COMSOL CONFERENCE 2018 BOSTON

Oakland UNIVERSITY

Fast Charging Strategy Optimization Based on Electrochemical Model and Dynamic Programming for a Lithium Ion Battery Cell

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Enabling Li-ion Battery Fast Charge?

⇨

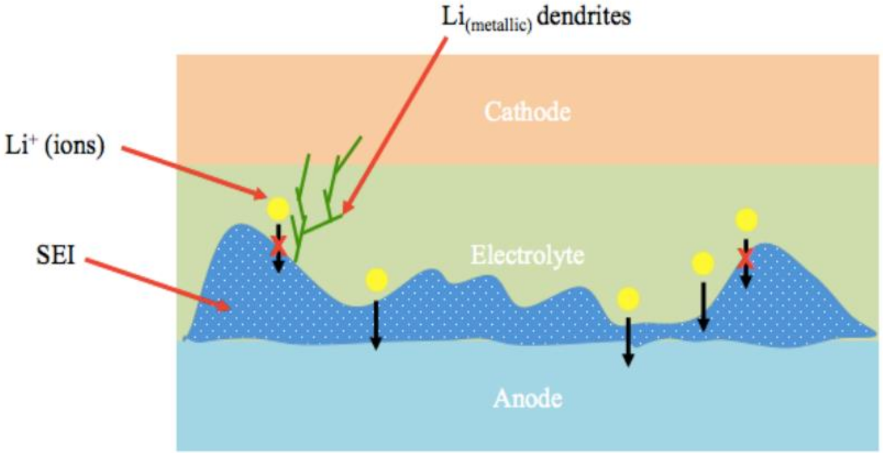
⇨ "Range Anxiety" ⇨ Fast Charge

Challenges of Fast Charge

Fast Charge → Heat generation → High temperature → Thermal runaway

Fast Charge → SEI growth → Degradation / Capacity fade

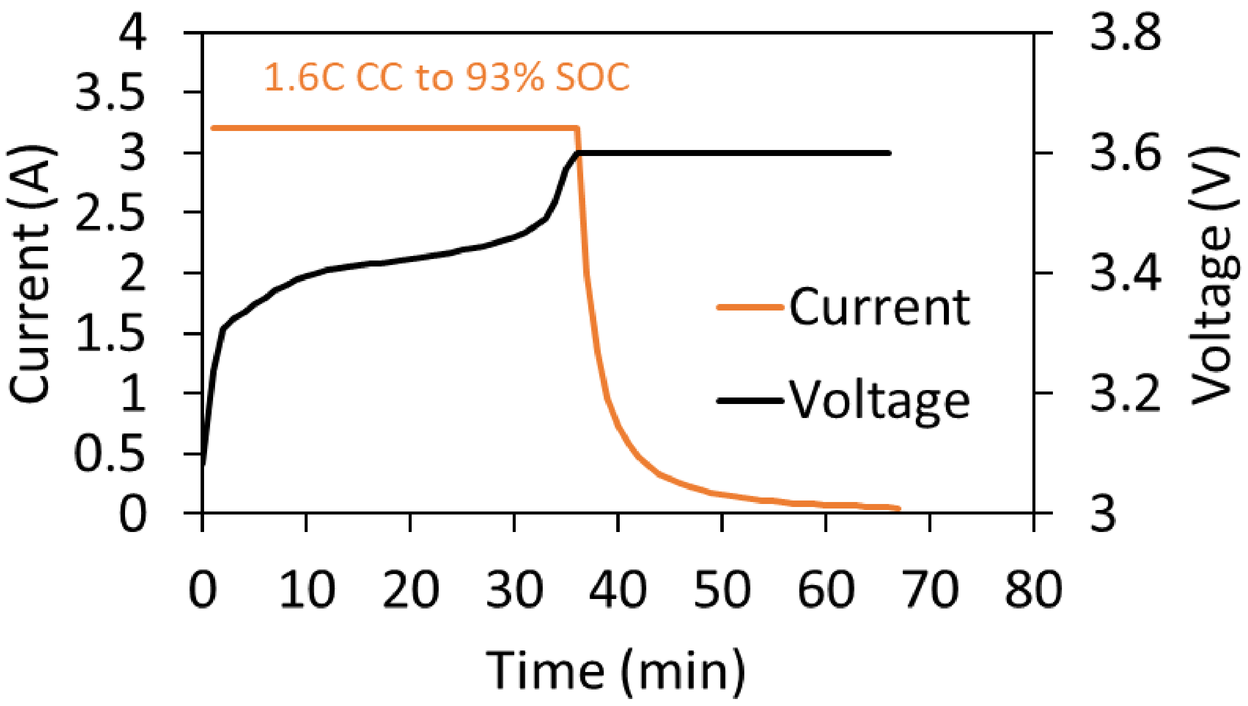
Fast Charge → Li plating



Charging Strategy Review

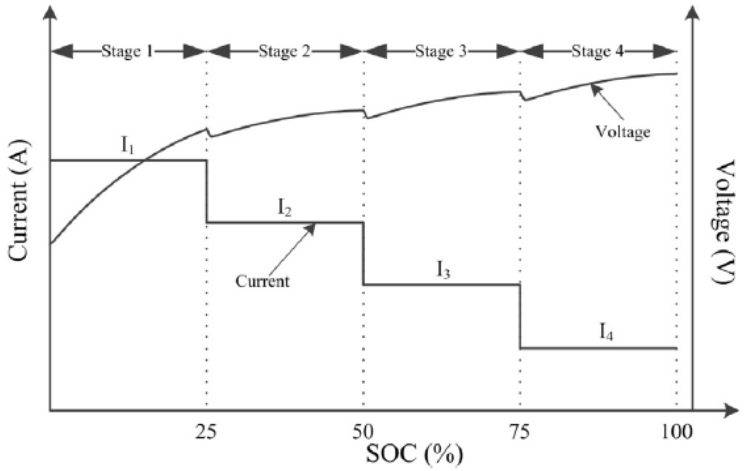
- Constant Current Constant Voltage (CCCV) Charging

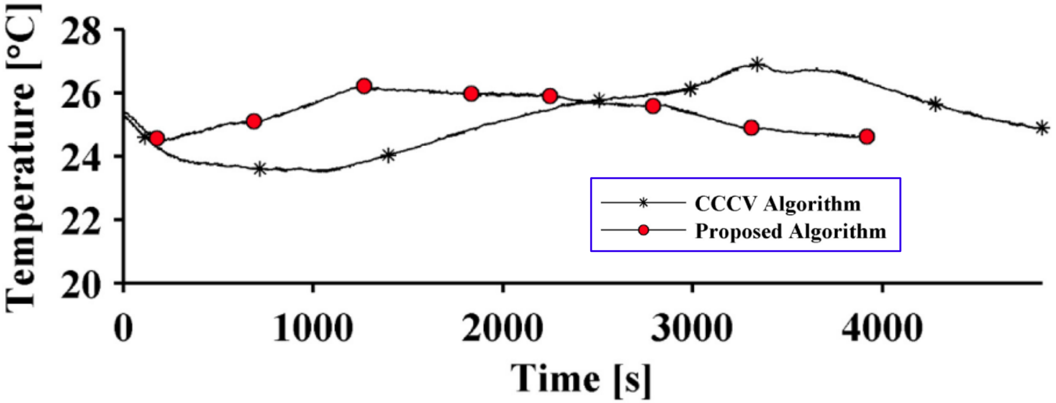
A123 26650 LFP Cell Data



Charging Strategy Review

- Multistage Constant Current Charging (MCC) (Vo et al. 2014)





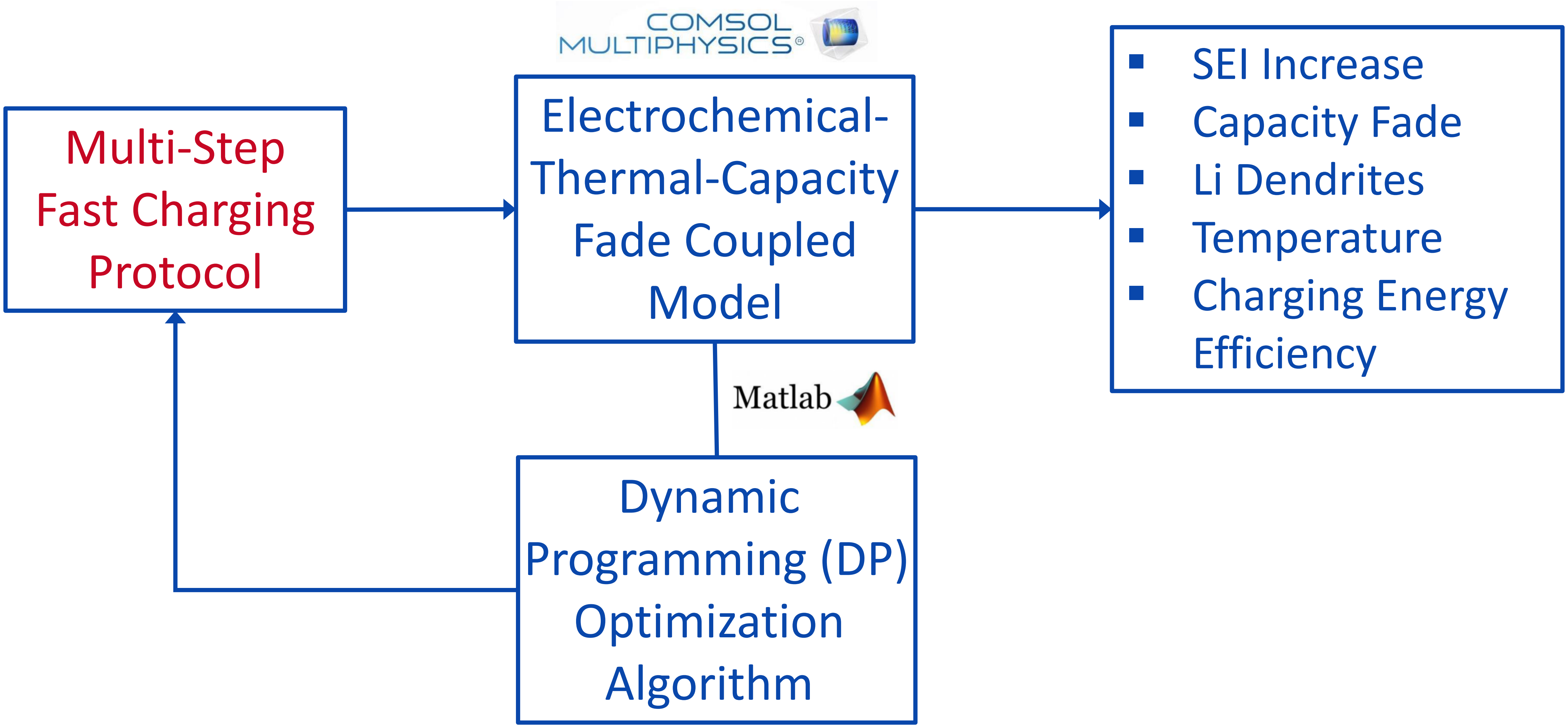
- Decrease charging time
- Low temperature rise
- High charging efficiency

Source: T.T. Vo, X. Chen, W. Shen, A. Kapoor, New charging strategy for lithium-ion batteries based on the integration of Taguchi method and state of charge estimation, J. Power Sources 273 (2015) 413-422

Objective

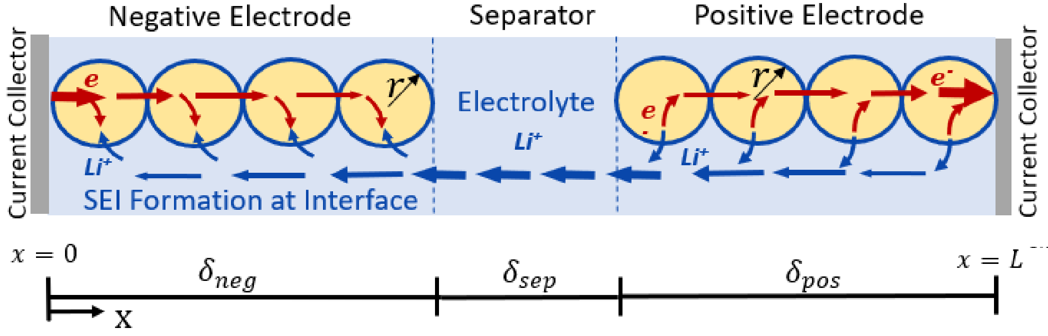
- To study the effect of charging protocol on capacity fade and thermal behavior by developing an electrochemical-thermal-capacity fade coupled model
- To optimize the charging protocol based on Dynamic Programming optimization algorithm

Methodology

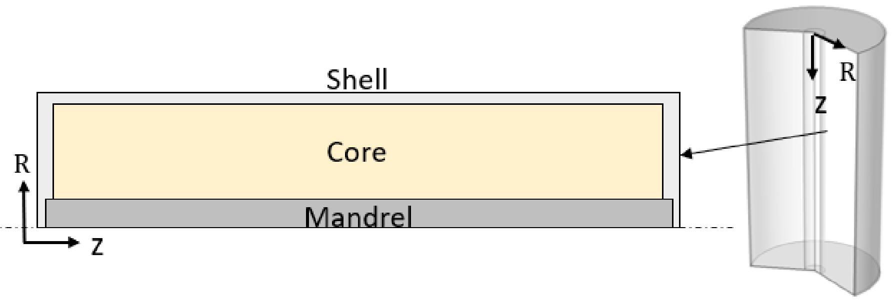


Methodology

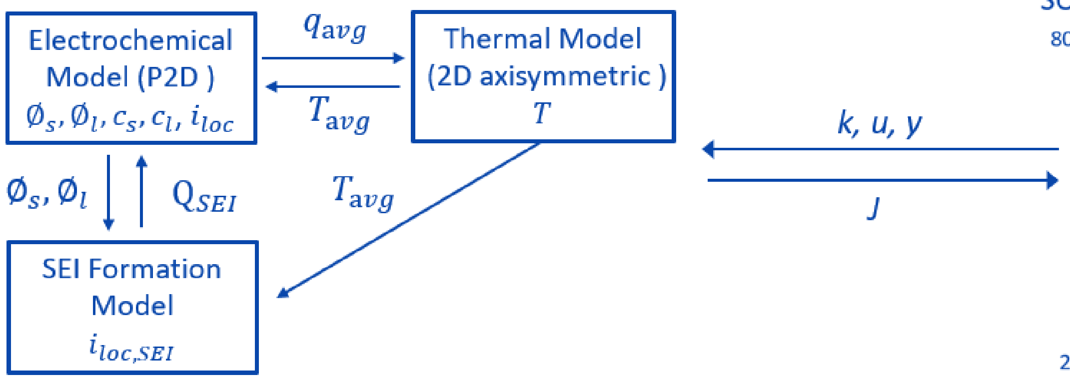
(a) *Electrochemical Model*



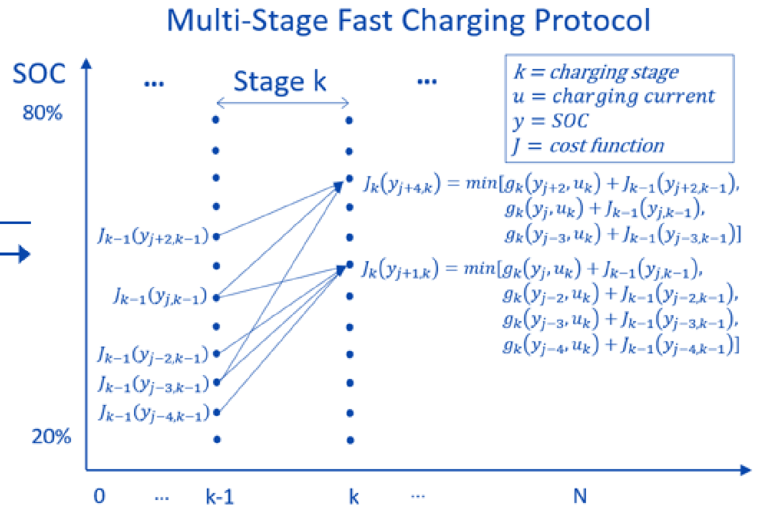
(b) *Thermal Model*



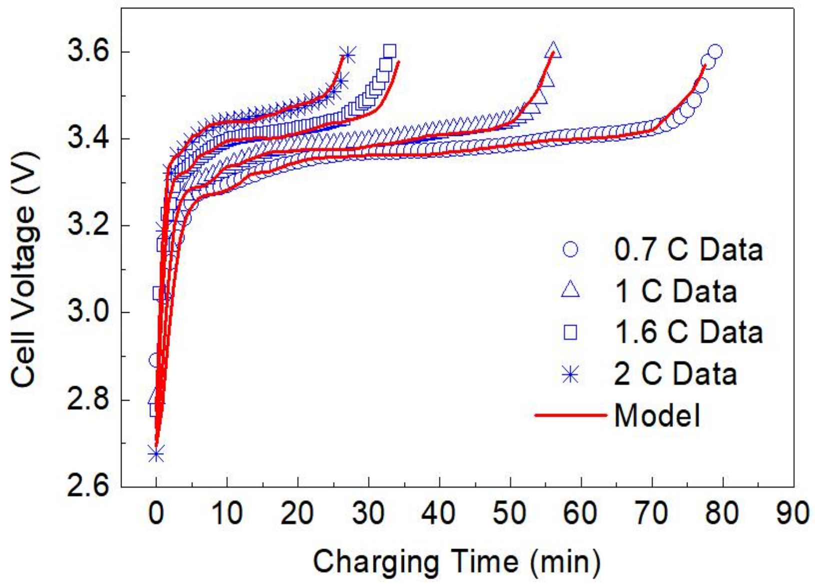
(c) *Model Coupling*

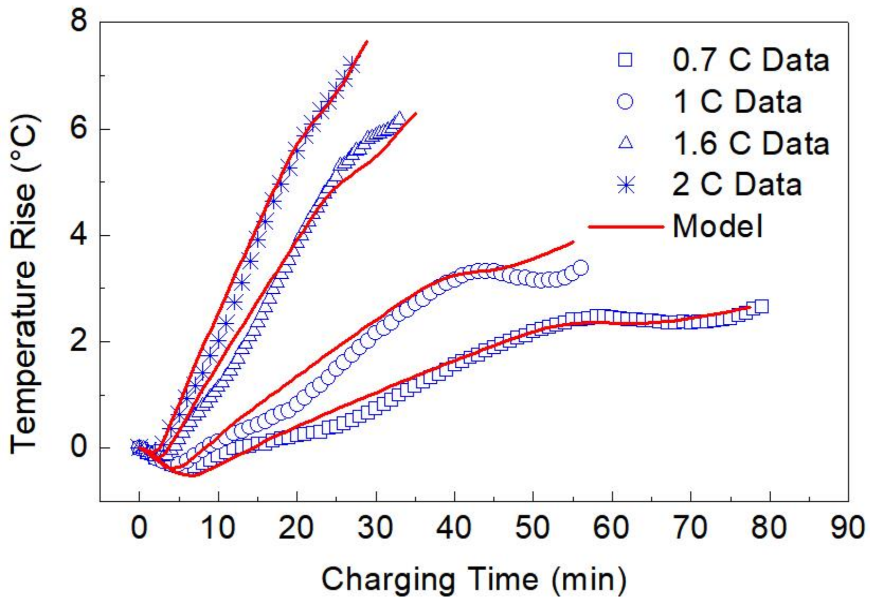


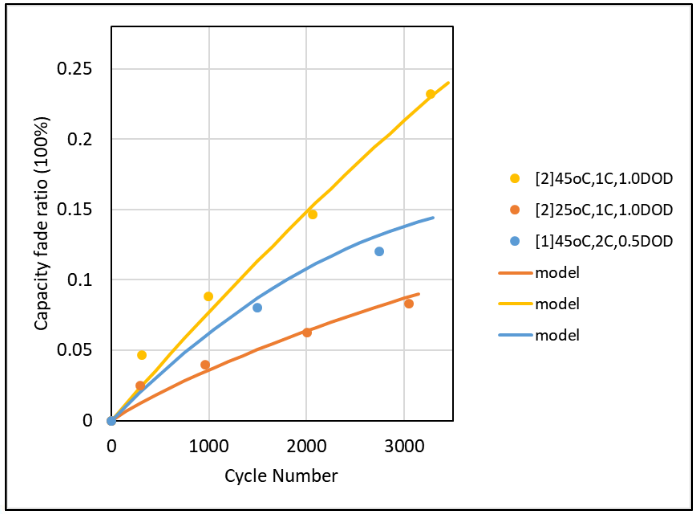
(d) *Dynamic Programming Optimization*



Model Validation





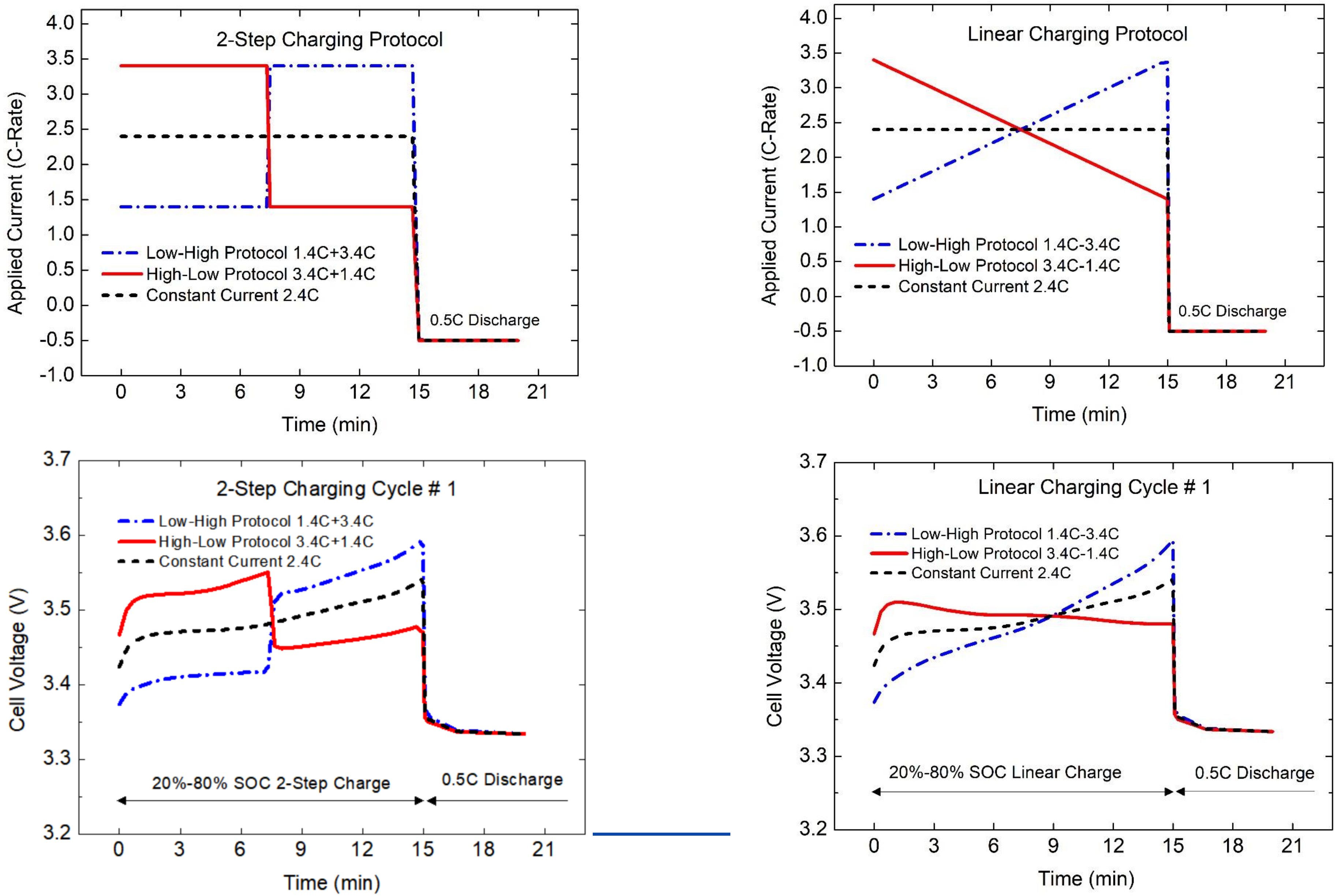


A123 2.3 Ah LFP 26650

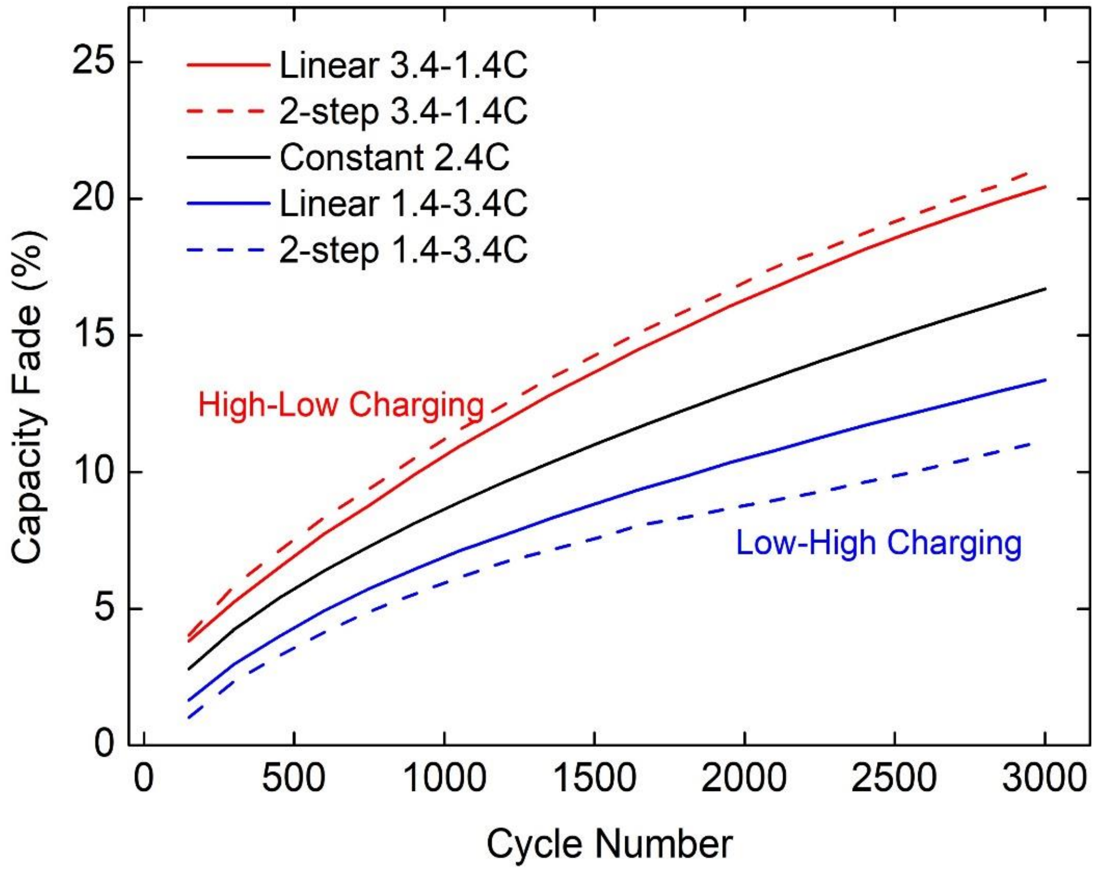
MACCOR system 4200
Battery test equipment

Source: T.T. Vo, X. Chen, W. Shen, A. Kapoor, New charging strategy for lithium-ion batteries based on the integration of Taguchi method and state of charge estimation, J. Power Sources 273 (2015) 413-422

15 minutes / 20% ~ 80% SOC Fast Charging Protocols



Impact of Cycle Number and Protocol on Capacity Fade



- Low-High charging protocols obtain lower capacity fade than High-Low protocols
- The 2-step Low-High protocol results in the lowest capacity fade

Dynamic Programming (DP) Optimization

Operating Conditions:

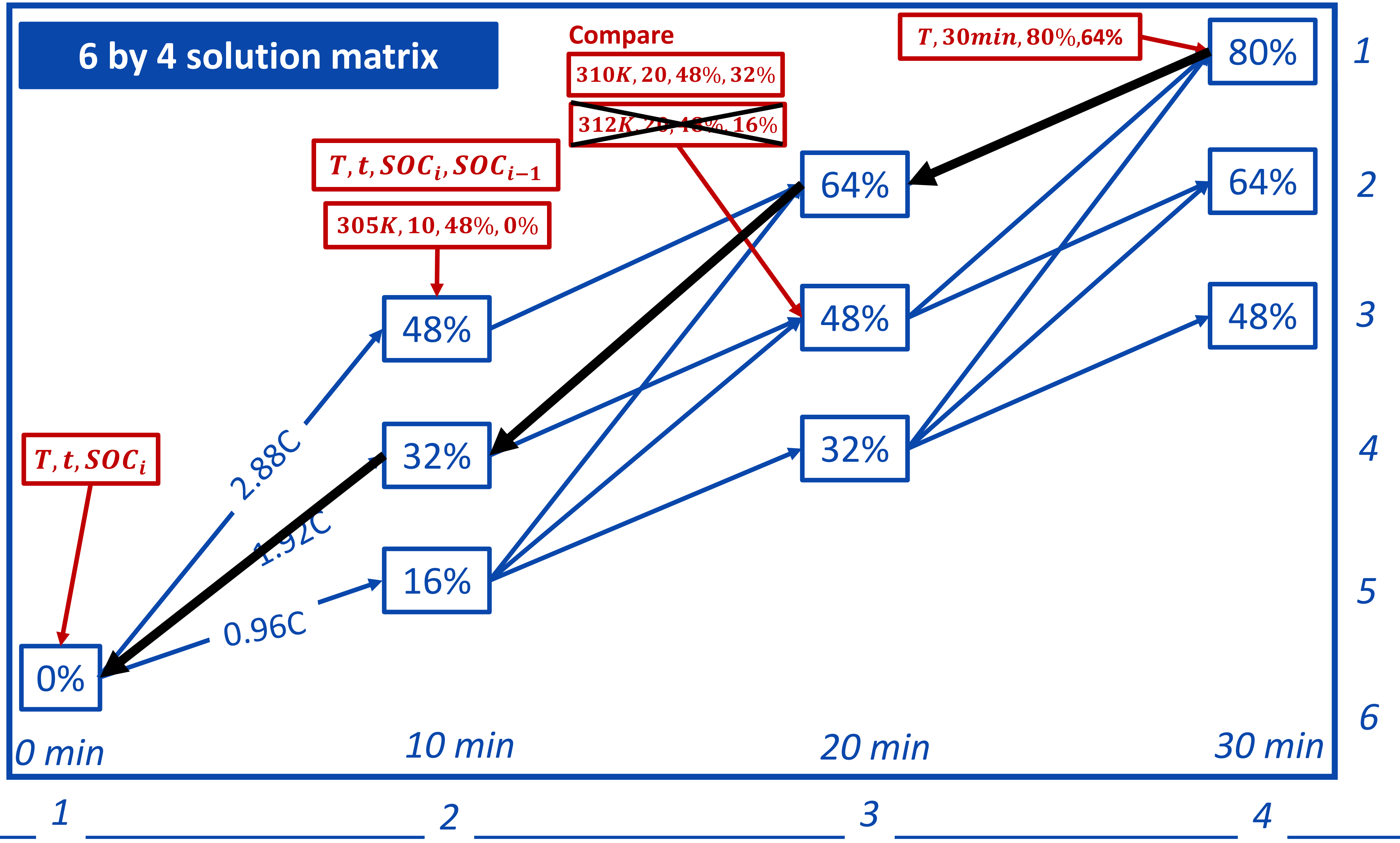
- Charging SOC = 0% ~ 80%
- Charging time = 30 mins
- Δt = 10 mins
- Charging step = 3
- Charging current = 0.96C, 1.92C, 2.88C
- ΔSOC = 16% (0.96C)

Goal:

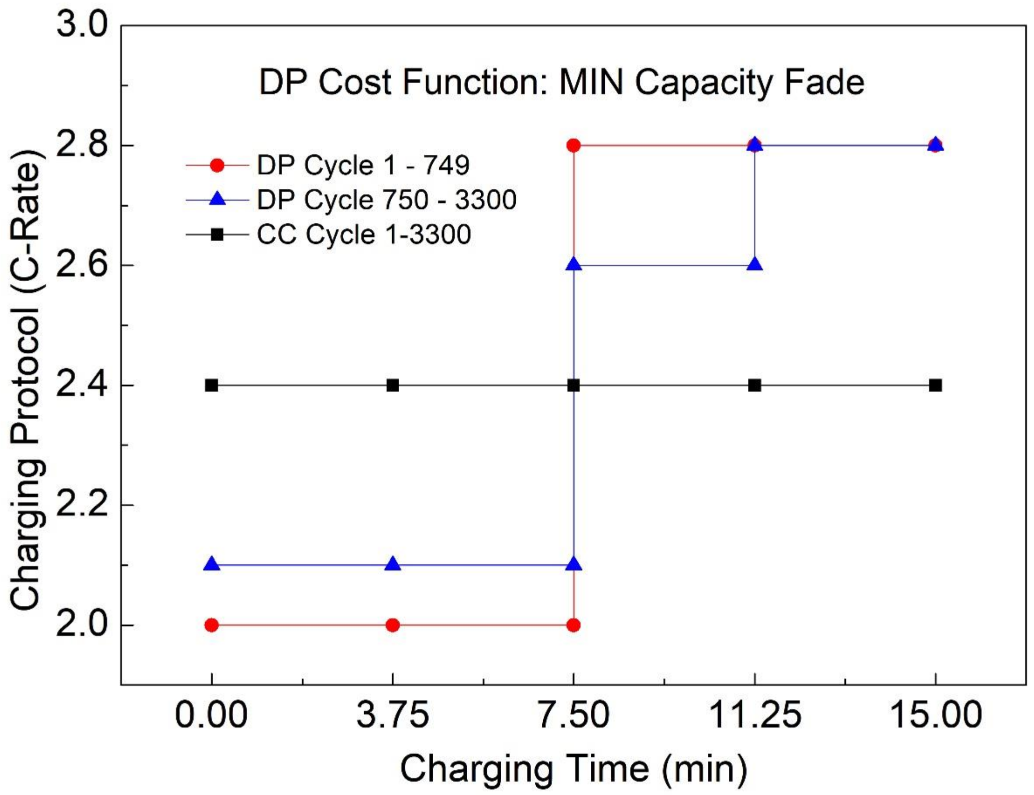
- $\min T(30min, 80\%)$

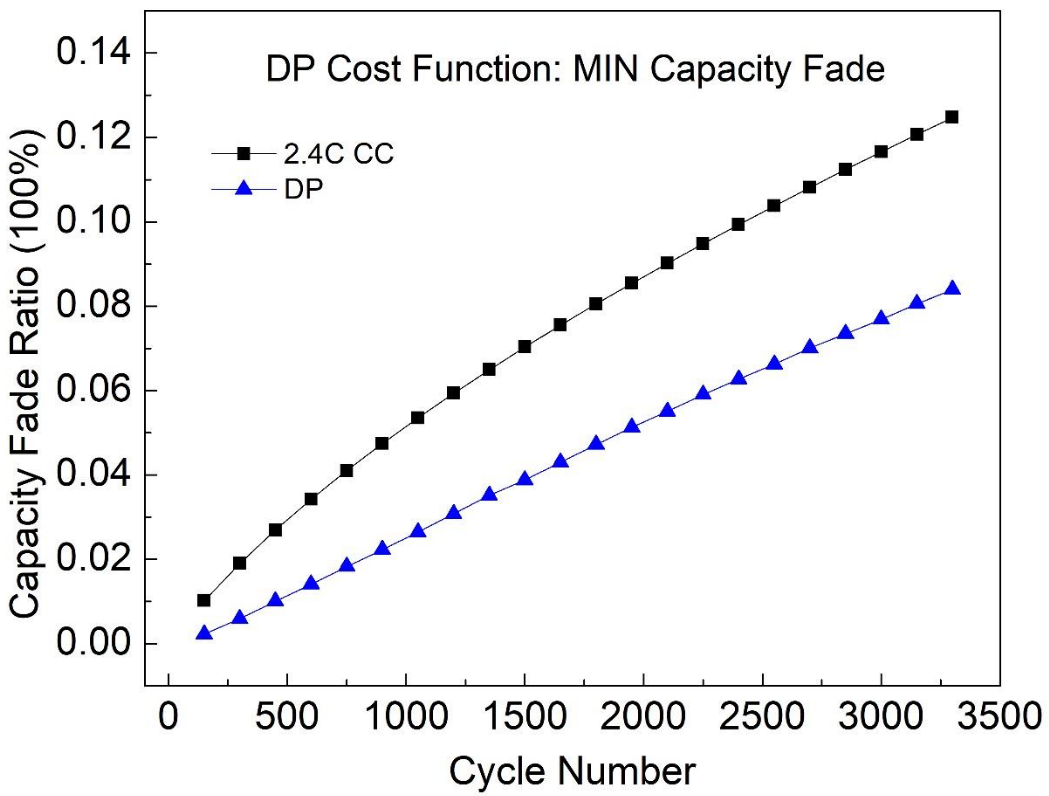
Constrains:

- $T < T_{max,\ cell}$
- SOC < 80%

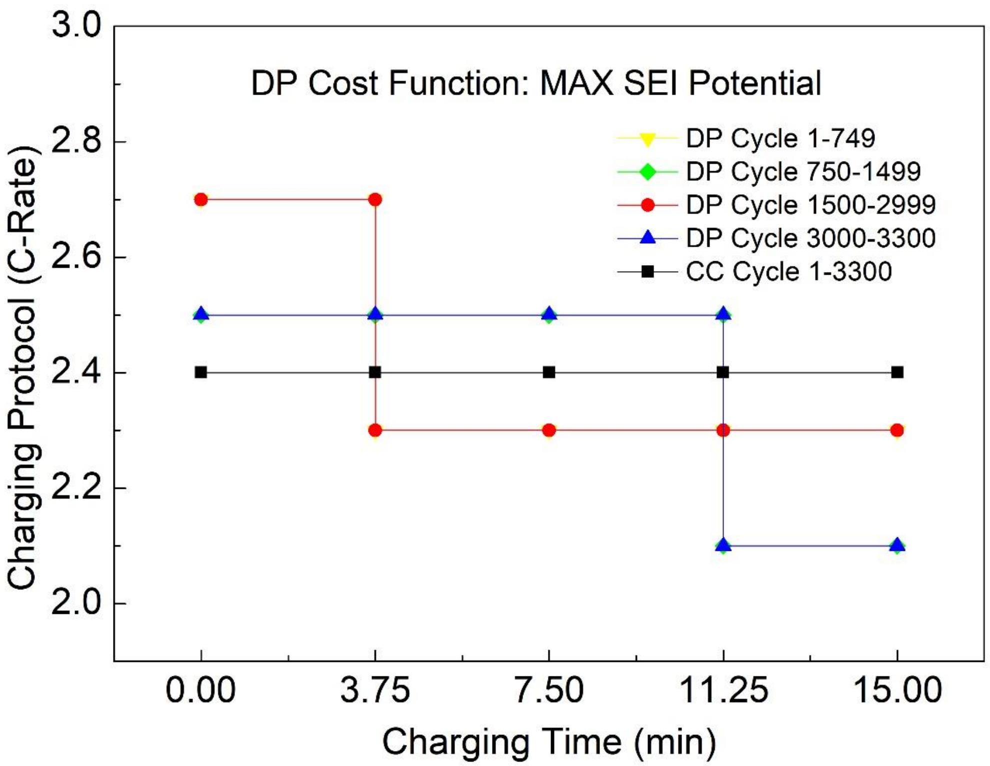


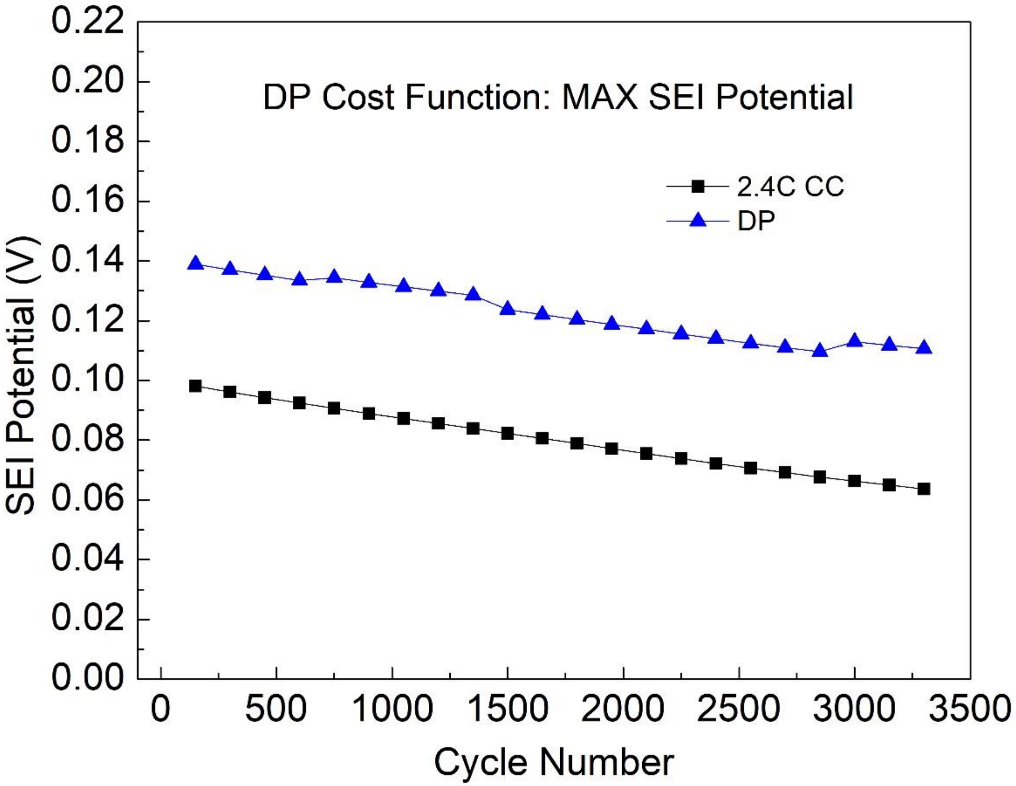
Capacity Fade Optimization



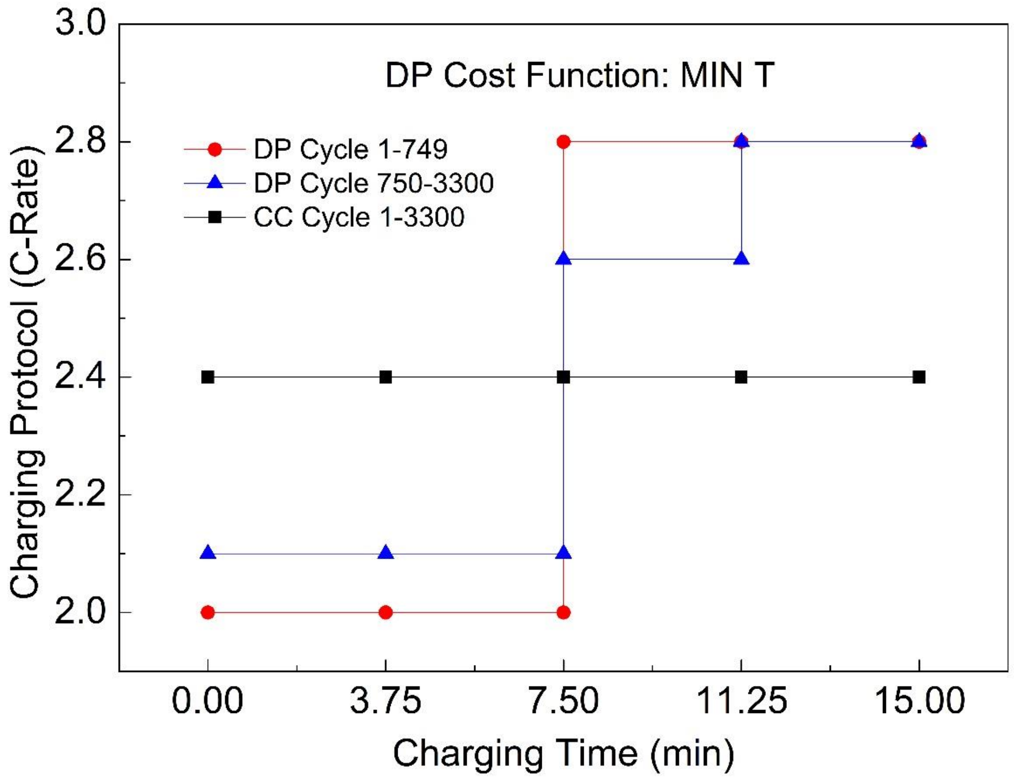


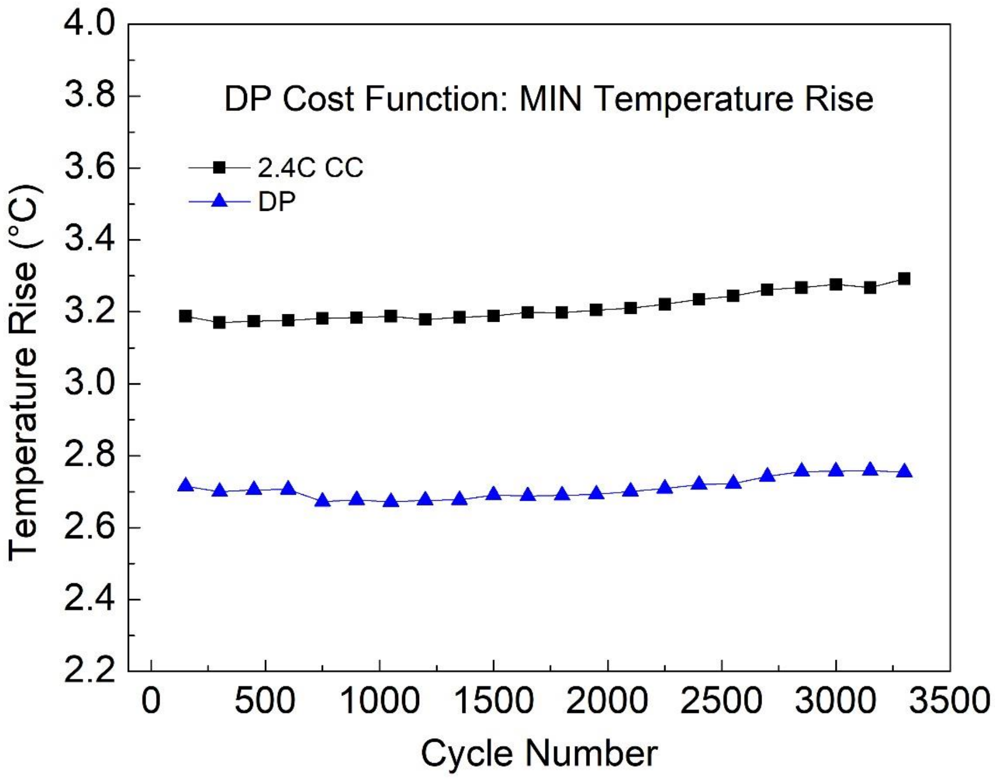
SEI Potential Optimization



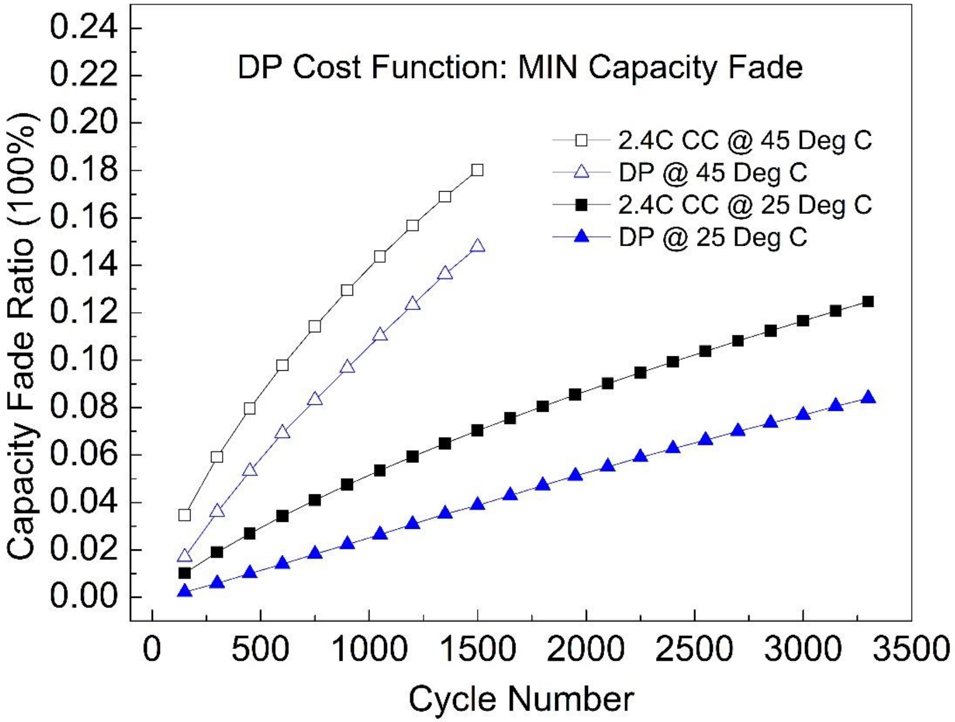


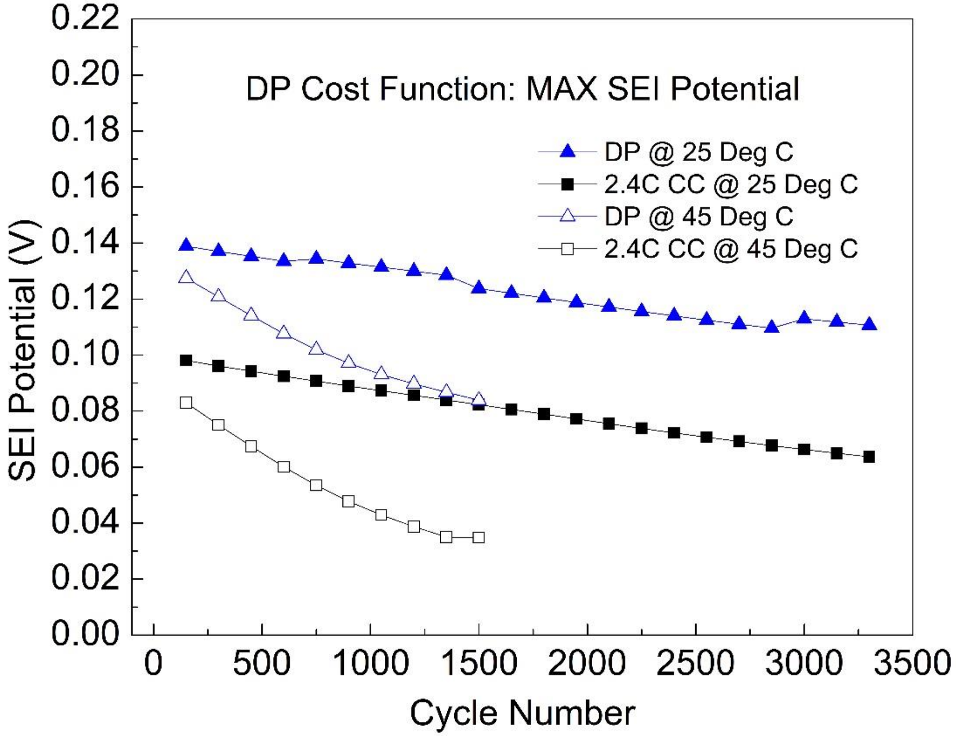
Temperature Rise Optimization





Optimization at Different Ambient Temperatures





Conclusions

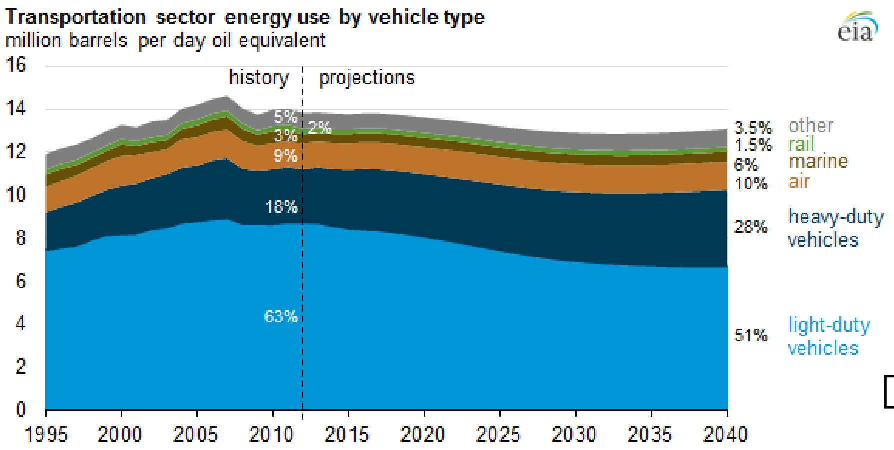
- An electrochemical-thermal-capacity fade coupled model for a Li-ion battery cell is developed using COMSOL Multiphysics
- The effect of fast-charging protocol on capacity fade with charging-discharging cycles is studied
- A Dynamic Programming Optimization algorithm is developed using COMSOL Livelink - MATLAB to optimize the fast charging protocol
- The cost function include capacity fade, SEI potential, and temperature rise.

Acknowledgement

Dr. Benjamin Reichman (BASF Battery Materials - Ovonic)

Thank you!

Enabling Li-ion Battery Fast Charge?



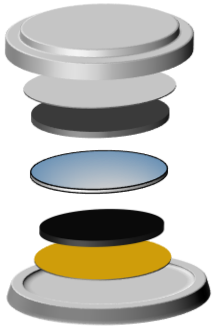
1% market share

- Cost
- "Range anxiety"

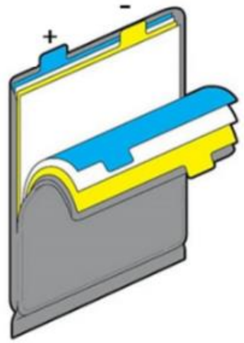
Fast charging Li-ion batteries …

Typical Lithium Ion Cells

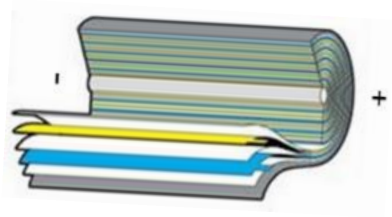
- ❑ Coin/Button Cell

- ❑ Prismatic Cell

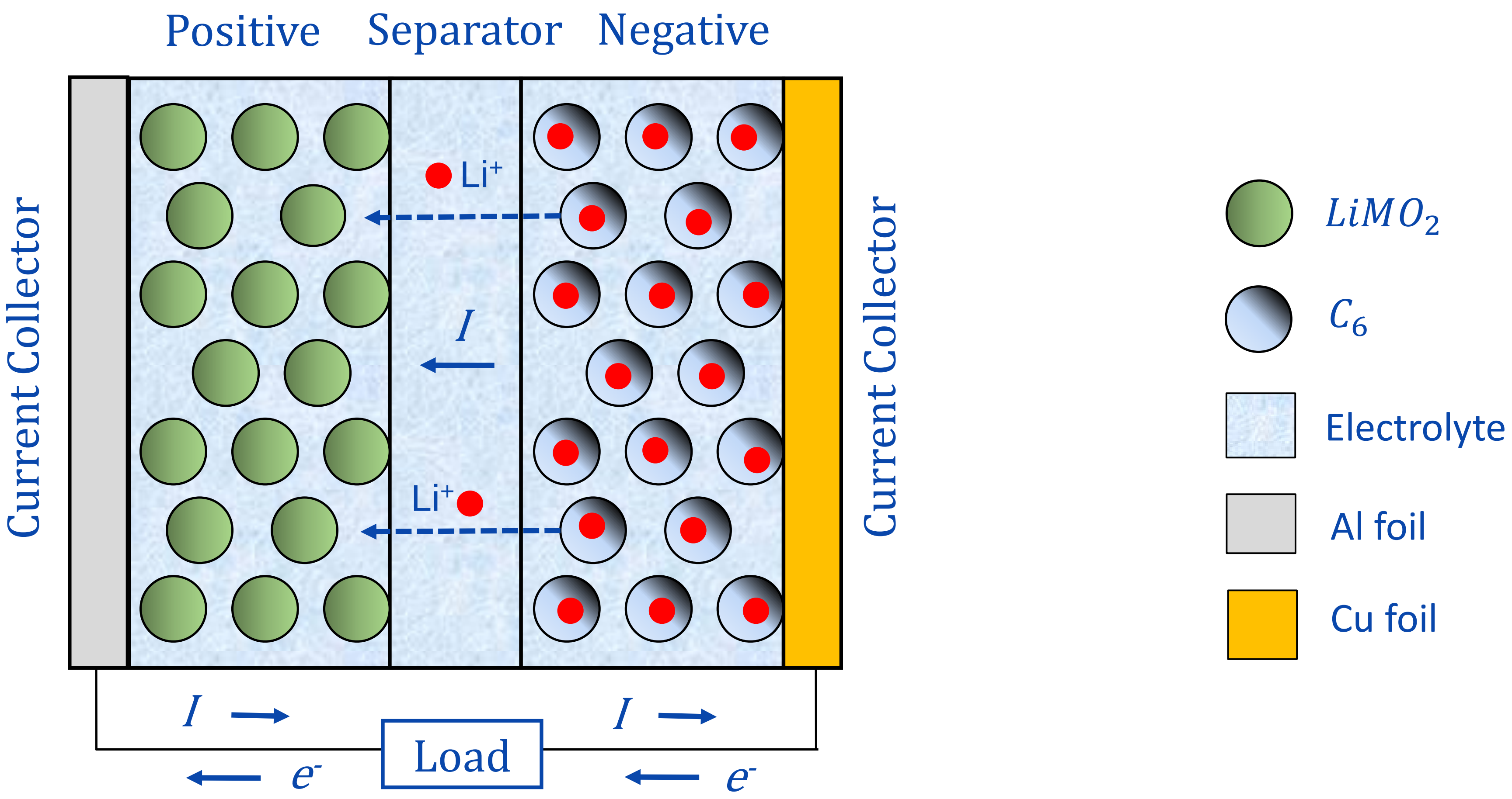



- ❑ Cylindrical Cell



- ❑ Pouch Cell

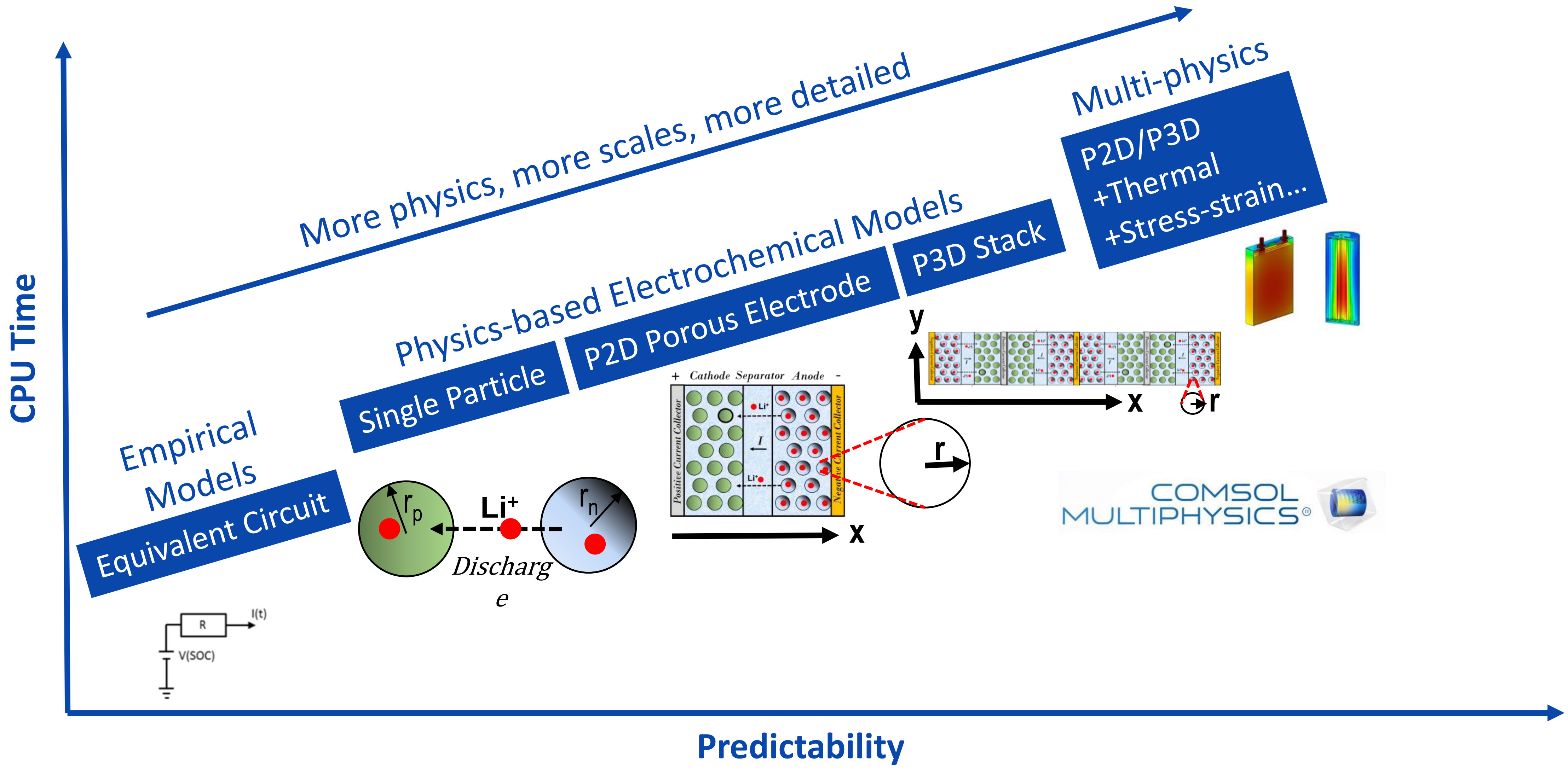

Lithium Ion Electrochemical Cell



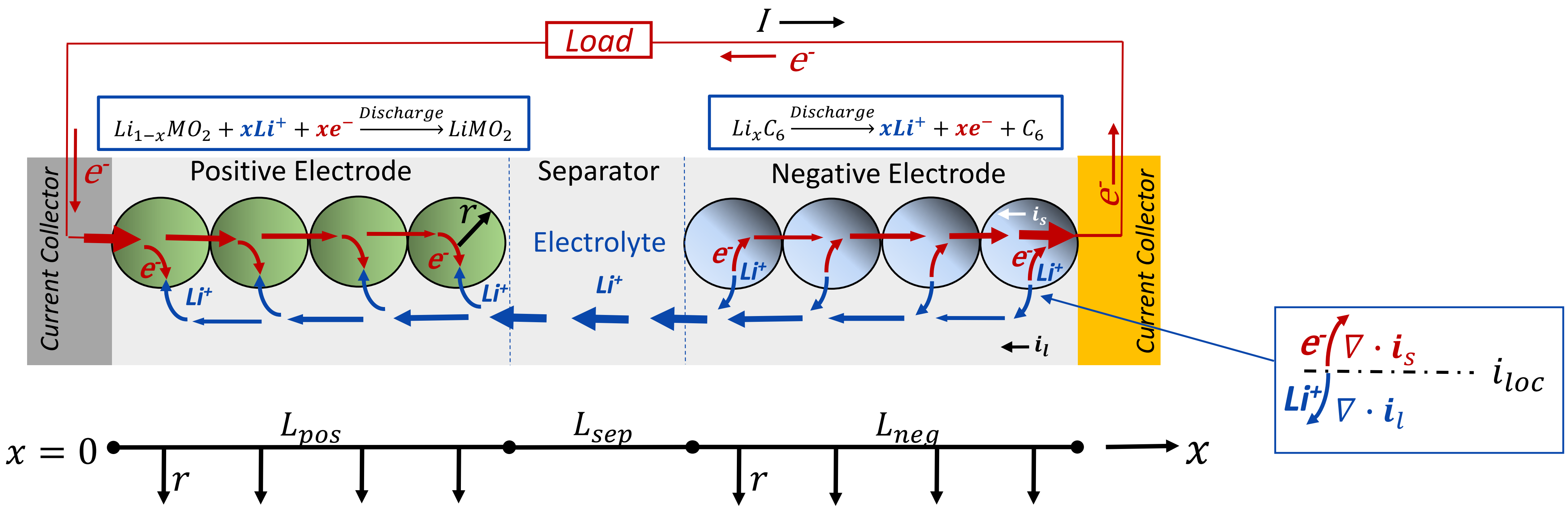
Positive Electrode: $Li_{1-x}MO_2 + xLi^+ + xe^- \xrightarrow{Discharge} LiMO_2$

Negative Electrode: $Li_xC_6 \xrightarrow{Discharge} \mathbf{xLi^+} + \mathbf{xe^-} + C_6$

Typical Lithium Ion Battery Models



P2D Electrochemical Model



Charge Conservation in x: $\nabla \cdot \boldsymbol{i}_s + \nabla \cdot \boldsymbol{i}_l = 0;$ $\nabla \cdot \boldsymbol{i}_s = -\alpha_v i_{loc};$ $\nabla \cdot \boldsymbol{i}_l = \alpha_v i_{loc}$

Mass Conservation in x: $\epsilon_l \frac{\partial c_l}{\partial t} + \nabla \cdot \boldsymbol{N}_l = \frac{\alpha_v i_{loc}}{F}$

Mass Conservation in r: $\frac{\partial c_s}{\partial t} + \nabla \cdot \left(-D_s \frac{\partial c_s}{\partial r}\right) = 0$

Electrochemical Kinetics: $i_{loc} = \mathrm{nF} k_0 c_l {c_s}^{\alpha_a} (1 - c_{s,max})^{1-\alpha_a} \left(C_R exp\left(\frac{\alpha_a F\eta}{RT}\right) - C_O exp\left(\frac{-\alpha_c F\eta}{RT}\right)\right)$

$\emptyset_s(x,t)$
$\emptyset_l(x,t)$
$c_l(x,t)$
$c_s(r,t)$

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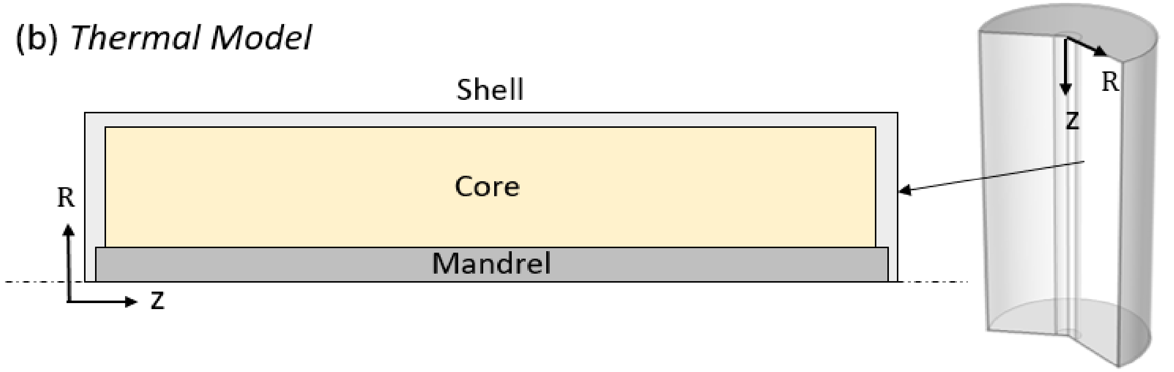
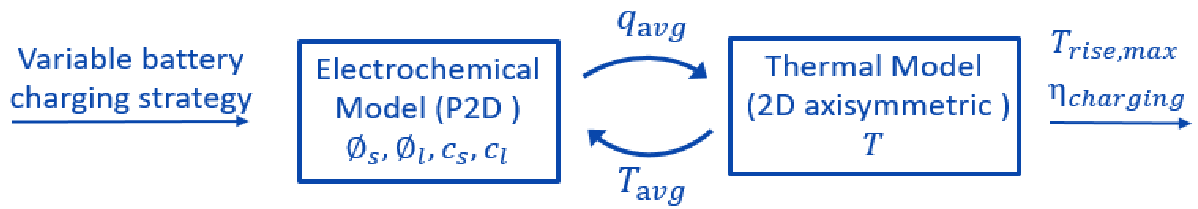
Thermal Model

(b) *Thermal Model*



(c) *Model Coupling*



Physics	Equations
Energy conservation	$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial R}\left(\lambda_R \frac{\partial T}{\partial R}\right) + \frac{\partial}{\partial Z}\left(\lambda_Z \frac{\partial T}{\partial Z}\right) + q_{tot}$
Local heat generation rate	$q_{tot} = q_{rev} + q_{irr} + q_{ohm}$
Reversible entropy heat	$q_{rev} = S_a j_{loc} T \frac{\partial U_{eq}}{\partial T}$
Irreversible reaction heat	$q_{irr} = S_a j_{loc}\left(\emptyset_s - \emptyset_l - U_{eq}\right)$
Irreversible ohmic heat	$q_{ohm} = q_{ohm,s} + q_{ohm,l}$
Electrical ohmic heat	$q_{ohm,s} = -i_s \cdot \nabla\emptyset_s = \sigma_s(\nabla\emptyset_s)^2$
Ionic ohmic heat	$q_{ohm,l} = -i_l \cdot \nabla\emptyset_l = \left(\kappa_{l,eff}\nabla\emptyset_l + \kappa_{D,eff}\nabla(\ln c_l)\right) \cdot \nabla\emptyset_l$

Capacity Fade Model

- In addition to the main graphite-lithium intercalation reaction on the negative electrode, the parasitic lithium/solvent reduction reaction is also included in the model:

$$S + Li^{+} + e^{-} \rightarrow P_{SEI}$$

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

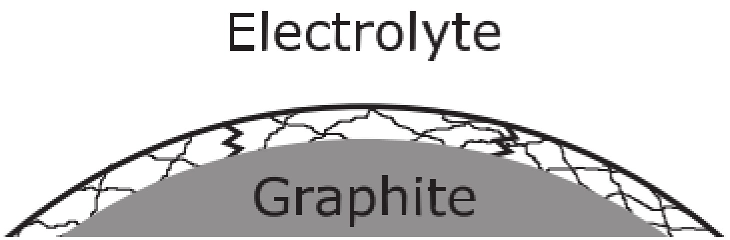
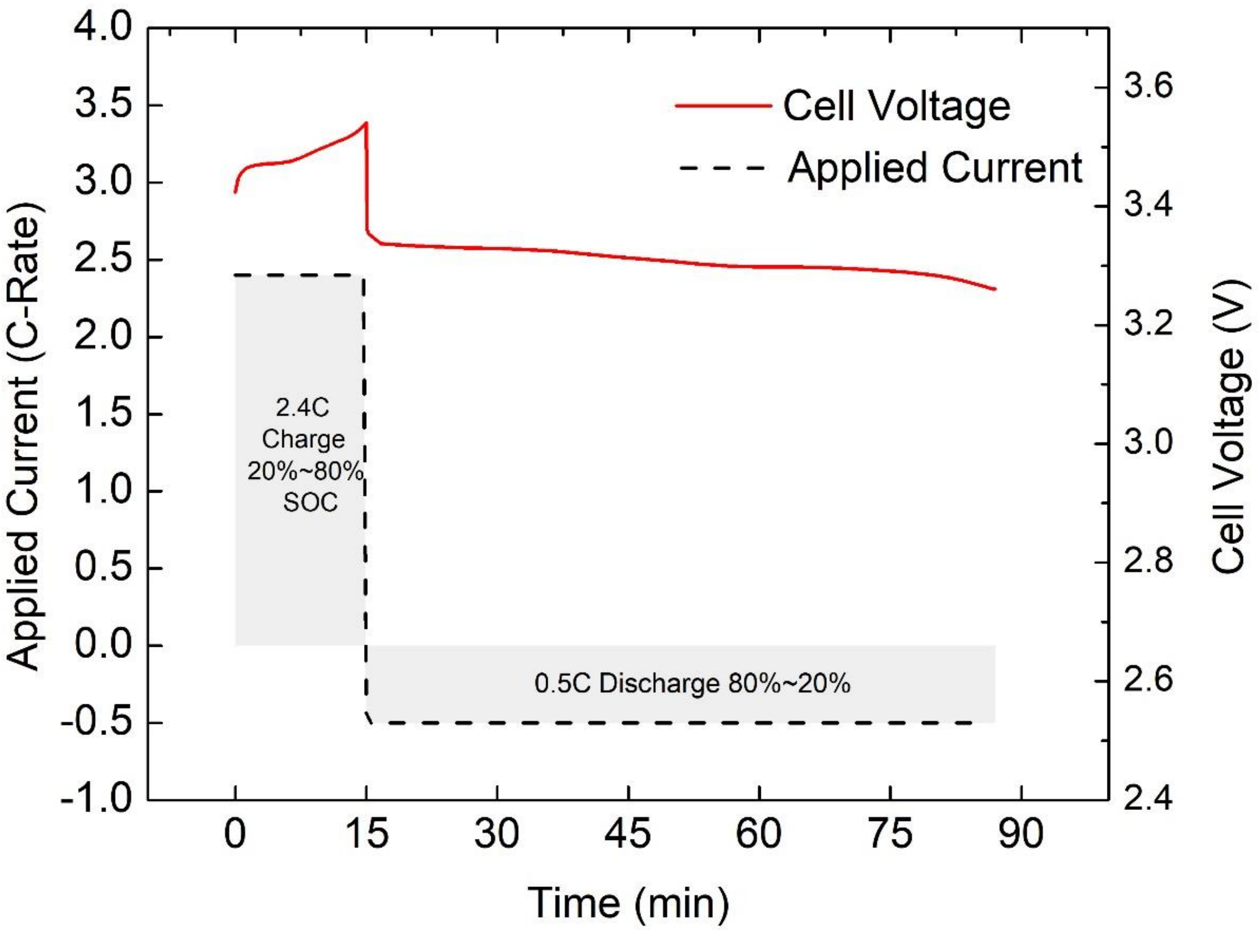
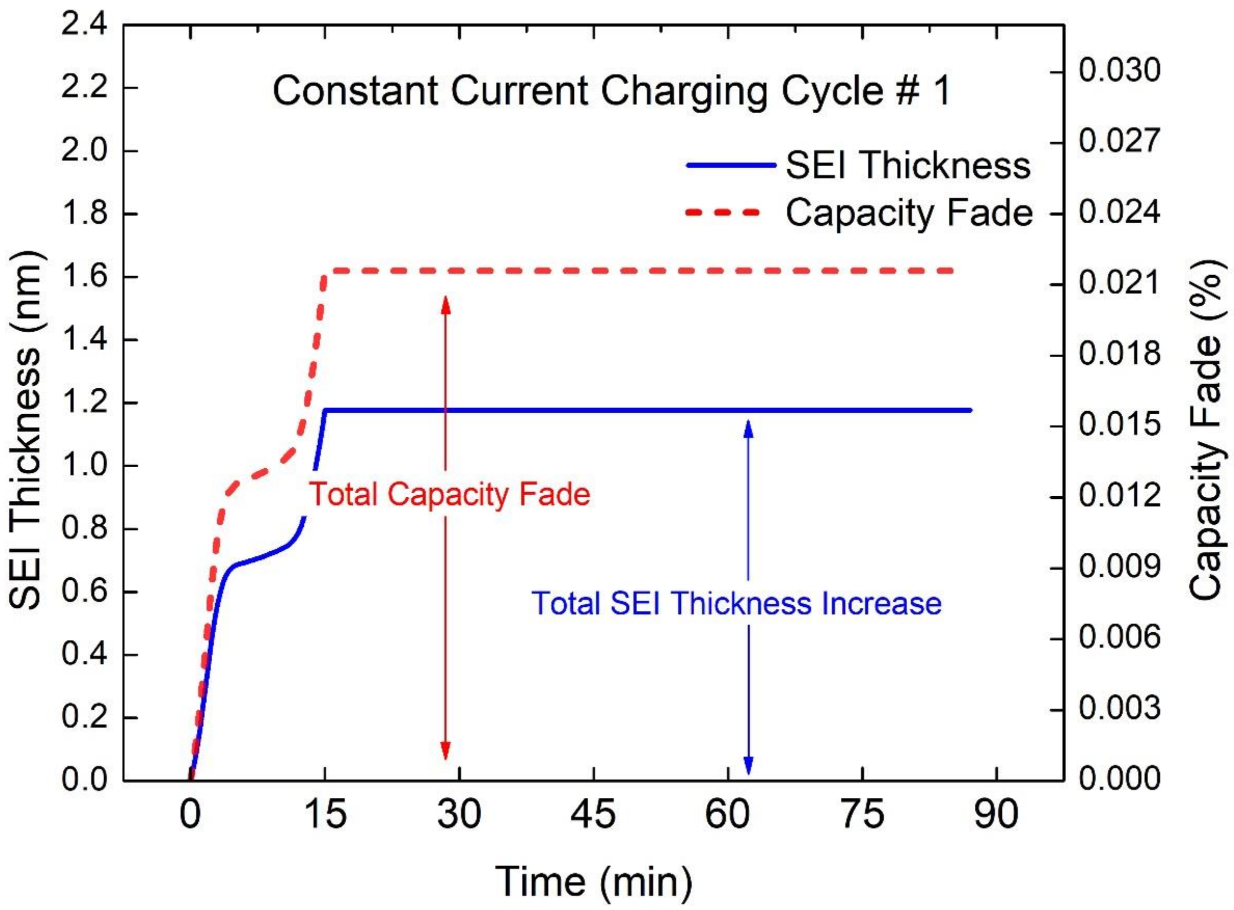


Figure 1. Cracks (macropores) formed in the microporous SEI layer due to expansion of the graphite particle during charge of the graphite electrode. The cracks enhance transport of the SEI layer forming species. The SEI layer is located between the graphite and the electrolyte.

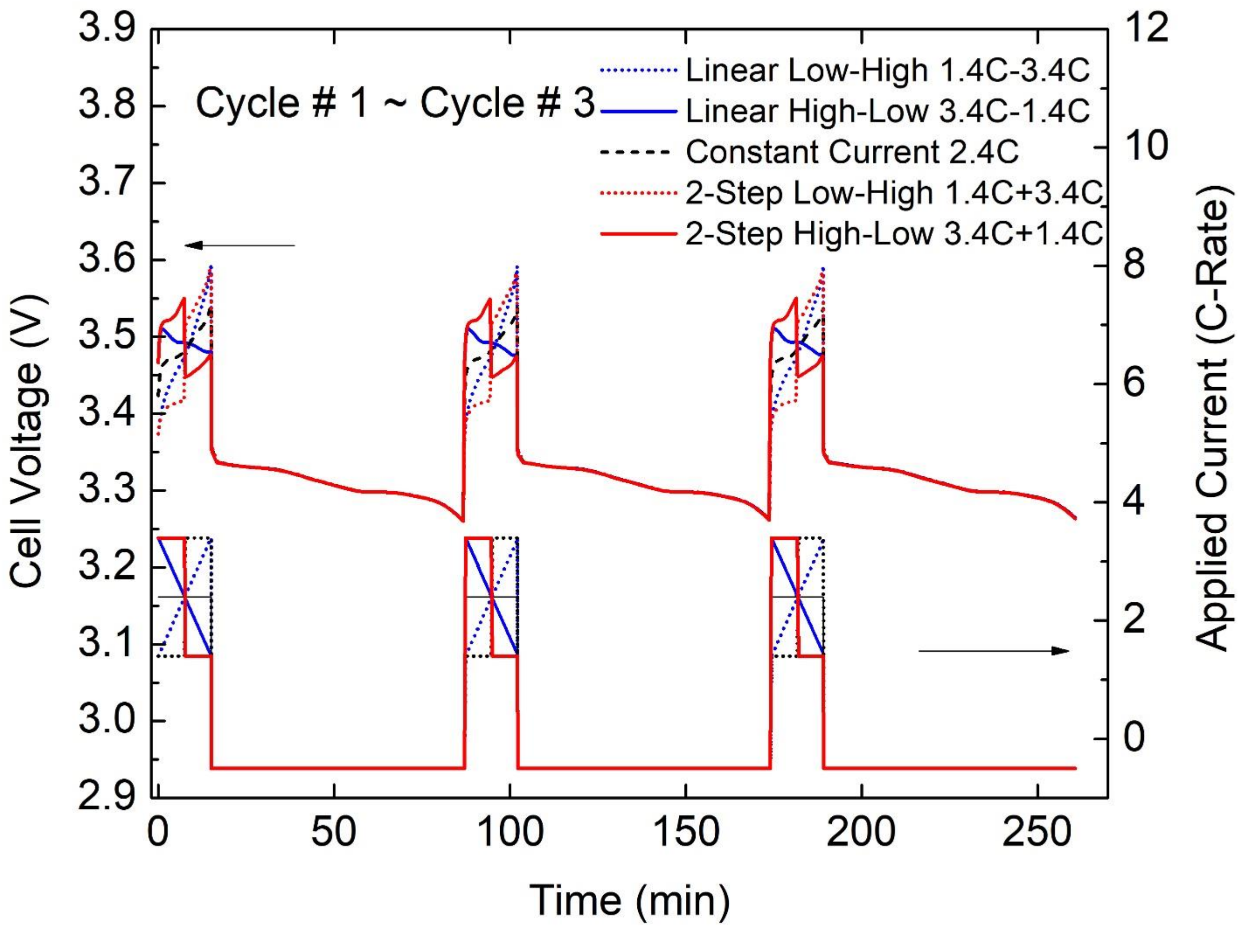
Source: Ekström, Henrik, and Göran Lindbergh. "A model for predicting capacity fade due to SEI formation in a commercial graphite/LiFePO4 cell." Journal of The Electrochemical Society 162, no. 6 (2015): A1003-A1007.

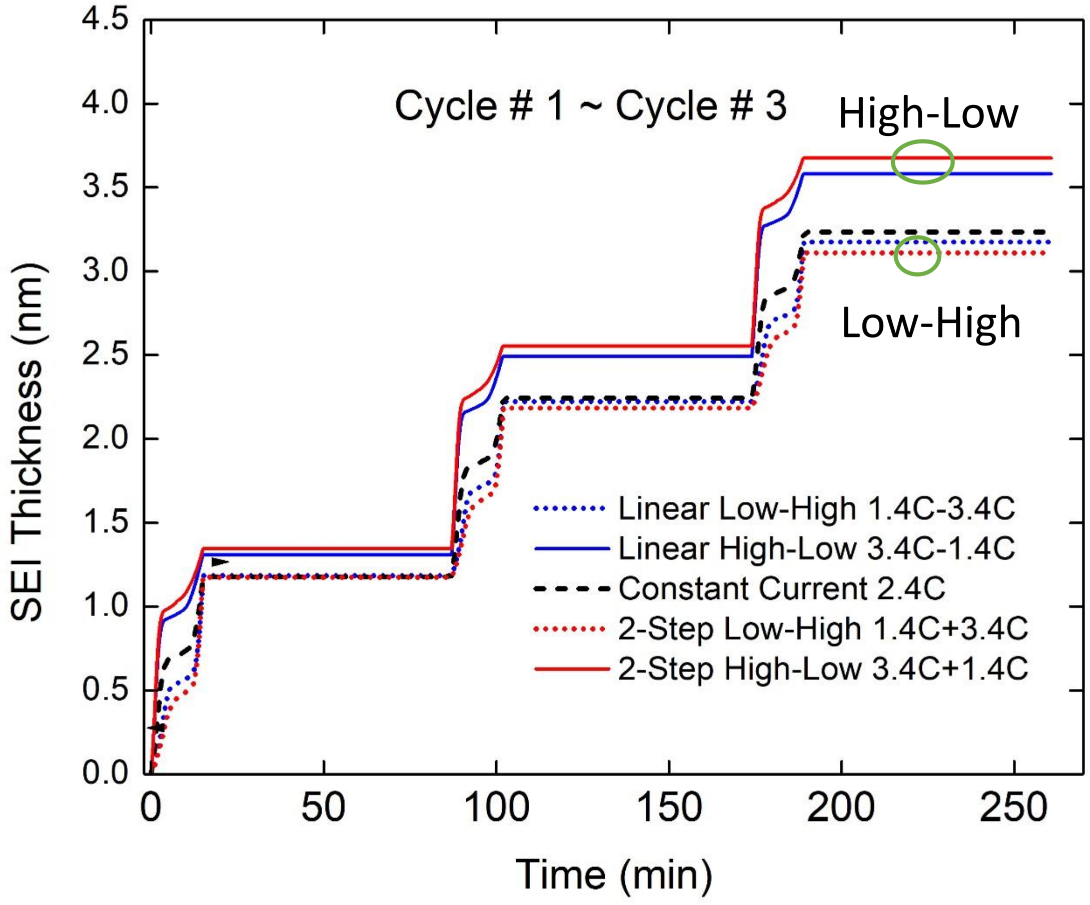
15 min 20 ~ 80% SOC Fast Charging Cycles





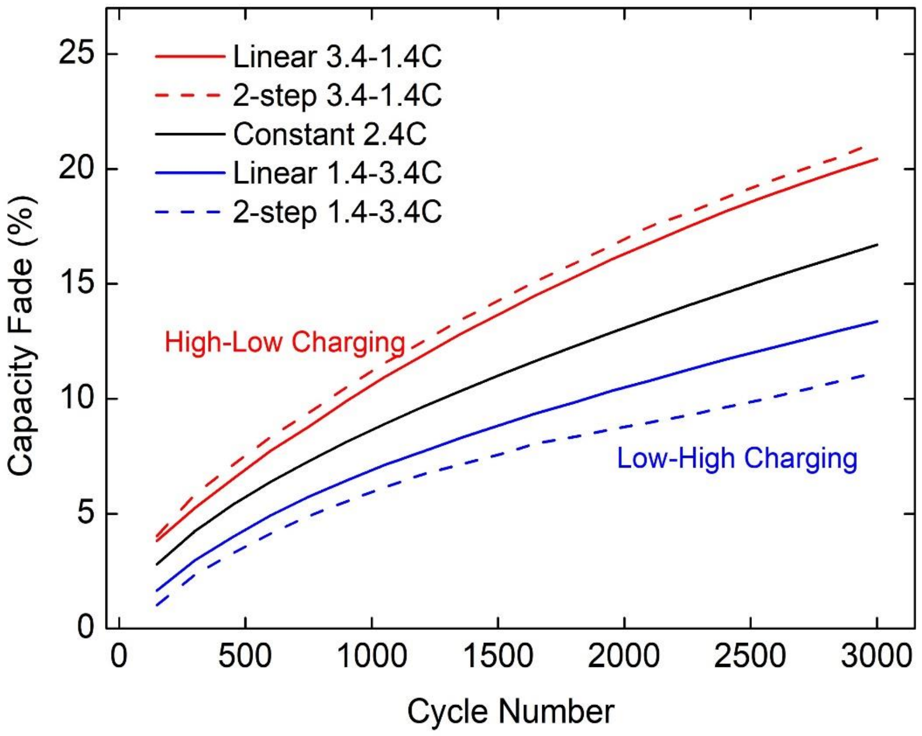
SEI Thickness Increase Cycle 1 – Cycle 3

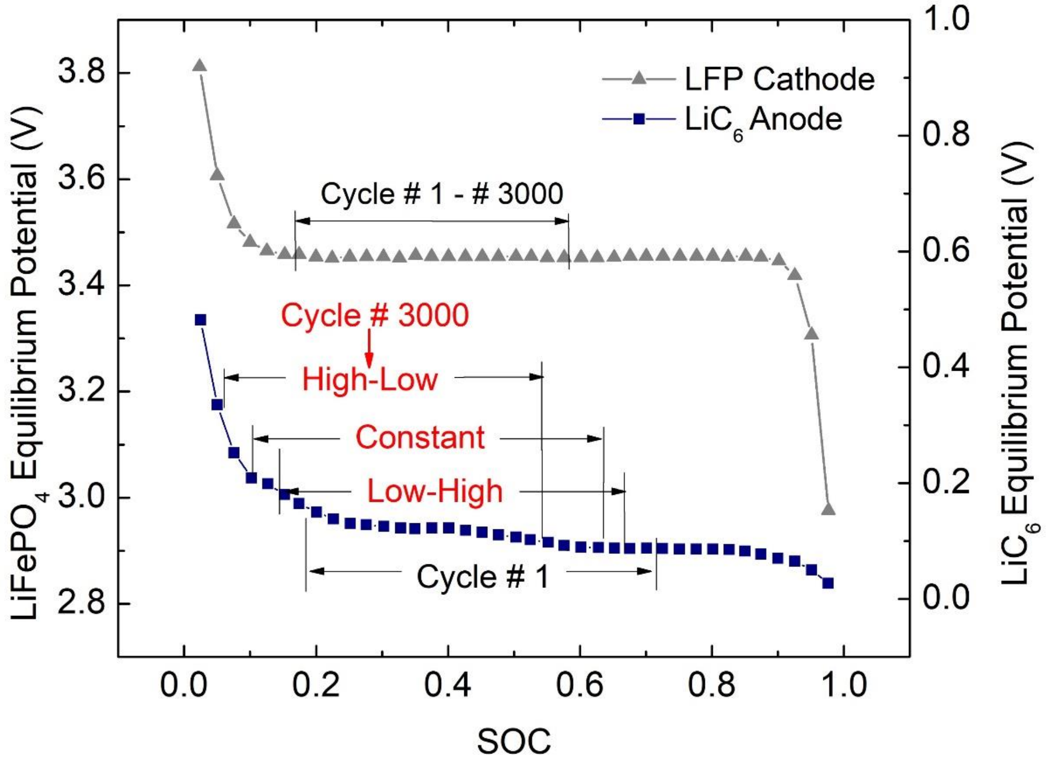




- SEI increases with cycles
- Low-High protocols have thinner SEI at cycle 3

Impact of Cycle Number and Protocol on Capacity Fade





- Low-High charging protocols obtain lower capacity fade than High-Low protocols
- The 2-step Low-High protocol results in the lowest capacity fade
- Utilization range shifts in the negative electrode

Optimization at Different Ambient Temperatures