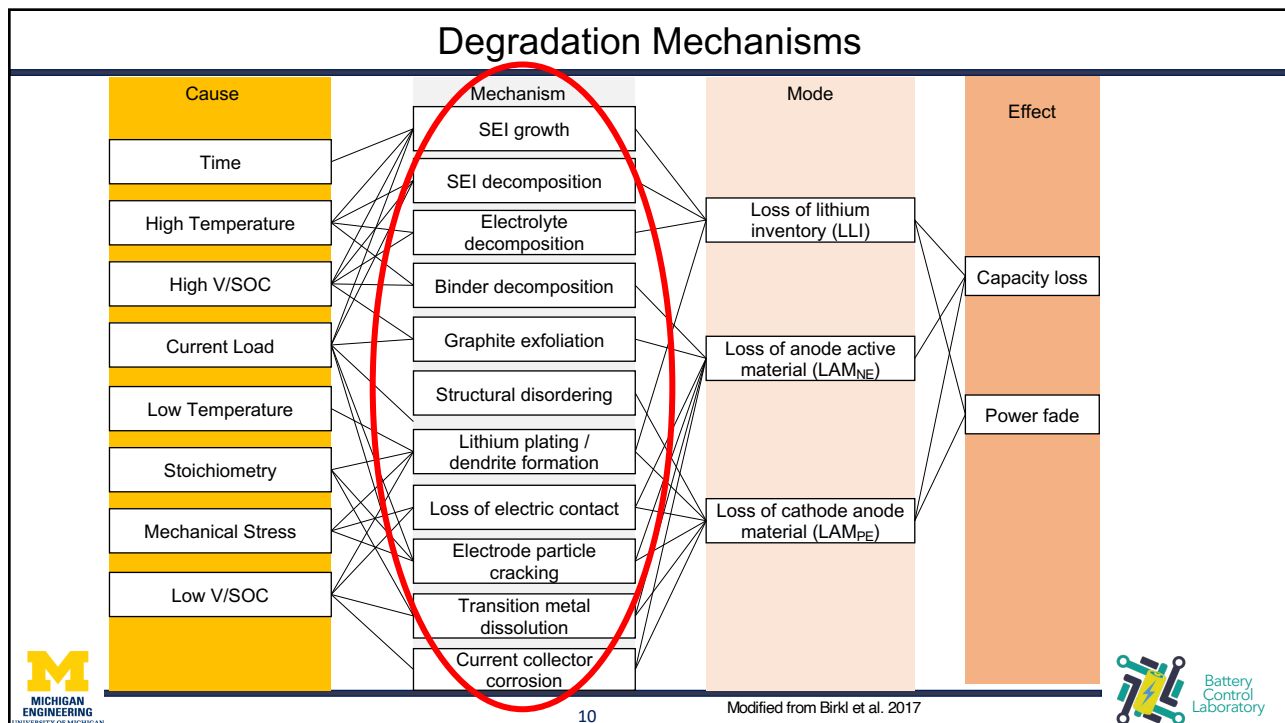
Modified from Birkel et al. 2017



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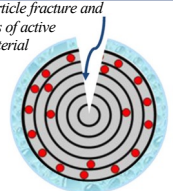


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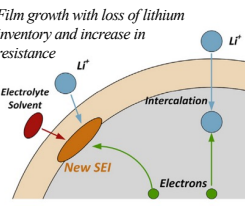
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## Battery Digital Twin



Particle fracture and loss of active material

Laresgotti, Izzaro, et al. "Modeling mechanical degradation in lithium-ion batteries during cycling: Solid electrolyte interphase fracture." *Journal of Power Sources* 300 (2015): 112-122.



Film growth with loss of lithium inventory and increase in resistance

Yang, Xiao-Guang, et al. "Modeling of lithium plating induced aging of lithium-ion batteries: Transition from linear to nonlinear aging." *Journal of Power Sources* (2017)

### Mechanical Degradation

$$\sigma_h(r, t) = \frac{2E\Omega}{3(1-\nu)} \left( \frac{1}{R_p^3} \int_0^{R_p} \rho^2 c_s(\rho, t) d\rho - \frac{c_s(r, t)}{3} \right)$$

$$\frac{dc_s}{dt} = \beta_{LAM} \left( \frac{\sigma_{h,surf}}{\sigma_{critical}} \right)^{m_{LAM}}$$

### SEI

$$j_{SEI} = -k_{SEI} c_{EC}^s \exp\left(\frac{-\alpha_{SEI} F}{RT} \eta_{SEI}\right)$$

$$-D_{SEI} \frac{c_{EC}^s - c_{EC}^0}{\delta_{film}} = -a_s j_{SEI}$$

$$\eta_{SEI} = \phi_s - V_R - U_{SEI}$$

$$\frac{\partial c_{SEI}}{\partial t} = \frac{-a_s j_{SEI}}{2}$$

$$\delta_{film} = \frac{1}{a_s} \left( \frac{c_{SEI} M_{SEI}}{\rho_{SEI}} \right)$$

$$R_{film} = \omega_{SEI} \frac{\delta_{film}}{k_{SEI}}$$

$$n_{Li,loss} = \int_0^{t_{end}} \left( \int_0^{l^-} A a_s \left( \frac{j_{SEI}}{2} \right) dx \right) dt$$

### Single Particle Model

$$\frac{\partial c_s}{\partial x}(r, t) = \frac{1}{r^2} \frac{1}{Dr} \left[ D_s r^2 \frac{\partial c_s}{\partial r}(r, t) \right]$$

$$\frac{\partial c_s}{\partial x}(0, t) = 0$$

$$D_s \frac{\partial c_s}{\partial r}(R_p, t) = -j_{tot}$$

$$c_s(r, 0) = c_{init}$$

$$a_s = \frac{3\epsilon_s}{R_p}$$

$$j_{tot} = \frac{I}{a_s l A}$$

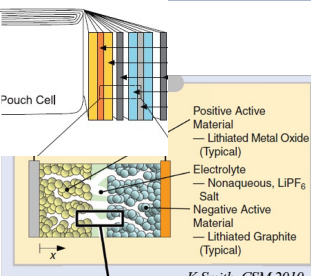
$$j = \frac{i_0}{F} \left( e^{\frac{(1-\alpha)F}{RT} \eta} - e^{-\frac{\alpha F}{RT} \eta} \right)$$

$$i_0 = k_0 (\bar{c}_e)^\alpha (c_{s,max} - c_{ss})^\alpha (c_{ss})^\alpha$$

$$\phi_s = \eta + V_R + U(c_{ss})$$

$$V_R = R_{film} F j$$

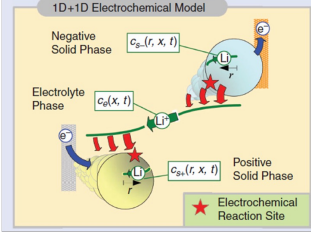
$$V(t) = \phi_s^+ - \phi_s^-$$



Pouch Cell

- Positive Active Material — Lithiated Metal Oxide (Typical)
- Electrolyte — Nonaqueous, LiPF<sub>6</sub> Salt
- Negative Active Material — Lithiated Graphite (Typical)

K. Smith, CSM 2010




1D+1D Electrochemical Model

Negative Solid Phase  $c_{e-}(r, x, t)$


Electrolyte Phase  $c_e(r, x, t)$

Positive Solid Phase  $c_{e+}(r, x, t)$

Electrochemical Reaction Site

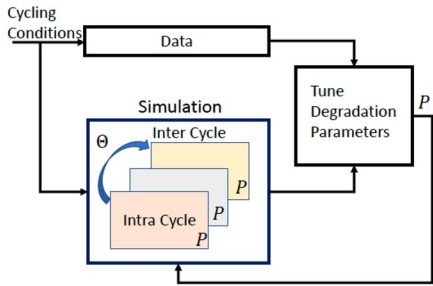


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## Calibrated Digital Twin Predicts Degradation over Life



Automatically tune degradation model parameters until a good fit with experimental data is found.

### Intra-cycle states

$$\mathbf{x} = \begin{bmatrix} C_s^+ \\ C_s^- \end{bmatrix}$$

### Inter-cycle states

$$\Theta = \begin{bmatrix} \delta_{SEI} \\ \epsilon_s^- \\ \epsilon_s^+ \\ n_{Li,s} \end{bmatrix}$$

### Parameters

$$\mathbf{P} = \begin{bmatrix} k_{SEI} \\ \beta_{LAM}^- \\ \beta_{LAM}^+ \end{bmatrix}$$

### Mechanical Degradation

$$\sigma_h(r, t) = \frac{2E\Omega}{3(1-\nu)} \left( \frac{1}{R_p^3} \int_0^{R_p} \rho^2 c_s(\rho, t) d\rho - \frac{c_s(r, t)}{3} \right)$$

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$$\phi_s = \eta + V_R + U(c_{ss})$$

$$V_R = R_{film} F j$$

$$V(t) = \phi_s^+ - \phi_s^-$$

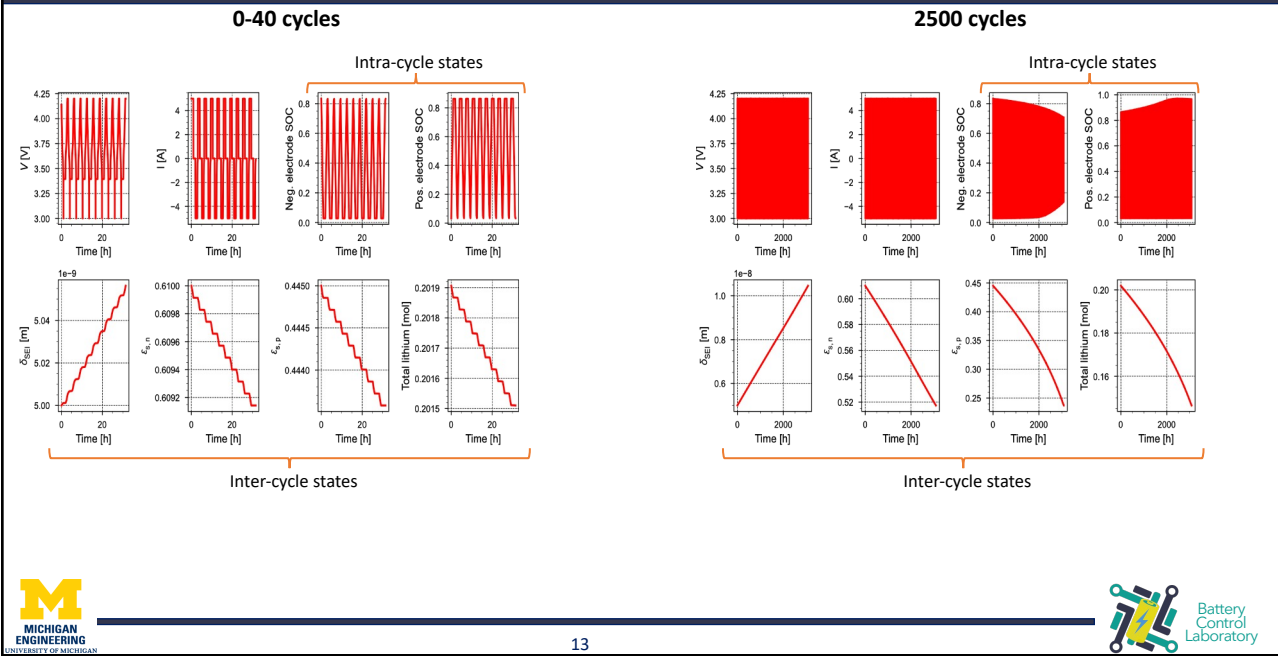


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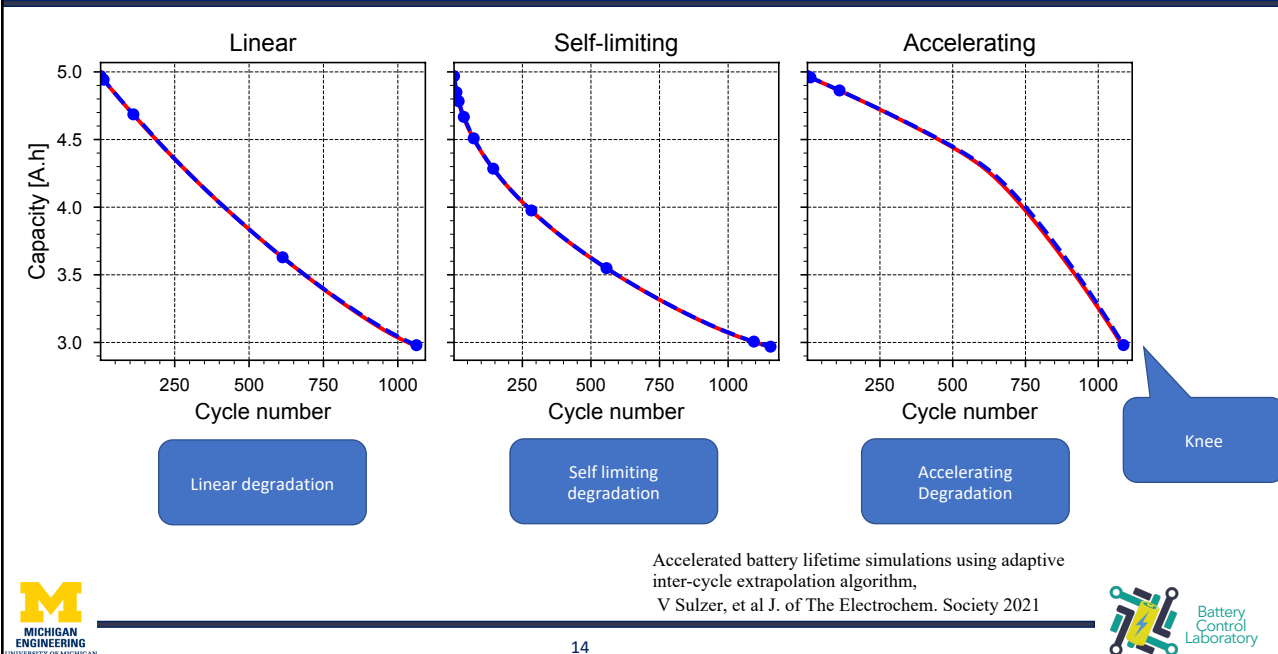
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# Intra-Cycle and Inter-Cycle Simulation of Battery Life



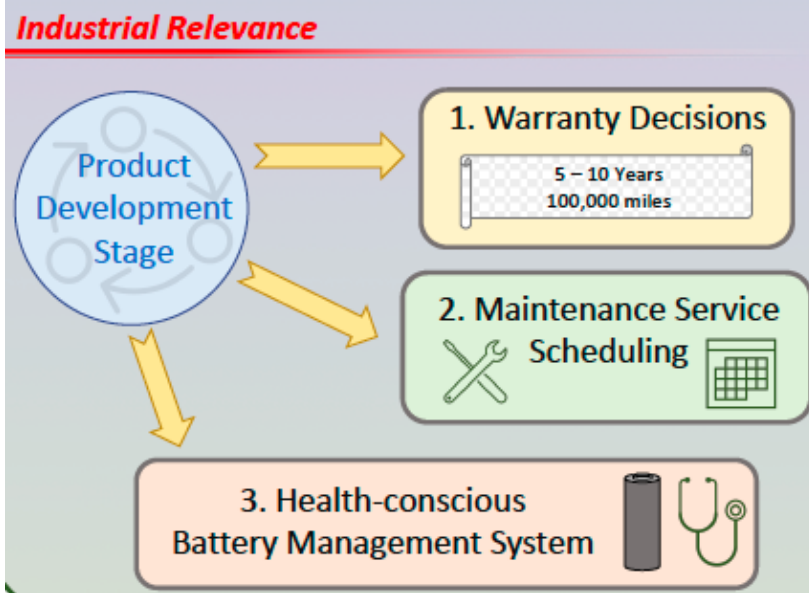
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# Degradation Patterns

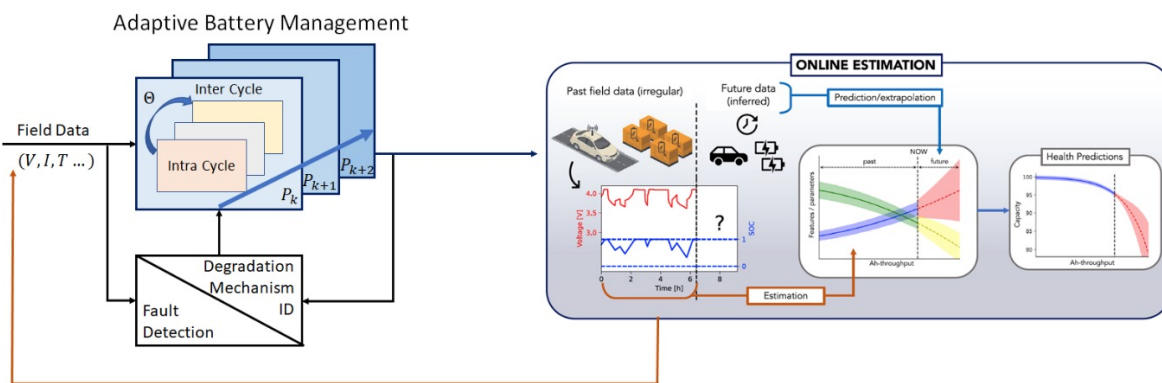


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# Value of Life Prediction to EV Manufacturers



# Monitoring Use & Predicting the Remaining Useful Life



Sulzer, V., et al. "Accelerated battery lifetime simulations using adaptive inter-cycle extrapolation algorithm". *JECSS21*  
 Pannala S. et al. "Methodology for Accelerated Inter-Cycle Simulations of Li-ion Battery Degradation with Intra-Cycle Resolved Degradation Mechanisms" *ACC 2022*





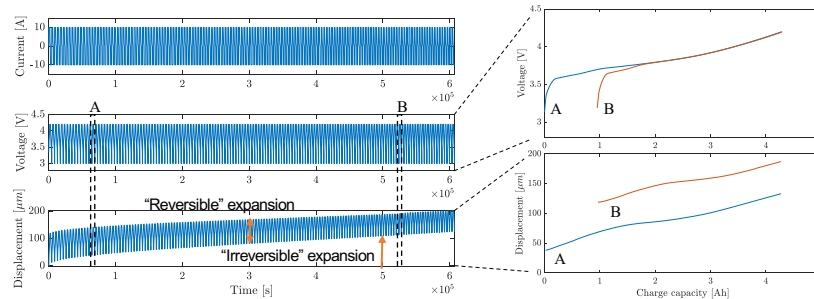
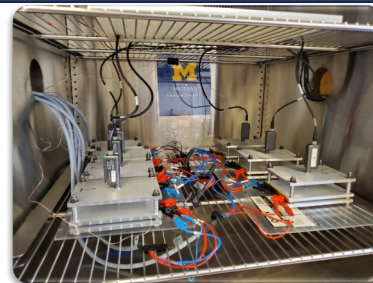
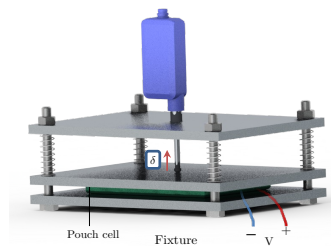
# Beyond Electrical Features The Mechanical Frontiers

## Degradation and Cell Expansion Cause or Effect?

Based on  
P. Mohtat, S. Lee, A. Stefanopoulou, J. Siegel,  
"Towards better estimability of electrode-specific  
state of health: Decoding the cell expansion,"  
*Journal of Power Sources* 427, 101-11 2019.



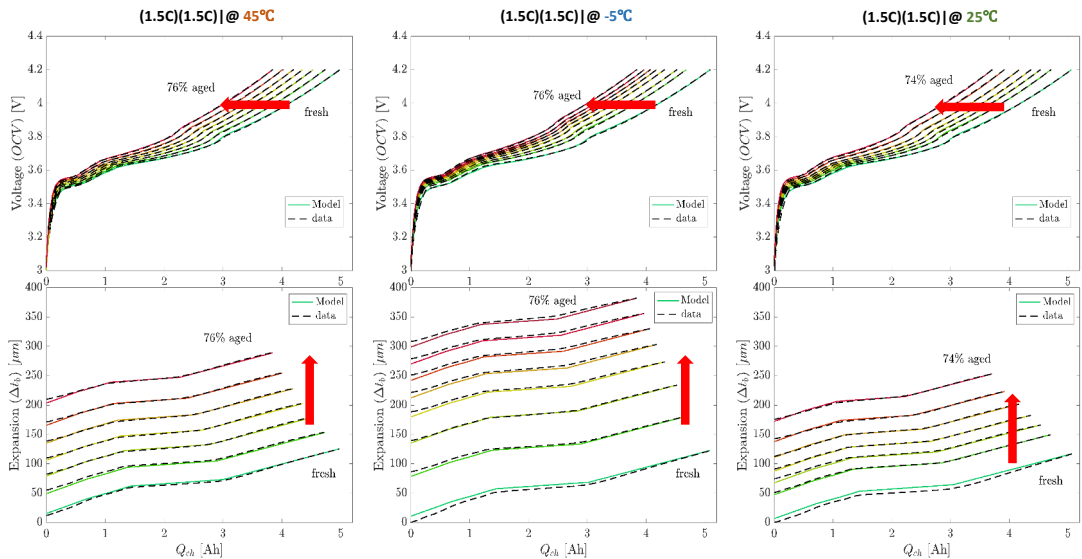
### Experiments: Cell Capacity, Resistance, & Thickness



# Aged Cells: Expanding in Thickness

Irreversible expansion from

- SEI growth
- particle fracture, and
- plating



P. Mohtat, et al(2021). "Reversible and Irreversible Expansion of Lithium-Ion Batteries Under a Wide Range of Stress Factors". *J. of Electrochem Soc.* 2021



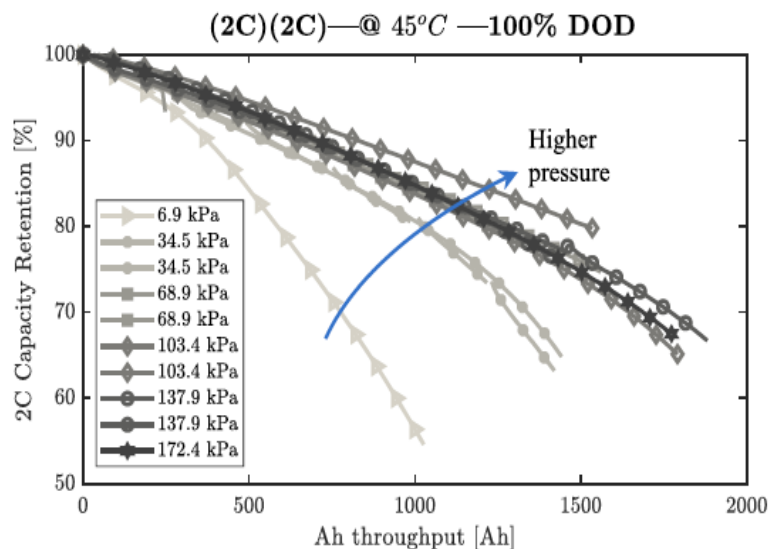
# Pressure Matters

Packaging:

- High Energy Density
- Protection
- Thermal Propagation
- Longevity
- Repair, ReMan, Refub,
- Recycle

The Goldilocks Principle:  
Pressure should neither be too low nor too high

P. Mohtat, et al(2021). "Reversible and Irreversible Expansion of Lithium-Ion Batteries Under a Wide Range of Stress Factors". *J. of Electrochem Soc.* 2021



## Expansion & Force Measurement

### Free Expansion (>100µm)

### Constrained Expansion

A Full HEV Ford Pack was instrumented with temp, expansion & force sensors

- Kim, et al., Optimal power management for a series hybrid electric vehicle cognizant of battery mechanical effects. ACC2014
- K. Oh, et al., "Phenomenological Force and Swelling Models for Rechargeable Lithium-Ion Battery Cells," JPS2016
- N. Samad, et al., "Battery Capacity Fading Estimation Using a Force-Based Incremental Capacity Analysis," JECSC2016
- Mohan, et al., A phenomenological model of bulk force in a Li-Ion battery pack and its application to state of charge estimation, JECSC2014
- Samad, et al., Parameterization and validation of a distributed coupled electro-thermal model for prismatic cells DSCC2014
- Mohan, S., et al., On improving battery state of charge estimation using bulk force measurements DSCC2015

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## ElectroChemical & ThermoMechanical Model Across Domains

Lattice

Particle

$$\frac{\partial c_{s,i}^p}{\partial t}(r,t) = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ D_i r^2 \frac{\partial c_{s,i}^p}{\partial r}(r,t) \right]$$

$$j_i^p(t) = \frac{i_0^p(t)}{F} \left( e^{\frac{\alpha_a F}{RT} \eta_i^p} - e^{-\frac{\alpha_c F}{RT} \eta_i^p} \right)$$

$$c_s^p \frac{\partial c_s}{\partial t}(x,t) = \nabla \cdot (D_i^e J \nabla c_s(x,t)) + \frac{1-r_0^e}{F} \nabla \cdot i_2(x,t)$$

$$\eta_i^p(x,t) = \Phi_1(x,t) - \Phi_2(x,t) - U_s(c_{s,e}^p(x,t)) - V_{R,i}^p(x,t)$$

Electrode

$$T(t) = \Delta t_{th} = \alpha_{th}(T - T_0)$$

$$\Delta t_e = \kappa_b \Delta t_{e_s}$$

$$\Delta t_p = \kappa_p (\Delta t_p + \Delta t_e)$$

Cell

$$\Phi_{1,1} = \Phi_{1,2} = \dots = \Phi_{1,N}$$

Fixture

Expansion

$$\Delta t_t = \Delta t_s + \Delta t_{th}$$

**Current (I) Flow:** Lattice → Particle → Electrode → Cell → Fixture

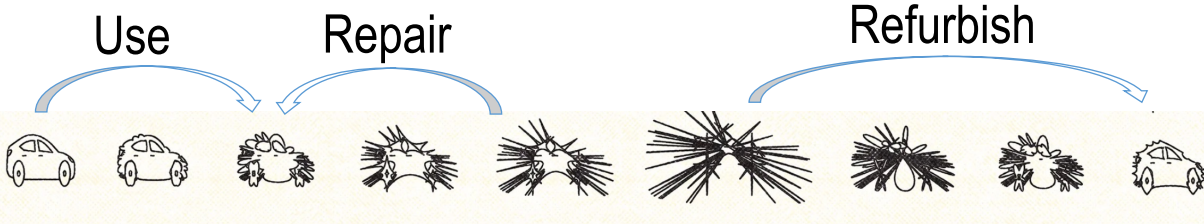
**Voltage Flow:** Cell → Fixture

**Expansion Flow:** Cell → Fixture

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## Second hand EVs: Repair & Refurbish

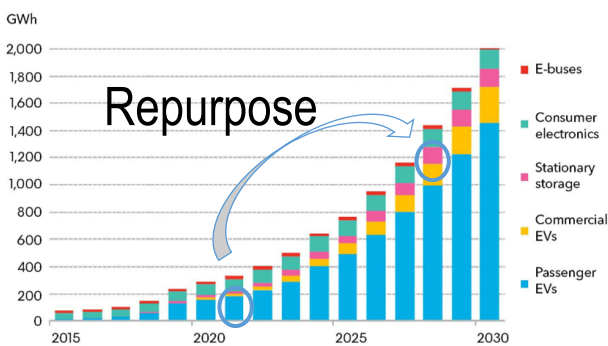


For Equitable Battery Ecosystem  
 Battery is 30-40% of EV cost  
 \$2.5B US industry in engine remanufacturing  
 6,000 machine shops in North America



## 2<sup>nd</sup> Life: Value of Repurposing

Annual lithium-ion battery demand



Source: Bloomberg NEF 2019 Electric Vehicle Outlook

Leveling battery competition between grid storage and EVs

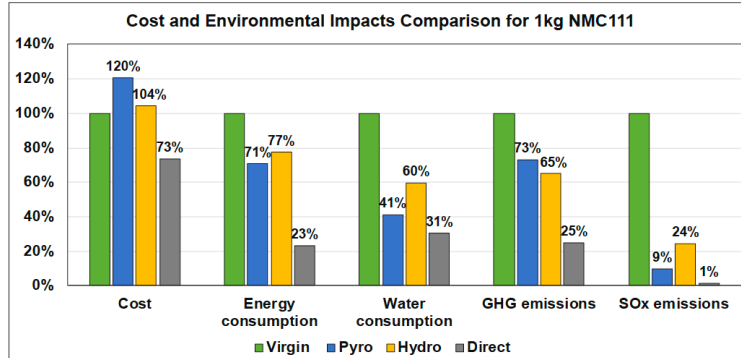
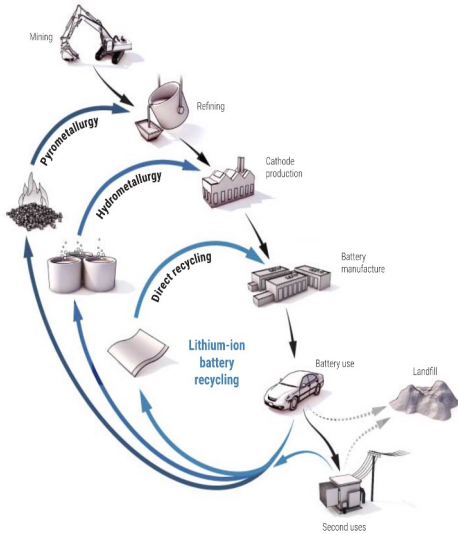
Decarbonizing the grid with frequency regulation & energy arbitrage

Improving fast charging economics

Supporting building decarbonization

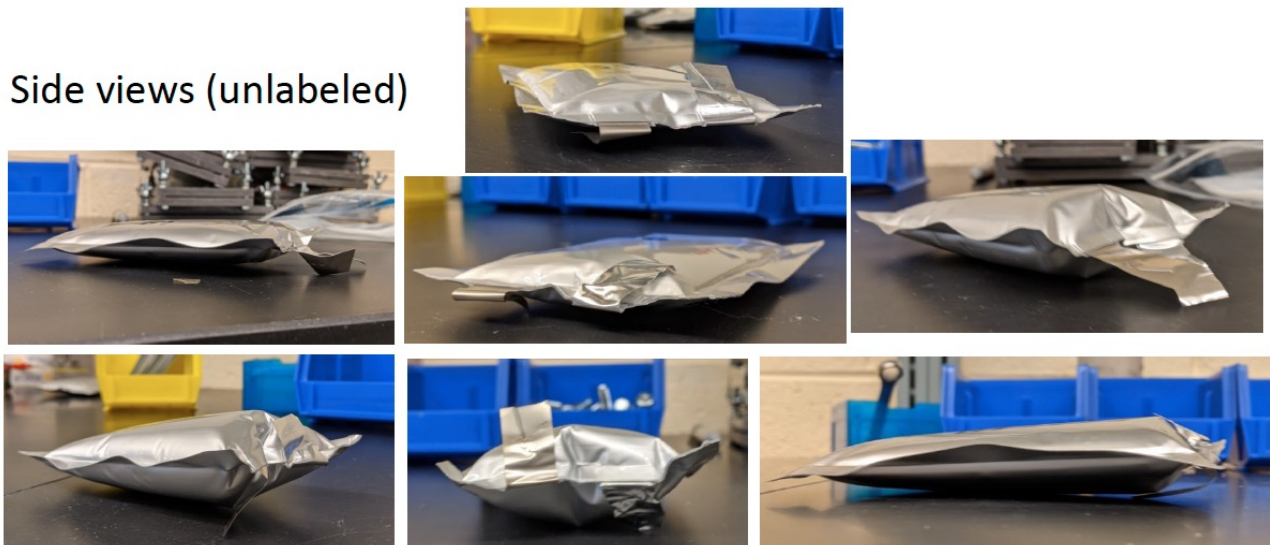


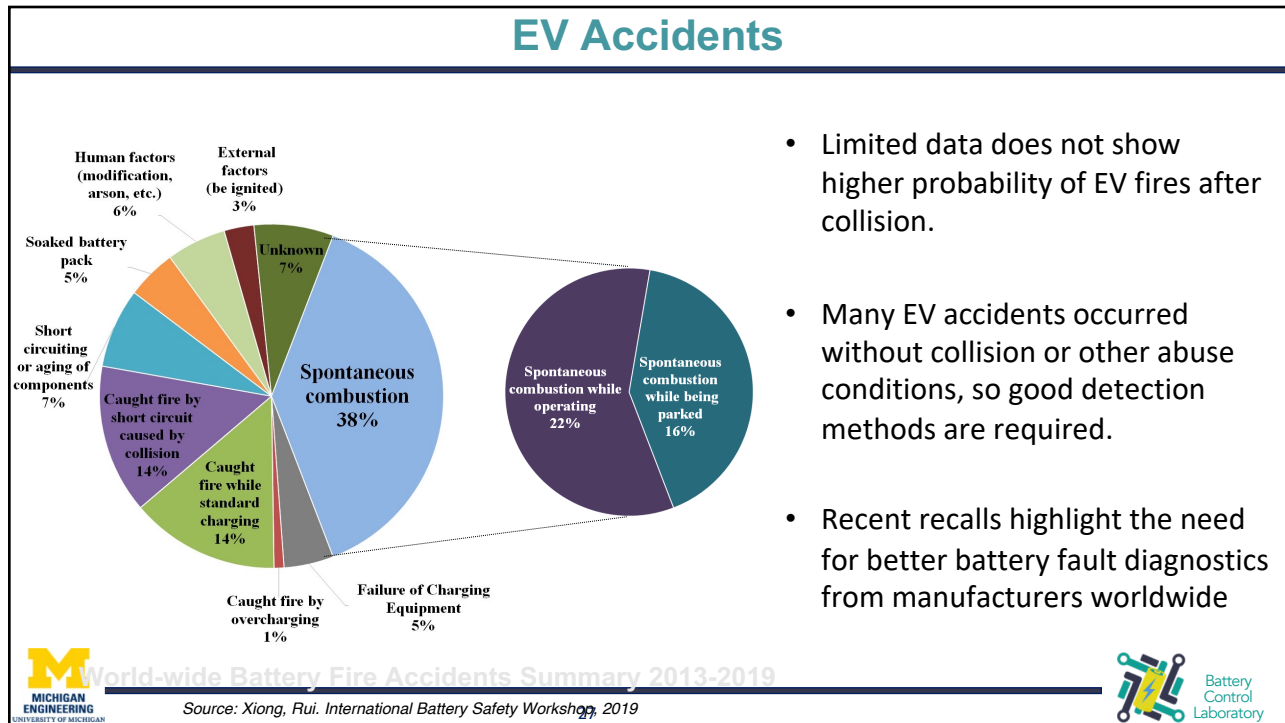
# Recycle



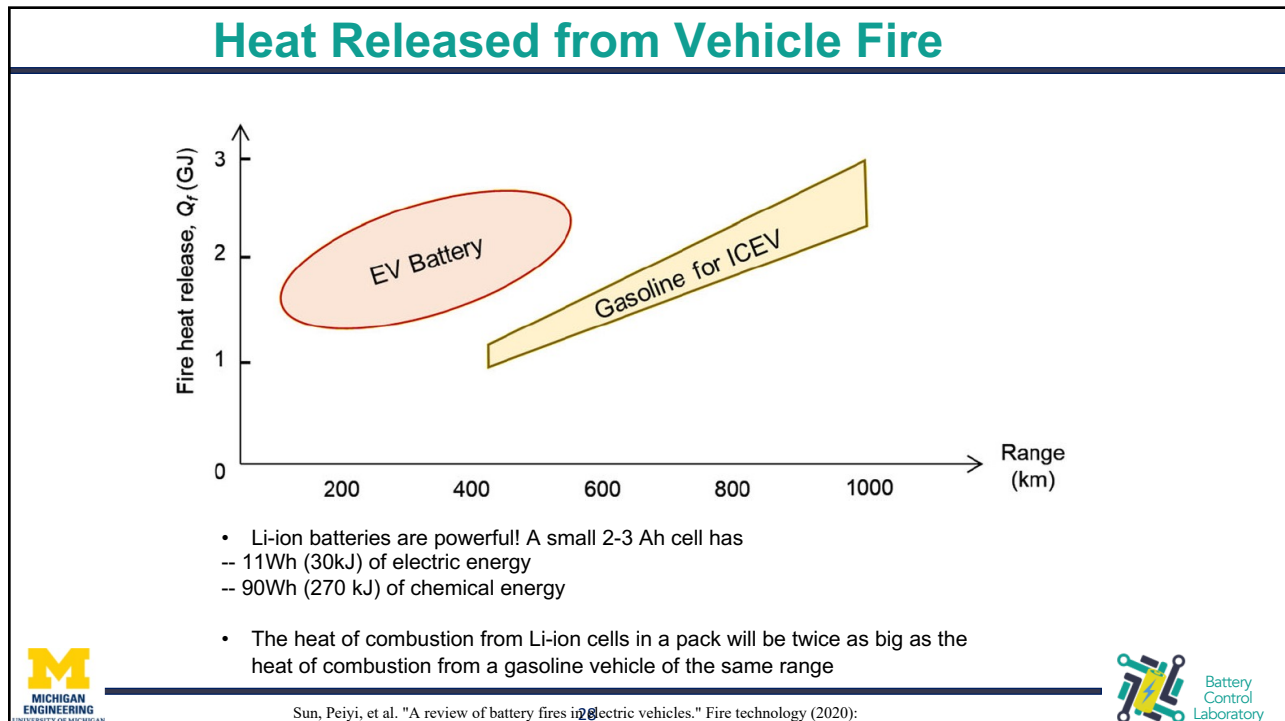
# Safe Handling and Transportation?

Side views (unlabeled)

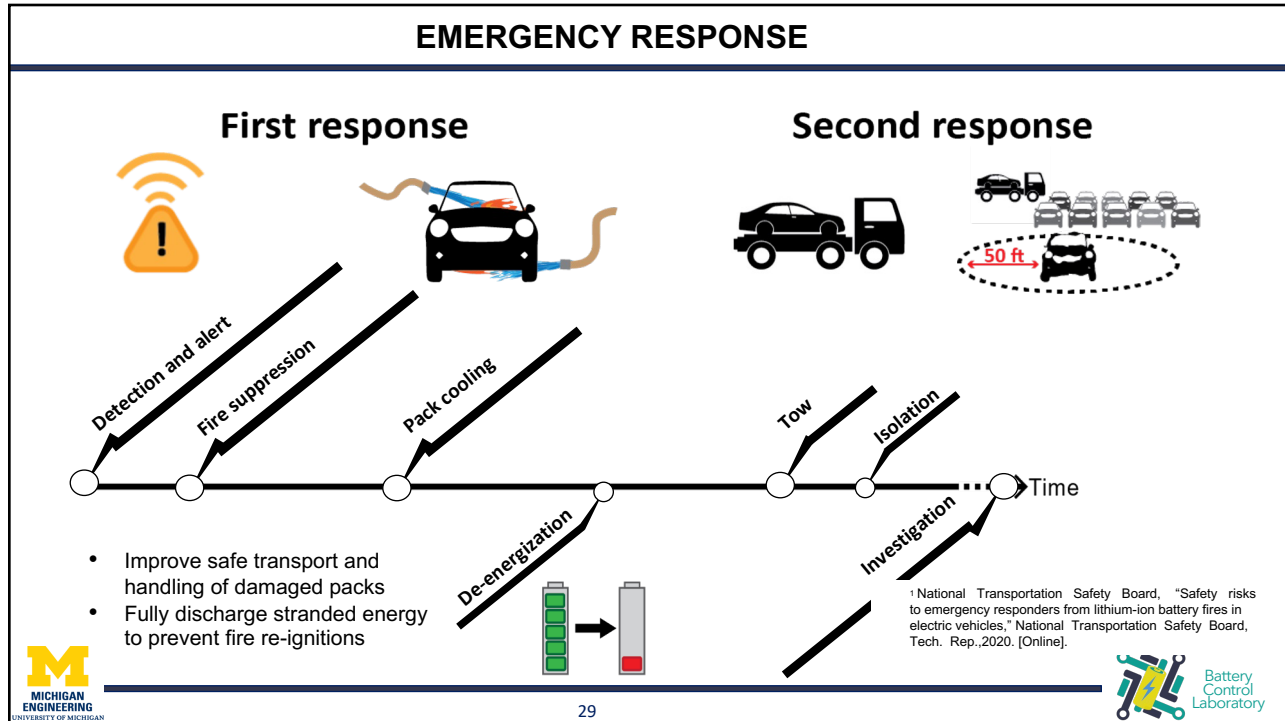




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## Existing methods are slow and resource intensive

### Discharge solutions at the pack-level:




**OEM discharge tools<sup>2</sup>**



Source: Team RRCO Battery Recycling Prize

Figure: Midtronics GRX-5100 EV/HEV Battery Service Tool (connected to a vehicle and discharging on right)  
Source: NHTSA Stranded Energy Assessment Techniques and Tools 2020

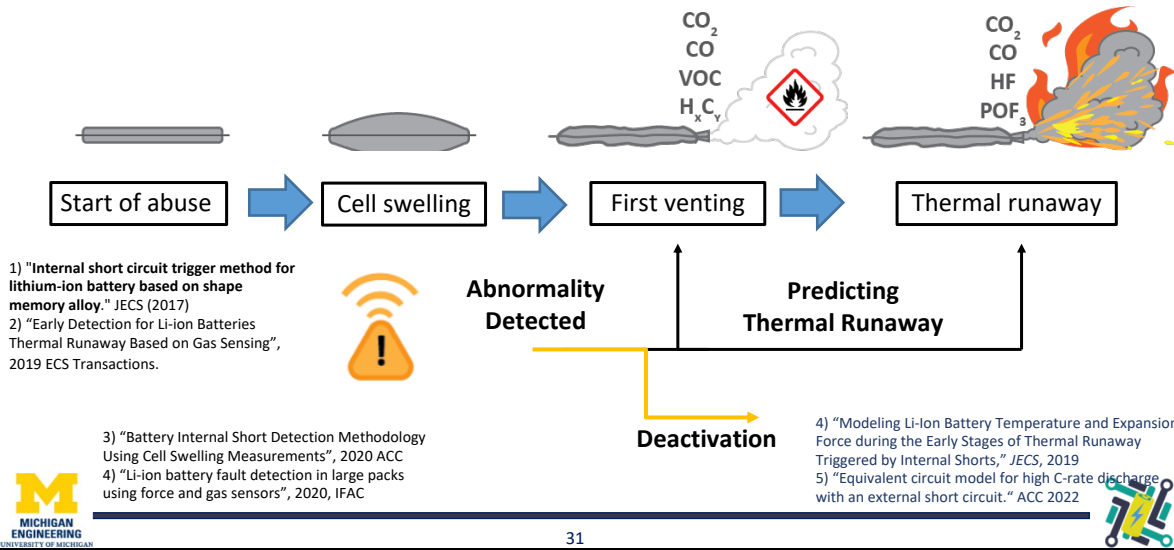



**Submersion in (salt) water**

In the Netherlands, crews load a BMW EV into a water bath after the battery began smoking inside a car dealership last spring. (Courtesy of Central and West Brabant Fire Brigade) Source: NEPA Journal

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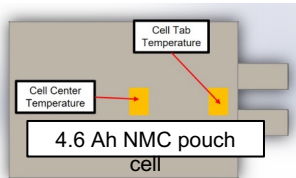
## Integrated Sensing: Pressure and Gas Sensing



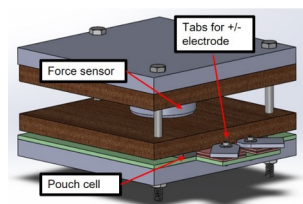
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## De-Energization with External Short circuit (ESC)

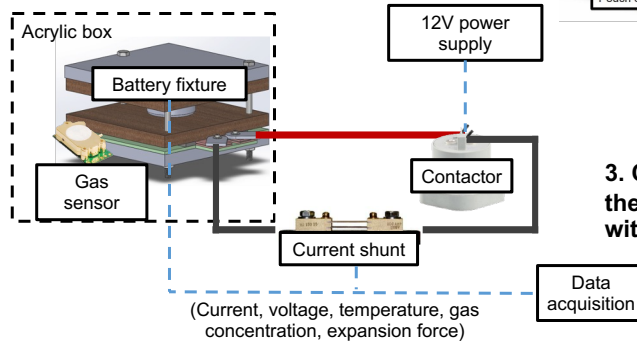
1. Attached K-type thermocouples to the cell



2. Secure the cell in the fixture instrumented with a load cell



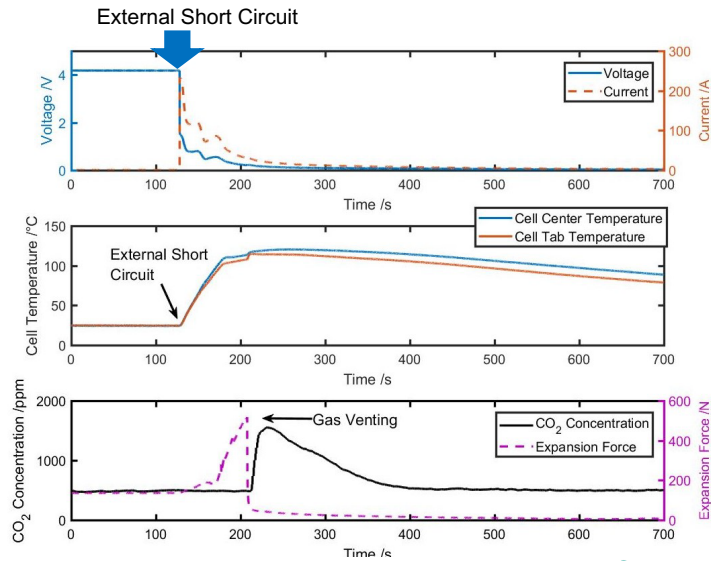
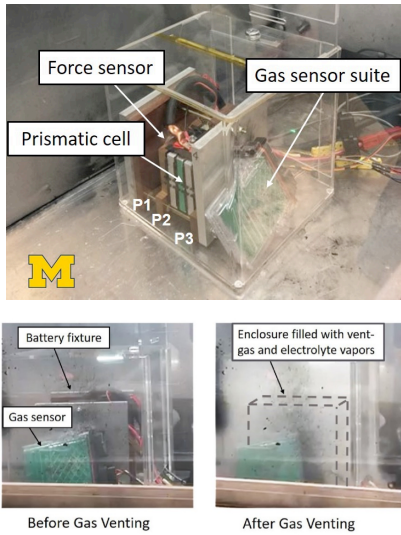
3. Connect the cell and place the fixture in an acrylic box with the gas sensing suite



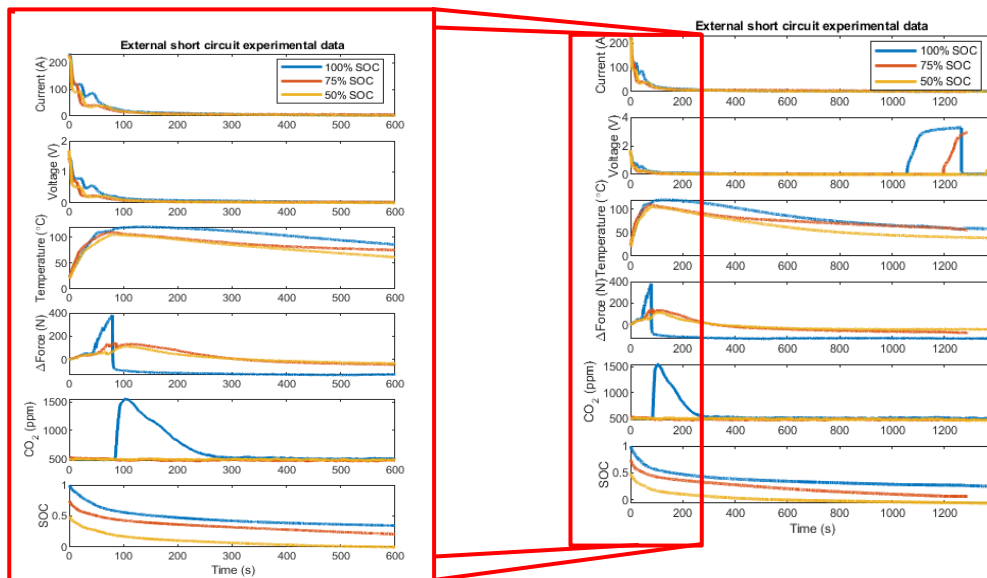
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# Cell External Short Circuit Experiment



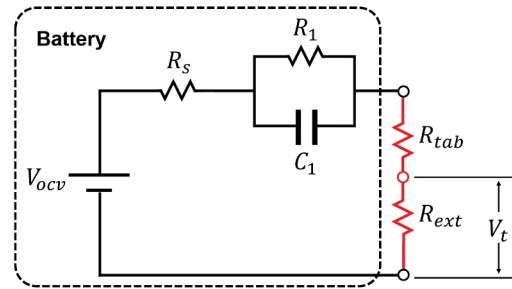
# Cell electrical, thermal, and mechanical response to ESC



# External short circuit electrical model

Nominal single RC equivalent circuit battery model:

$$\begin{aligned} \dot{SOC} &= -\frac{1}{Q} I(t) \\ \dot{V} &= -\frac{1}{R_1 C_1} V_1 + \frac{1}{C_1} I(t) \\ V_t(t) &= V_{ocv} - V_1 - (R_s + R_{tab}) I(t) \end{aligned}$$



External short circuit elements:

$$R_{tab} = \frac{1}{I_0} (V_{ocv}(SOC_0) - V_{t,0}) - R_s(SOC_0)$$

$$R_{ext} = \frac{V_{t,0}}{I_0}$$

RC modification for diffusion-limited current:

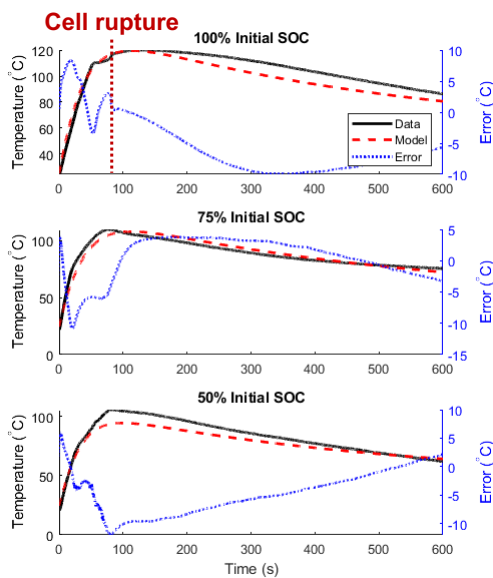
$$R_1 = a\tilde{R}_1(SOC)$$

$$C_1 = b\tilde{C}_1(SOC)$$

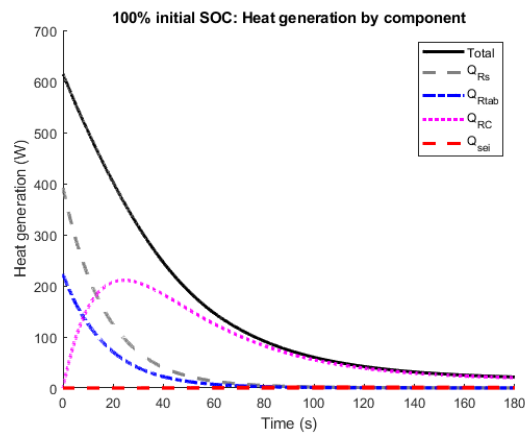
- Nominal consists of only 2 ODEs and 5 parameters
- $R_s$ ,  $R_1$ , and  $C_1$  are functions of SOC
- With a current pulse, we can estimate all nominal parameters at the current SOC except capacity



# Thermal model validation



- Almost all heating is from Ohmic heat
- Error in current will strongly propagate to the thermal model



# Overview of the internal pressure model

**First Venting Model**

Battery

$T(t)$

$P_{total}$

$n(CO_2)$

**Timing & Gas Release Prediction**

- $t_{vent}(P_{total} > P_{crit})$
- $n(CO_2)$  released

**Expansion force (N)**

Peak expansion of 517 N is used to calculate  $P_{crit} = 158 \text{ kPa}$

**CO<sub>2</sub> concentration (ppm)**

Peak CO<sub>2</sub> is calculated to be 0.8 mmol

M MICHIGAN ENGINEERING UNIVERSITY OF MICHIGAN

Cai, Ting, et al. "Modeling Li-ion Battery First Venting Events Before Thermal Runaway." Modeling, Estimation and Control Conference 2021.

Battery Control Laboratory

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# Modeling cell internal pressure

**Internal cell pressure:**  
 $P_{total} = P_{sat} + P_{CO_2}$

**Critical venting pressure:**  
 $P_{crit} = \frac{F_{max}}{A_{surf}} + P_{atm}$

**Electrolyte vapor saturation pressure:**  
 $P_{sat} = y_{EC} \cdot P_{sat,EC} + y_{DMC} \cdot P_{sat,DMC}$

**Gas pressure from generated CO<sub>2</sub>:**  
 $P_{CO_2} = \frac{n(CO_2)RT}{V_h}$

**Electrolyte component saturation pressure:**  
 $\log(P_{sat}/kPa) = A - \frac{B}{T/K + C}$

Component	A	B	C
DMC	6.4338	1413.0	-44.25
EC	6.4897	1836.57	-102.23

**Amount of CO<sub>2</sub> from gas evolution model:**  
 $n(CO_2) = \frac{m_{an}(x_{SEI,0} - x_{SEI})}{2M_{C_6}}$   
 $\frac{dx_{SEI}}{dt} = -A_{SEI} \cdot x_{SEI} \cdot \exp\left(-\frac{E_{SEI}}{k_b T}\right)$

**Cell head volume from expansion:**  
 $V_h = V_{h,0} + A_{surf} \times (\Delta d - \alpha_{cell} \cdot \Delta T)$   
 $\Delta d = L \frac{\Delta \sigma}{E}$   
 $\Delta \sigma = \max\left(P_{total} - \sigma_0 - P_{atm}, \frac{E \cdot \alpha_{cell} \cdot \Delta T}{L}\right)$

**Active material**  
Before → After

$\Delta d$

$\alpha_{cell} \Delta T$

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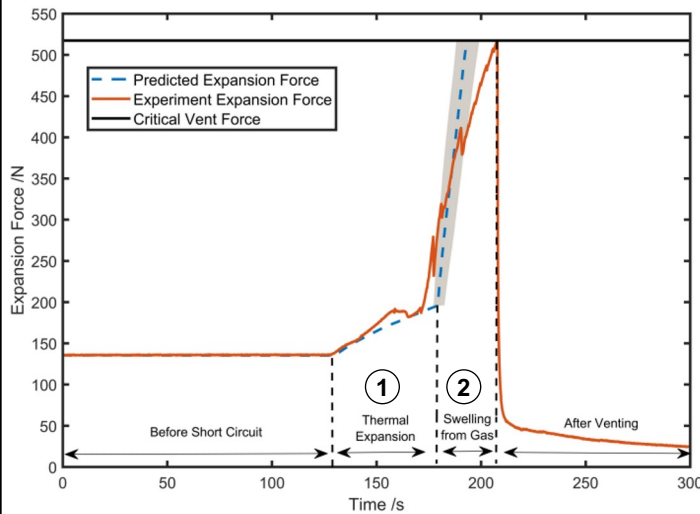
Cai, Ting, et al. "Modeling Li-ion Battery First Venting Events Before Thermal Runaway." Modeling, Estimation and Control Conference 2021.

Battery Control Laboratory

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## Model results: Expansion and total CO<sub>2</sub> gas release



- Two expansion force measurement slopes due to
  1. Thermal expansion of the active material
  2. Cell swelling due to gas generation
- Measured peak CO<sub>2</sub> concentration is within the predicted range accounting for K-type thermocouple accuracy ( $\pm 2.2^\circ\text{C}$ )

Table 3. CO<sub>2</sub> Gas Generation from Model Prediction and Experiments (mmol)

	Model		Experiment
CO <sub>2</sub> amount before venting	CO <sub>2</sub> amount after venting	Total CO <sub>2</sub> amount	Total CO <sub>2</sub> amount
0.25 - 0.42	0.35 - 0.55	0.6 - 0.97	0.8

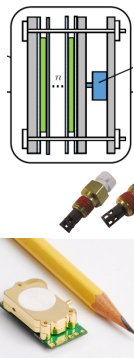
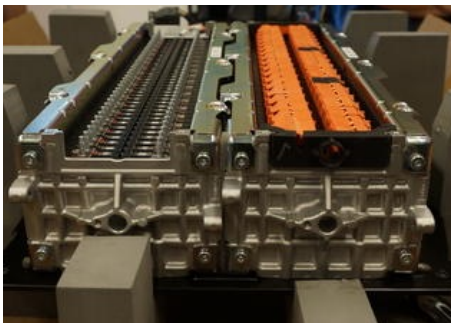


Cai, Ting, et al. "Modeling Li-ion Battery First Venting Events Before Thermal Runaway." Modeling, Estimation and Control Conference 2021.

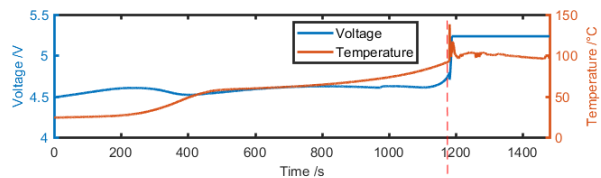


## A Multi-Sensory Approach (I,V,T,F/P,G) for Pack Safety

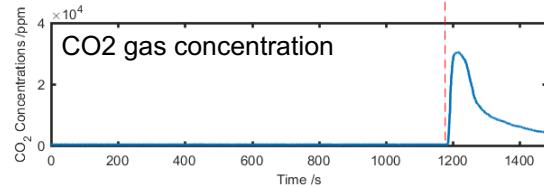
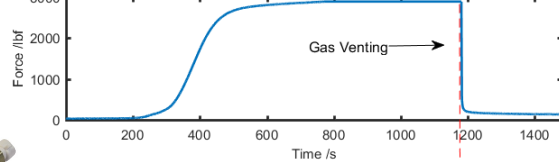
- Cell overcharged to 4.8 volts before gas venting occurs
- Force shows good response during overcharging, and drops rapidly after gas venting
- Gas detection shows rapid response after the force drops



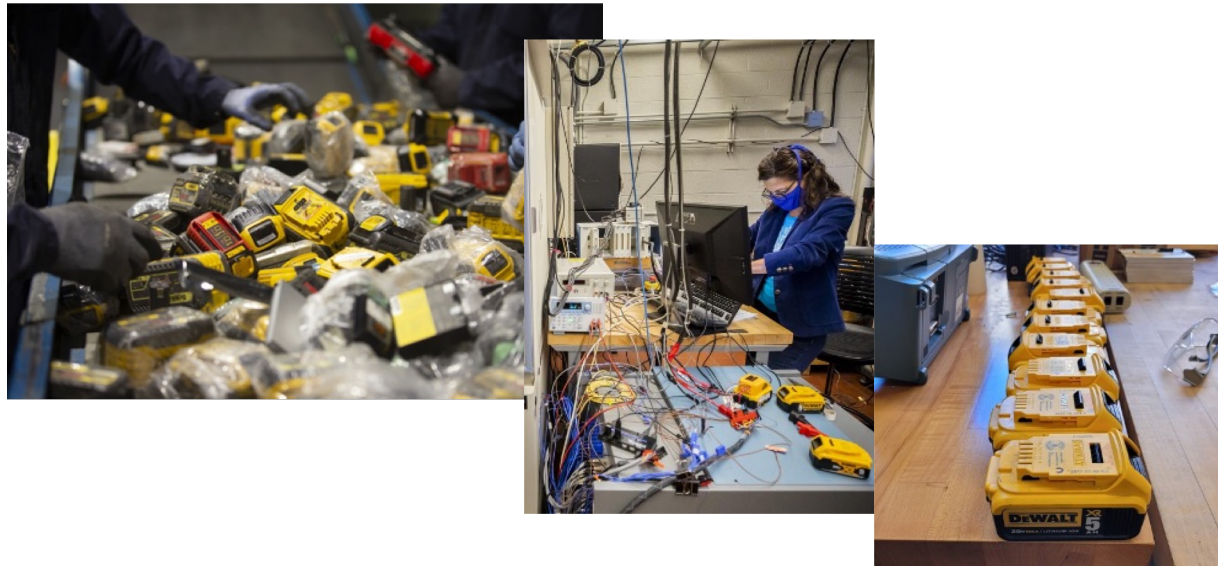
Voltage, Temperature



Cell Swelling Force



# Managing Discarded Batteries



# Policy & Labeling for Waste Management

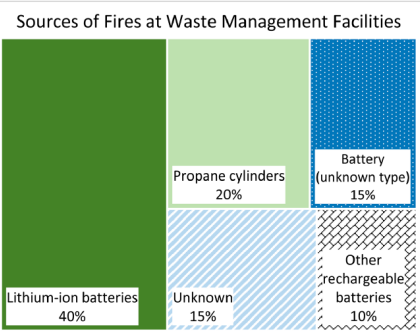


Figure 4: Sources of Fires at California waste management facilities, according to a 2018 survey by the California Product Stewardship Council



Figure 7: Locations of LIB-caused fires across the United States, 2013-2020

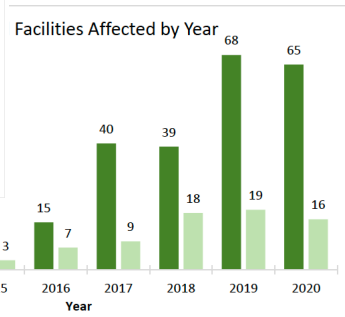


Figure 5: Facilities affected and number of fires by year

An Analysis of Lithium-ion Battery Fires in Waste Management and Recycling, EPA Office of Resource Conservation and Recovery, EPA 530-R-21-002, July 2021



## Safety ... for Next Gen Batteries

**Oxygen**

- Cathodes such as NMC, NCA, LCO used in LIBs contain and can release oxygen
- If the cell packaging is compromised, oxygen is present in ambient air

**Heat**

- External sources such as a garage fire
- Internal sources
  - Exothermic chemical reactions such as SEI formation/degradation
  - Electrical short in battery resulting in large currents
    - $Heat=i^2RT$  (Joule's Law)

Solid State Electrolyte

**Fuel**

- Many components in the cell can burn, but the most flammable is the liquid organic electrolyte
- If the cell is heated, the electrolyte is also volatile resulting in high pressure that can rupture the cell forming a flammable aerosol

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## Auto Manufacturing & Repair Employment

**State-Level Employment in Internal Combustion Engine (ICE) Related Parts Manufacturing & Repair**

- 0-1,000 Workers
- 1,001 - 5,000 Workers
- 5,001 - 10,000 Workers
- 10,001 - 20,000 Workers
- 20,001 - 40,000 Workers

**Manufacturing Locations**

- ★ EV Battery Plants, Current &
- Announced
- EV Production, Current & Announced
- Hybrid / Hybrid & ICE Production
- ICE (Gas, Diesel) Production Only

1.8 million

US Jobs in Auto Manufacturing & Repair

303,000

of these Auto Jobs are in ICE-Related Transition.

How many

Jobs will be created in a Battery Economy?

44

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# Battery industry survey confirms lack of workforce with necessary skills

- ~75% of respondents are planning to hire <1 year & 71% have hired in the past year
- 90% identified limited # of applicants with required skills
- 44% did not find local applicants with required skills

	2-year Community College (n=35)	4 Year College/ University (n=43)
Battery materials (chem engineering, mat science)	12	32
Mining	5	7
Electrical	13	15
Power Electronics	11	17
Software/Battery Management	12	22
System Design	8	21
Prototyping	11	18
Battery Testing	21	23
Safety (electrical, hazmat, fire, etc.)	15	14
Application of batteries (installation, operation, etc.)	12	13
Design for Waste management	9	16
Battery Recycling	13	18
Environmental engineering	4	14
Project management	12	16
Technical lead/ management	7	19
Supply chain management	11	16
Manufacturing including plant design	10	22
Installation of battery systems	14	8
Operation and Maintenance of systems	11	10
Electrical skills for battery technicians (high voltage)	20	13
First response to battery fires	13	8



Member Survey (n=67, r=40%)



By Alyssa McQuilling - Southernresearch.org



# Team Effort

## Teaching Battery Control and Systems: Dr. Jason Siegel

For Senior, Ms, PhD students In campus and On line since 2011.

### Lecture 5: Autoregressive battery model for tracking resistance increase

Electric resistance (R) varying Resistance depends on temperature

- Gradual → Degradation: State of Health
- Abrupt → Coolant fault

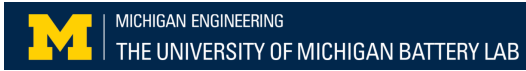


Search this recording

Time	Text	Score
0:00	Administrative Matters	0:00
0:00	Find the R, R, C parameters with Voltage and Current...	0:00
0:25	Find the R, R, C parameters...	0:25
4:13	Recall from Session 4: Find the R, R, C parameters...	4:13
8:05	Recall from Session 4: Find the R, R, C parameters...	8:05
8:06	Find the R, R, C parameters...	8:06
8:42	Recall from Session 4: Find the R, R, C parameters with Voltage and Current...	8:42
8:42	Find the R, R, C parameters...	8:42
16:42	Recall from Session 4: Find the R, R, C parameters...	16:42
22:57	Recall from Session 4: Find the R, R, C parameters...	22:57
33:13	Generalized Equivalent Circuit Model in State Space...	33:13



# Thank you!



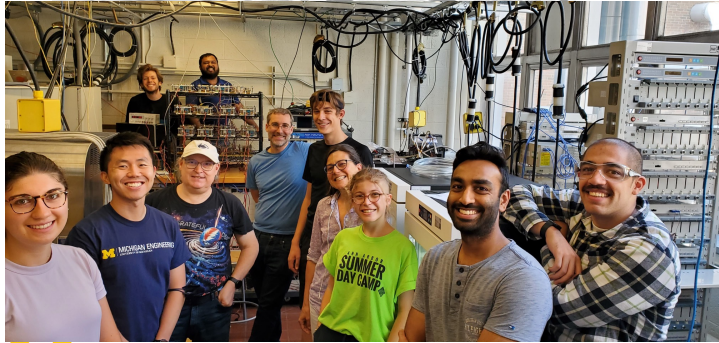
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Tino Sulzer, Rebecca Pickens*

*Sravan Pannala, Vivian Tran,  
Andrew Weng*



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**A123, Navitas, Samsung, and LG**

