Impact of Battery Operation and Manufacturing Process on Battery Performance over Lifetime

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Project Goals

M-ERA.NET Joint Call 2021

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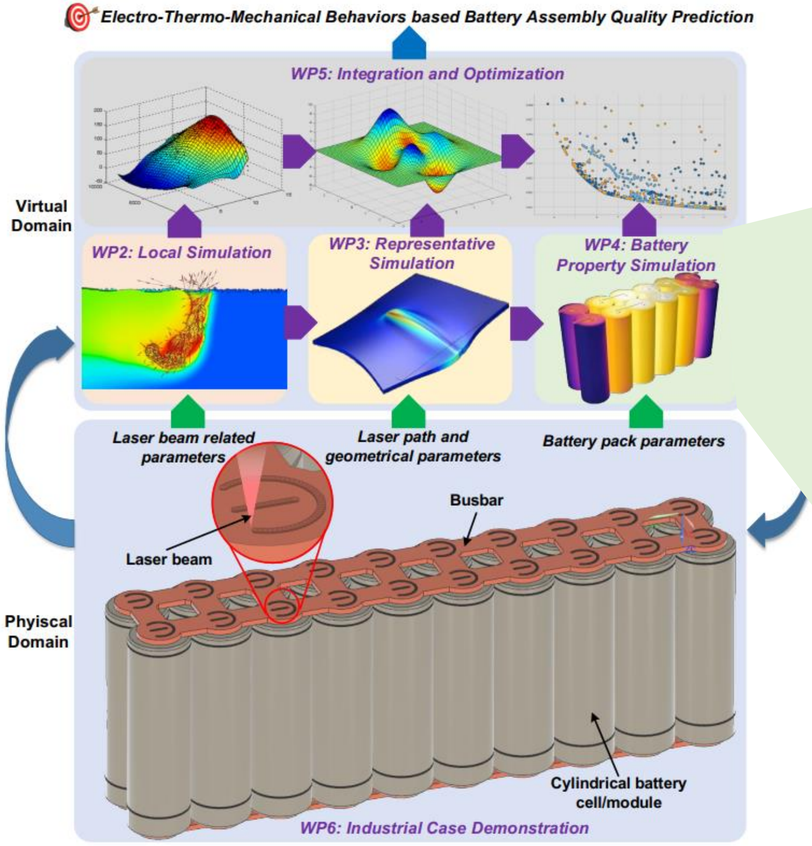
Project: Multi-scale simulation of laser welding for optimal battery pack manufacturing

VOLVO, UNIVERSITY OF SKÖVDE, DTU, Aurobay, resolvent



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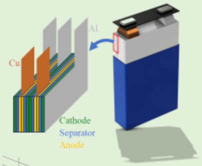
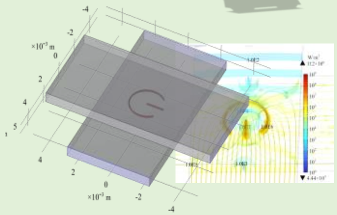
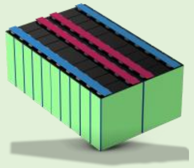


Battery cell performance



Busbar/tab joint performance



System performance

Design Tool

PRESENTATION & POSTER

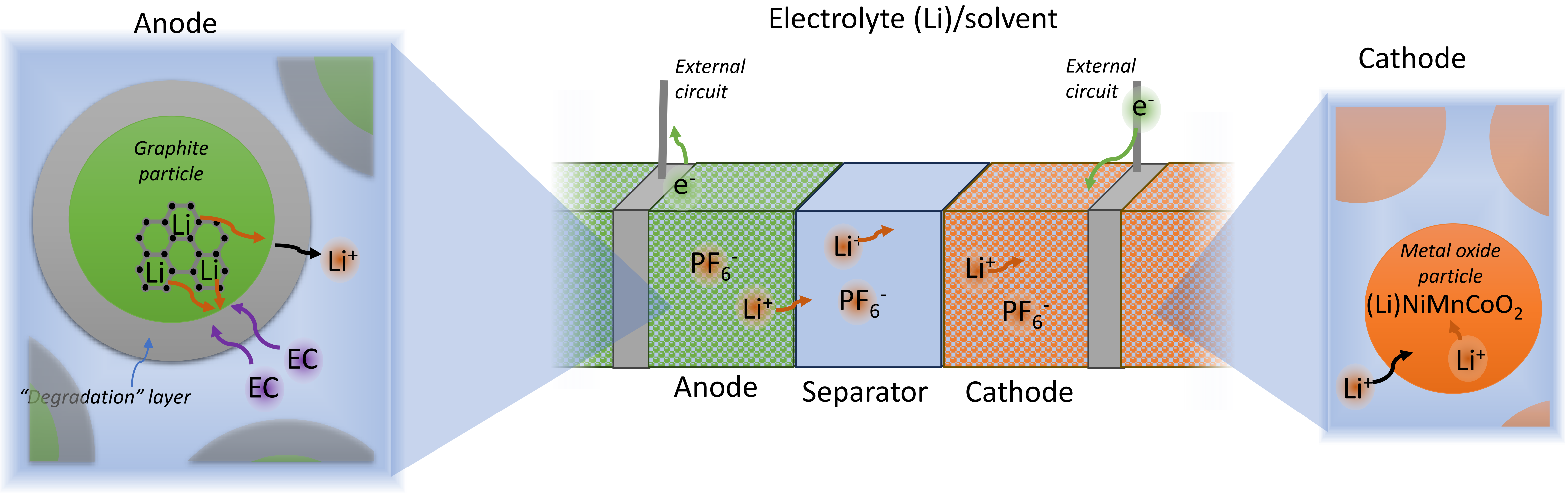
PRESENTATION

Andre G. Steckel

PRESENTATION

Martin R. Nielsen

Electrochemical Battery Model



Lithium diffusion
Ionic current distribution
Degradation
Intercalation
Electric current distribution

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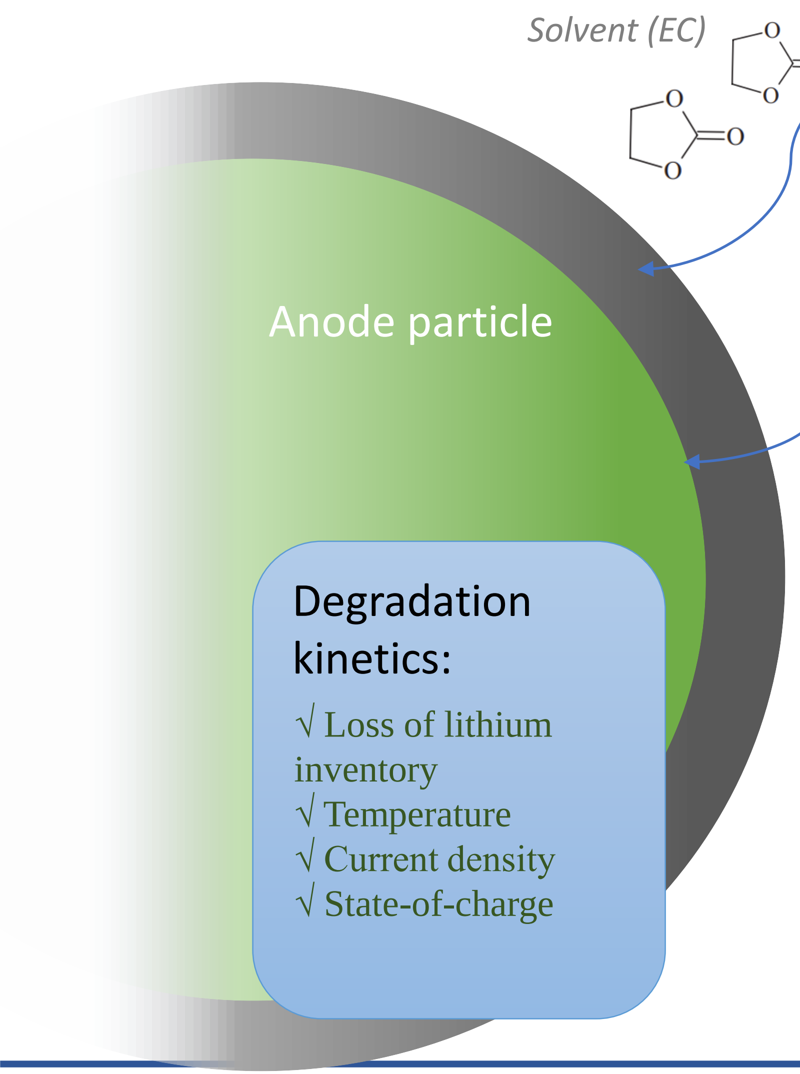
Electrochemical Battery Model



Solvent diffusion through SEI layer

$$\frac{\partial c_{EC,P}}{\partial t} = \frac{\partial}{\partial r}\left(D_{EC,P}\frac{\partial c_{EC,P}}{\partial r}\right) - \frac{d\delta_{SEI}}{dt}\frac{\partial c_{EC,P}}{\partial r}$$

$$\frac{d\delta_{SEI}}{dt} = -\frac{i_s}{2\mathcal{F}}\frac{M_{SEI}}{\rho_{SEI}}$$

Reaction on particle surface

SEI Layer formation $2EC + 2e^- + 2Li^+ \rightarrow SEI + C_2H_4(g)$

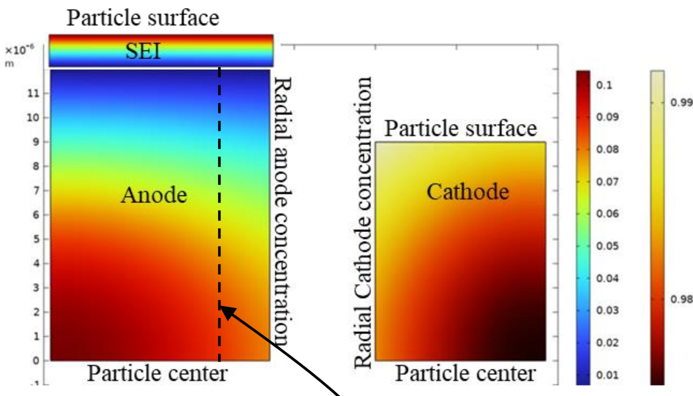
$$i_s = -Fk_{f,s}c_{EC}\exp\left[-\frac{\beta F}{RT}\left(\phi_{S,n} - \frac{\delta}{\kappa_{SEI}}i_{tot}\right)\right]$$

Intercalation $LiC_6(s) \leftrightarrow C_6(s) + Li^+(soln) + e^-$

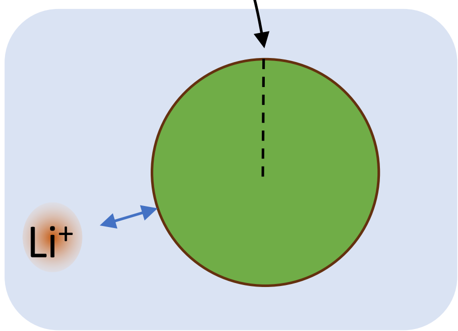
$$i_{int} = i_{int,0}\cdot 2\sinh\left[\frac{0.5F}{RT}\left(\phi_{S,n} - \phi_{E,n} - U_{0,n} - \frac{\delta}{\kappa_{SEI}}i_{tot}\right)\right]$$

Total $i_{tot} = i_s + i_{int}$

EC concentration at particle surface



Spherical Electrode Particles



Mass balance in particle surface:

Lithium: $\left(-D_{eff,s}\,r^2\frac{\partial c_P}{\partial r}\right)|_{r=\delta_{P,p}} = -\delta_{P,j}^2\frac{i_{tot,j}}{\mathcal{F}}$

Solvent: $\left(-D_{EC}\frac{\partial c_{EC}}{\partial r} + c_{EC}\right)|_{r=\delta_{P,p}} = i_s/F$

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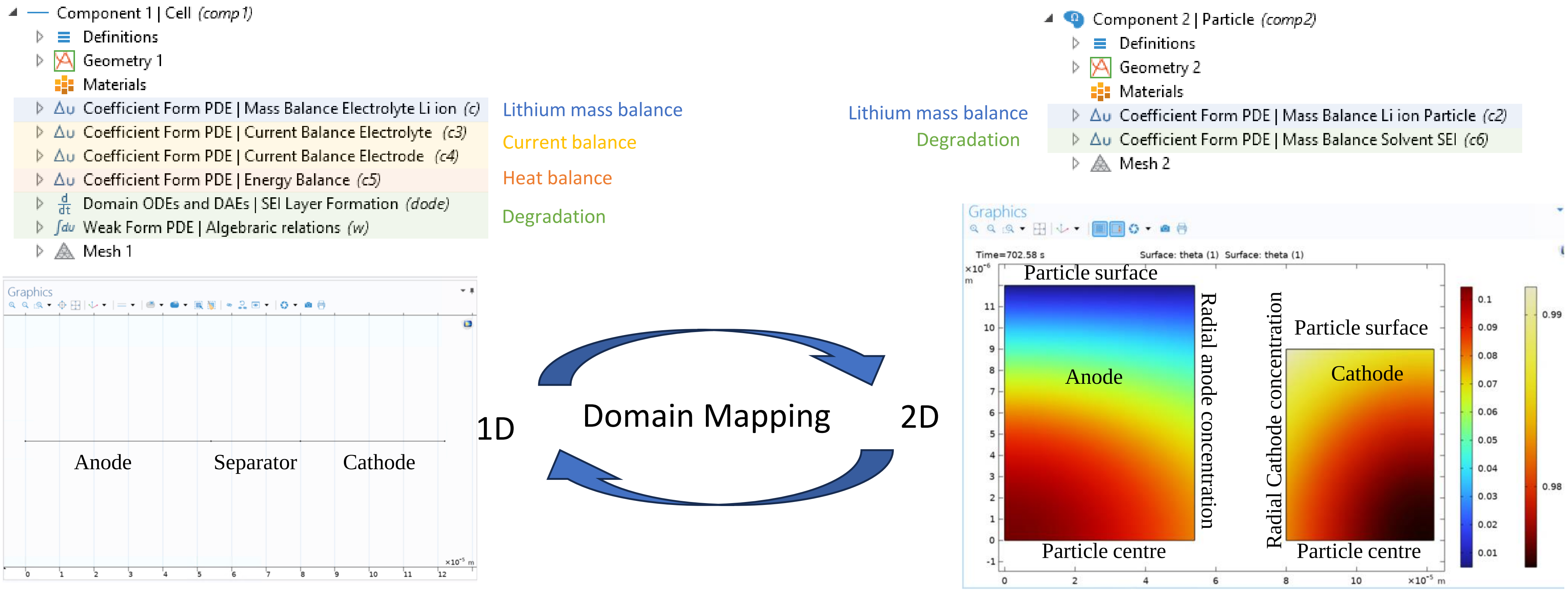
Safari et al., Journal of The Electrochemical Society, 156 3 A145-A153 2009.

COMSOL Implementation

Electrochemistry & Degradation

Particle and SEI Layer Diffusion



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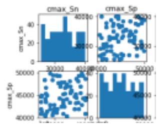
COMSOL Implementation



Parameter set Sample generation
- *Python*
- *SALib [1]*

LHS Samples
csv file

Experimental data
- *Battery Archive [2]*

Experimental Timeseries data
csv file

Simulation instance manager
- *Windows /COMSOL [3]*

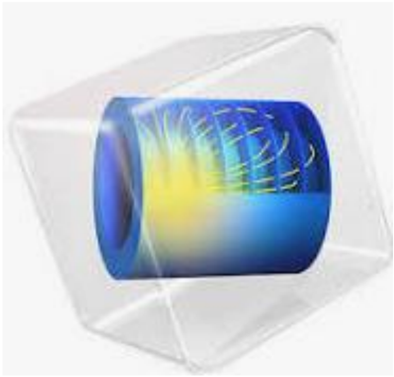
Stop Signal
csv file

COMSOL Multiphysics

Application Builder

Application Builder

Application Builder



- *Model Builder*
- *Application Builder*

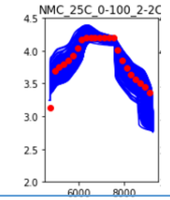
Application Builder

Application Builder

Model Builder

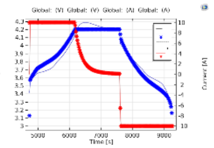
Simulation Timeseries data
csv file

Cost Functions
csv file



Post processing
- *Python*
- *SALib [1]*

Final simulation



Analysis
- *COMSOL*

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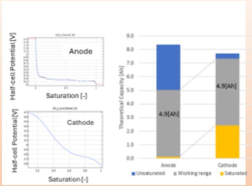
[1] https://salib.readthedocs.io/en/latest/ ; [2] www.batteryarchive.org; [3] COMSOL documentation

Parameter Fitting Method

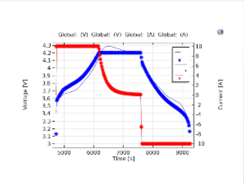
Pre-Cycling



- *Open cell voltage*
- *Half cell voltage*
- *SEM micrographs*
- *Design /Manufacturer data*

First-principles parameters

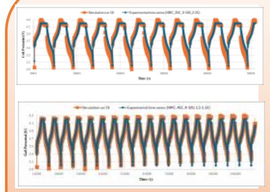
Single Cycle ("Fresh")



- *Fresh battery*
- *Time-potential-current time series data*
- *Charge /Discharge /Rest*
- *Varying conditions (temperature, C-rates, SOC min /max)*

System parameters
Temperature dependent kinetics and diffusion
$(k_n, E_{kn}), (k_p, E_{kp}),$
$(D_n, E_{Dn}), (D_p, E_{Dp}),$
R_{cell}

Multiple Cycles



- *Multiple cycling data*
- *Time-potential-current time series data*
- *Charge /Discharge /Rest*
- *Varying conditions (temperature, C-rates, SOC min /max)*

System Parameters
Degradation
$D_{EC,SEI}$
k_{SEI}

1. Sample

N samples

2. Simulate

M datasets

3. Evaluate

$$F_{cost} = \frac{1}{M}\sum_{j=1}^{M}\frac{1}{N}\sum_{i=1}^{N} w_{ij}(U_{ij} - \tilde{U}_j)^2$$

Uniform weight $w_j = 1$

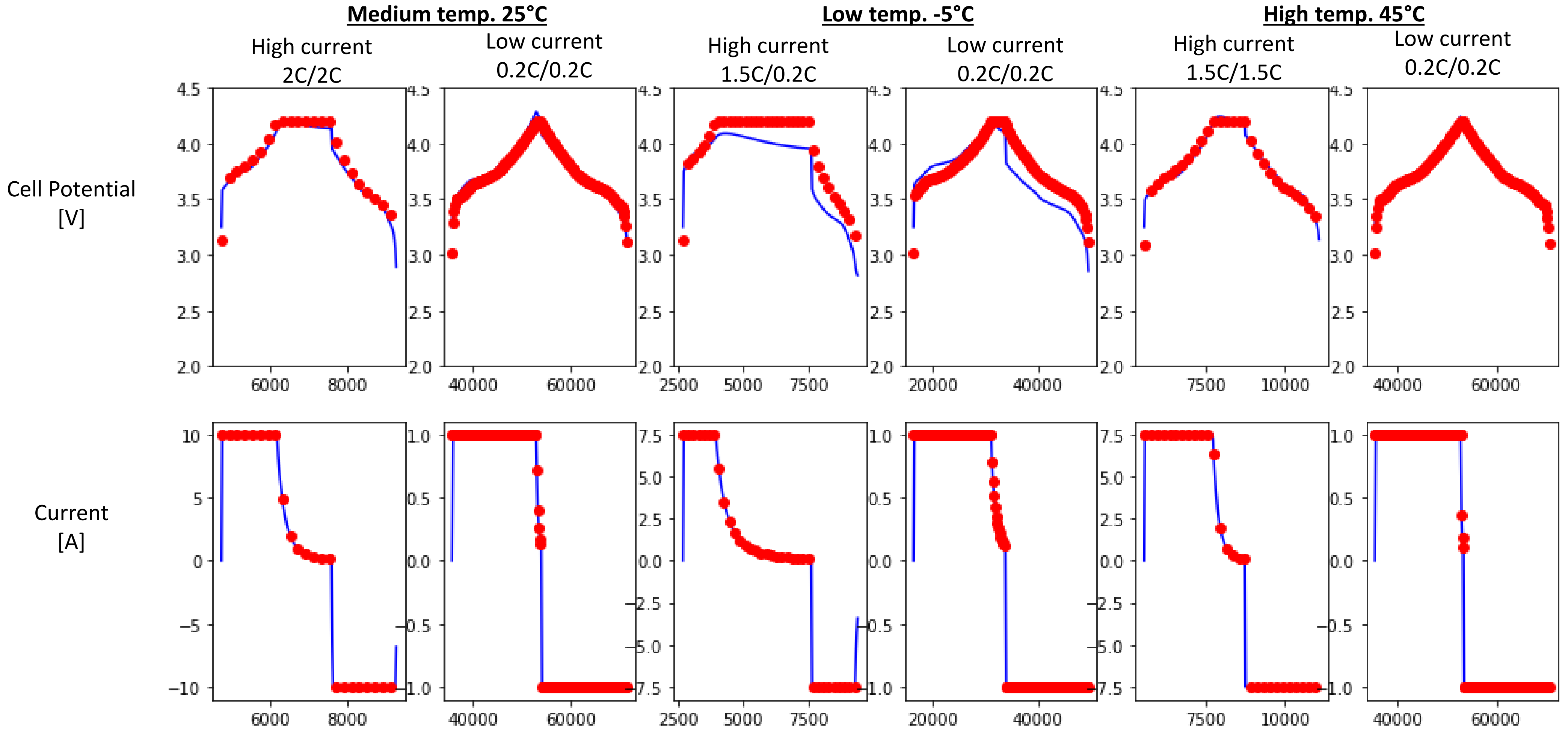
Acceptable F_{cost}?

No

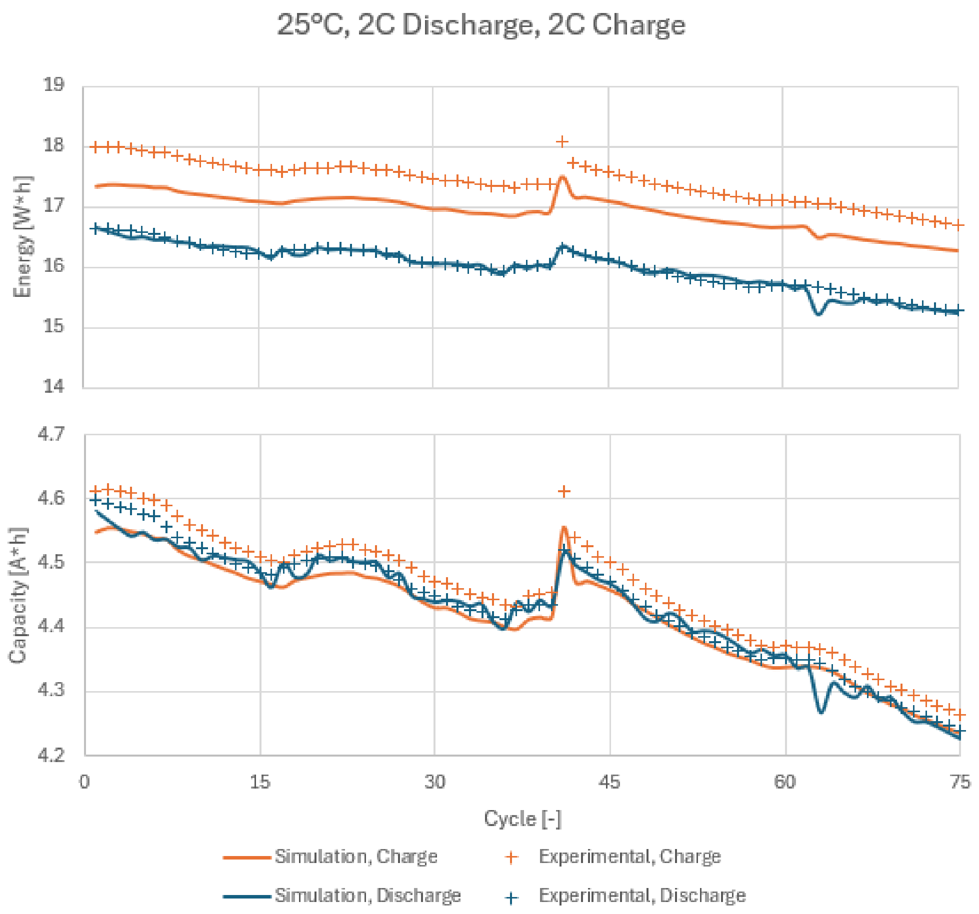
Yes

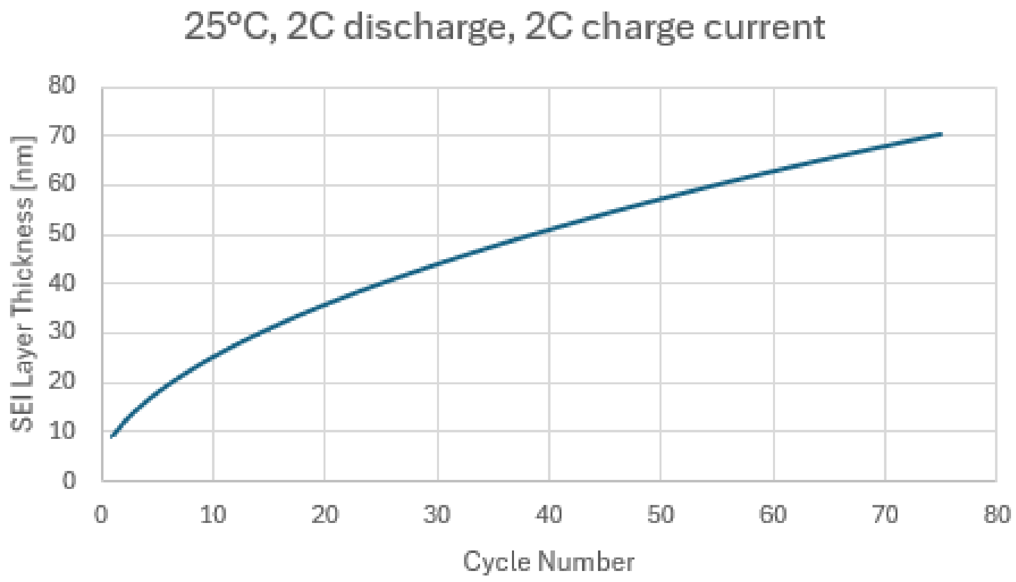
Finish

Expected vs Obtained Results



Expected vs Obtained Results





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Quality of Fit

Fresh Battery

$N = 600$ (samples)
$M = 6$ (datasets)

$$\min F_{cost} = 0.012[V^2]$$

Degradation

$N = 25$ (samples)
$M = 2$ (datasets)
$CYC = 75$ (cycles)

$$\min F_{cost} = 0.667[V^2]$$

Uncertainty and Sensitivity Analysis

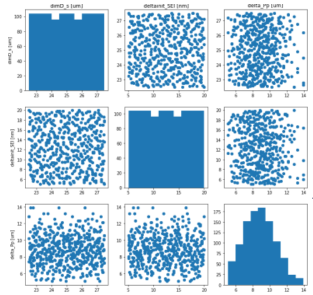
Inputs – Manufacturing Parameters

1. **Mechanical process tolerances**
   Separator thickness variations
   $L_s \sim \mathcal{U}(22.5[\mu m]; 27.5[\mu m])$

2. **Cell Storage Conditioning variations**
   Initial SEI layer thickness
   $\delta_{SEI,init} \sim \mathcal{U}(5[nm], 20[\text{nm}])$

3. **Electrode process parameter limits**
   Positive electrode particle radius
   $\delta_{P,p} \sim \mathcal{N}(8.4[\mu m]; (2.5[\mu\text{m}])^2)$

Uncertain Parameter Sampling

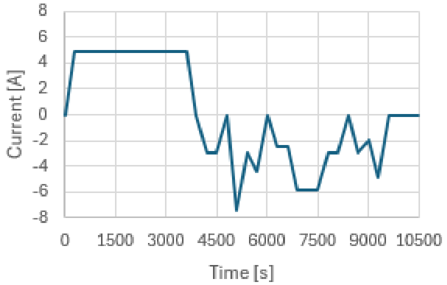


Sample size=1024

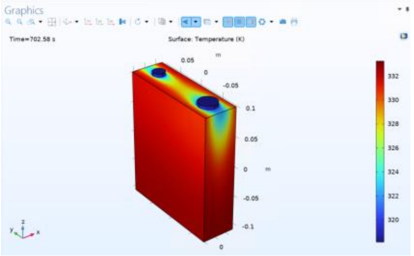
Inputs – Operating Parameters

1. **Charge: 1C**
2. **Discharge conditions: Varying**
3. **Temperature: 25°C**

Load curve

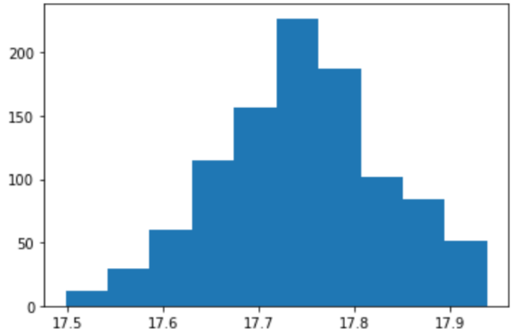


Battery Cell Electrochemical Model



Outputs – Cell Quality Control

Uncertainty Analysis



Sensitivity Analysis

Sobol indices [1]:

S_{1i} = Contribution to output variance

S_{Ti} = Overall effect

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[1] Sobol', I.M., 2001. "Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates"

Uncertainty and Sensitivity Analysis

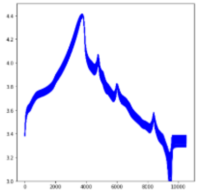
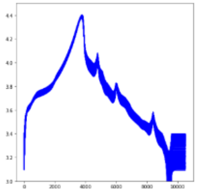
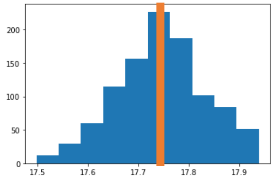
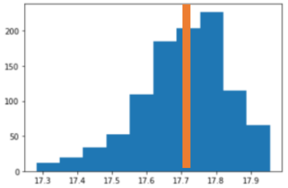
Ranking of variables for importance on output variance:

- 1 cycle: $L_s > \delta_{SEI,init} > \delta_{P,p}$
- 25 cycles: $\delta_{P,p} > \delta_{SEI,init} > L_s$

Optimization

- Manufacturing cost example based on product specification:
  $Cost = Cost_{nomial} + Cost_{oversize}$
  $Cost_{nomial} = f(\mu, \ldots)$
  $Cost_{oversize} = f(\sigma^2, \ldots)$

Reduce $Cost_{oversize}$ by reducing variance on cathode particle size distribution.

Variable	1st cycle		25th cycle	
Potential				
Histogram				
Discharge energy 95% confidence interval [W*h]	17.60 ≤ 17.75 ≤ 17.89		17.46 ≤ 17.71 ≤ 17.89	
Sensitivity [1]	$S_{1i}^{cycle=1}$	$S_{Ti}^{cycle=1}$	$S_{1i}^{cycle=25}$	$S_{Ti}^{cycle=25}$
L_s	0.36	0.97	0.03	0.36
$\delta_{SEI,init}$	0.38	0.86	0.30	0.78
$\delta_{P,p}$	0.33	0.69	0.39	0.90

[1] Sobol', I.M., 2001. "Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates"

Conclusions

- Successful implementation of an electrochemical model of a battery including degradation
- Robust framework for parameter fitting
- Parameters successfully tuned for data set (incl. temperature dependency)
- Uncertainty/Sensitivity Analysis to quantify performance parameter variance
- Uncertainty/Sensitivity Analysis to prioritize optimization efforts on e.g., manufacturing process

- COMSOL Application Builder offers excellent freedom and flexibility for handling large data sets and complex scenario simulations

Acknowledgement

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Project: Multi-scale simulation of laser welding for optimal battery pack manufacturing

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