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Real-time Parameter Estimation of Lithium-Ion Battery Models Using a Novel Tanks-in-Series Approach

Modeling, **A**nalysis, and **P**rocess-control **L**aboratory for **E**lectrochemical systems

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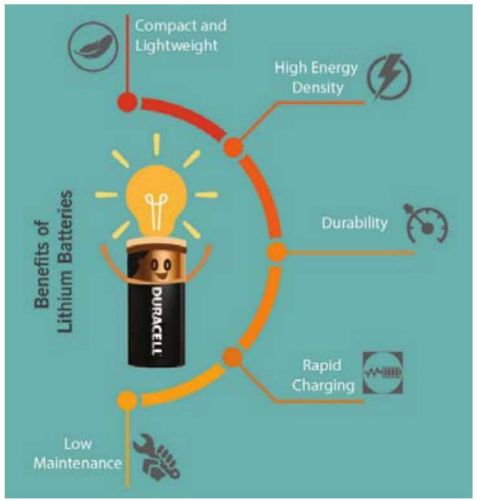
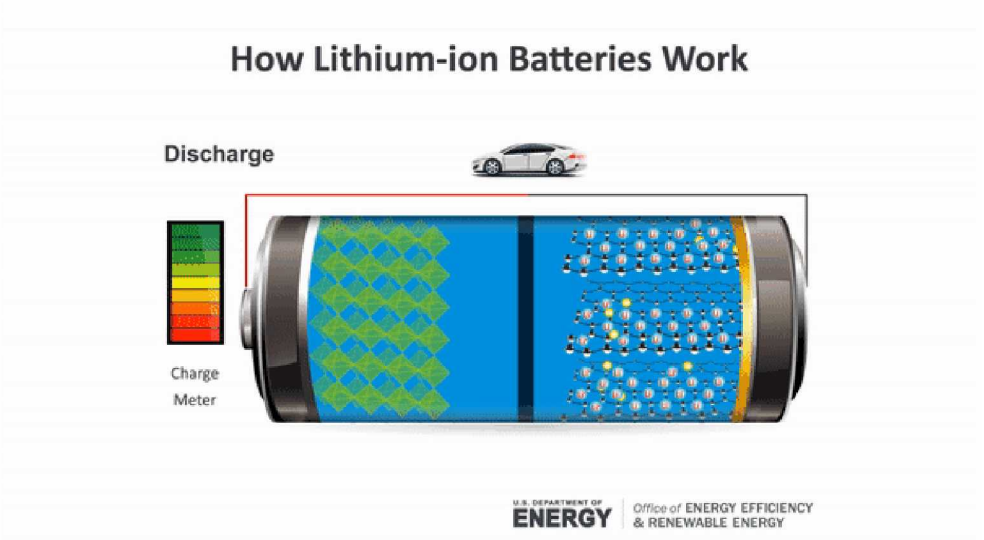
Overview

- Introduction
- Background
- Novel Tanks-in-Series model
- Problem Formulation
- Proposed Methodology
- Results and Discussions
- Conclusion

Introduction

- **Lithium-Ion batteries are becoming increasingly popular.**



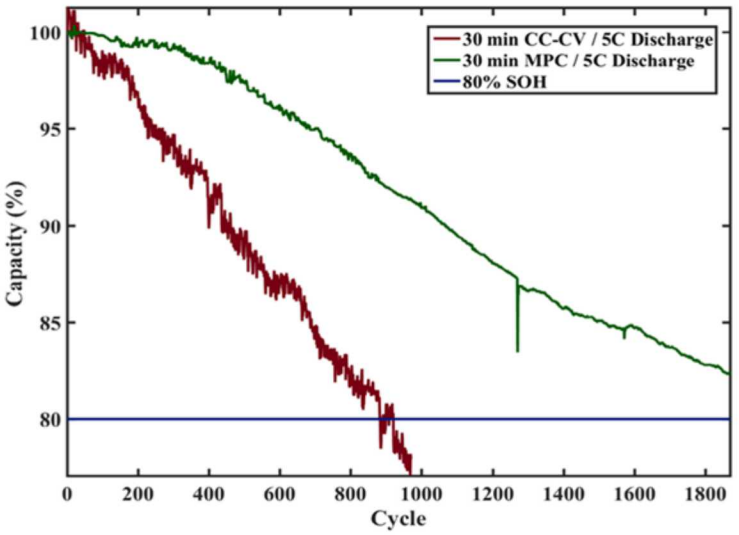


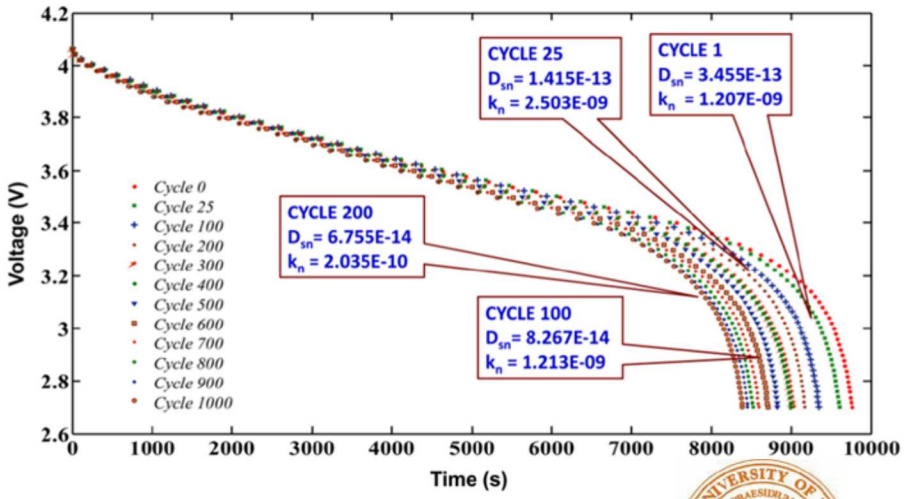
- **To monitor, control, and predict the performance of Li-ion batteries, advanced electrochemical model-based battery management systems (BMS) play a vital role.**

Ref: https://www.energy.gov/eere/articles/how-does-lithium-ion-battery-work
https://www.annova.biz/en/top-5-benefits-of-lithium-batteries

Physics Based Battery Management System

- Model-based BMS can double the cycle life.
- Physics-based battery models are complex, and parameters change over cycles.
- Accuracy of the model parameters determines model's predictability of internal states.

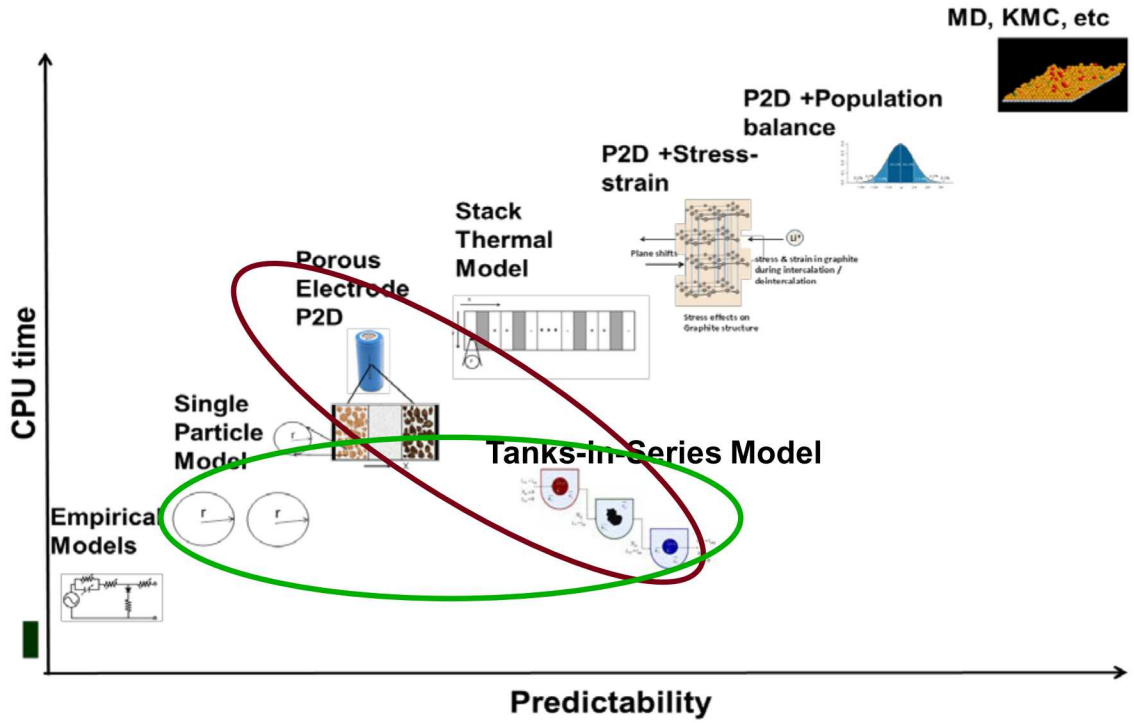




Ref: Pathak, M. *et. al.* (2017). ECS transactions, 75(23), 51.
Ramadesigan, V. *et. al.* (2011). JES, 158(9), 1048-1054.

Speed Vs Accuracy

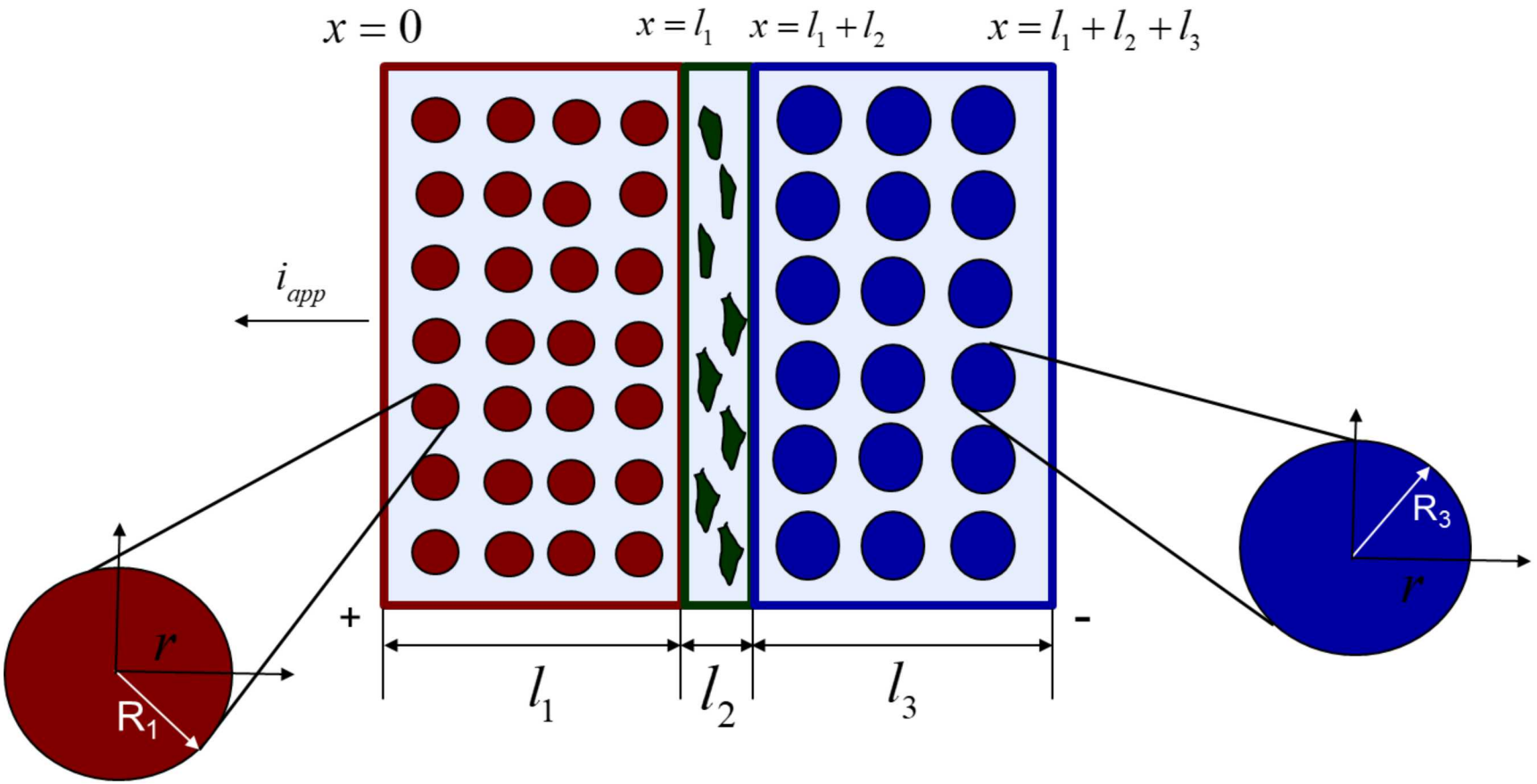
- **Trade-off between CPU time vs. predictability.**



- **Develop a robust approach for estimating the parameters of physics-based lithium-ion battery model.**

Ref: Subramaniam, A. et. al. (2020). JES, 167(1), 013534.

The p2D Model For Lithium-ion Batteries



The p2D Li-ion Battery Model

- **Coupled Conservation Laws :**

Electronic Charge :

$$\sigma_{\text{eff,p}} \frac{\partial^2 \Phi_1}{\partial x^2} = a_{\text{p}} F j_{\text{p}}; \ \Phi_1 \text{ is the solid-phase potential}$$

Overall Charge :

$$-\sigma_{\text{eff,p}} \frac{\partial \Phi_1}{\partial x} - \kappa_{\text{eff,p}} \frac{\partial \Phi_2}{\partial x} + \frac{2\kappa_{\text{eff,p}} RT}{F}\left(1 - t_+\right) \frac{\partial \ln c}{\partial x} = I;$$

Φ_2 is the liquid phase potential

Electrolyte Mass:

$$\varepsilon_{\text{p}} \frac{\partial c}{\partial t} = D_{\text{eff,p}} \frac{\partial^2 c}{\partial x^2} + a_{\text{p}} \left(1 - t_+\right) j_{\text{p}};$$

c is the electrolyte concentration

Parameters and Constitutive Equations

$$\kappa_{\text{eff,p}} = \varepsilon_{\text{p}}^{\ \text{brugg}_{\text{p}}} \kappa = 0.01775 \times \begin{pmatrix} 4.1253\times10^{-2} + 5.007\times10^{-1} c - 4.7212\times10^{-1} c^2 \\ +1.5094\times10^{-1} c^3 - 1.6018\times10^{-2} c^4 \end{pmatrix}$$

Solid Phase Mass:

$$\frac{\partial c_p^s}{\partial t} = D_{\text{s,p}} \left(\frac{\partial^2 c_p^s}{\partial r^2} + \frac{2}{\text{r}} \frac{\partial c_p^s}{\partial r} \right); \ c_p^s \text{ is the solid phase concentration}$$

$$j_{\text{p}} = 2k_{\text{p}} \left(c_{\text{s,max,p}} - c_p^s\right)^{0.5} c_p^{s\,0.5} c^{0.5} \sinh\left[\frac{0.5F}{RT}\left(\Phi_1 - \Phi_2 - U_{\text{p}}\right)\right]$$

$$U_{\text{p}} = f(SOC)$$

Computational Complexity has spurred active investigation of different simplification and reformulation techniques

[J. S. Newman+, (1993-2012)]

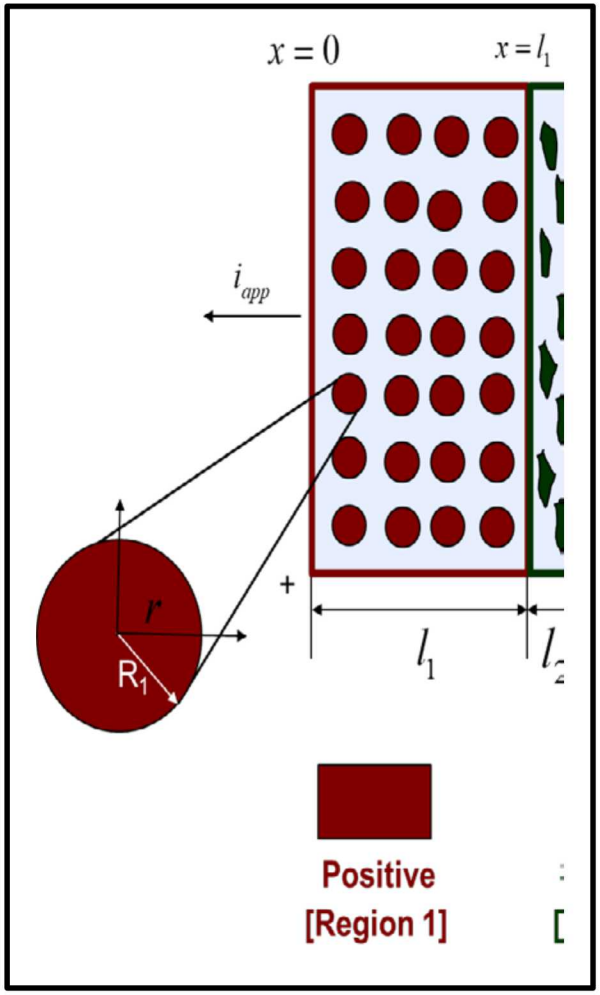
The Single Particle Model

Neglect Electrolyte Effects:

$$\frac{\partial c_1^s}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D_1^s \frac{\partial c_1^s}{\partial r} \right)$$

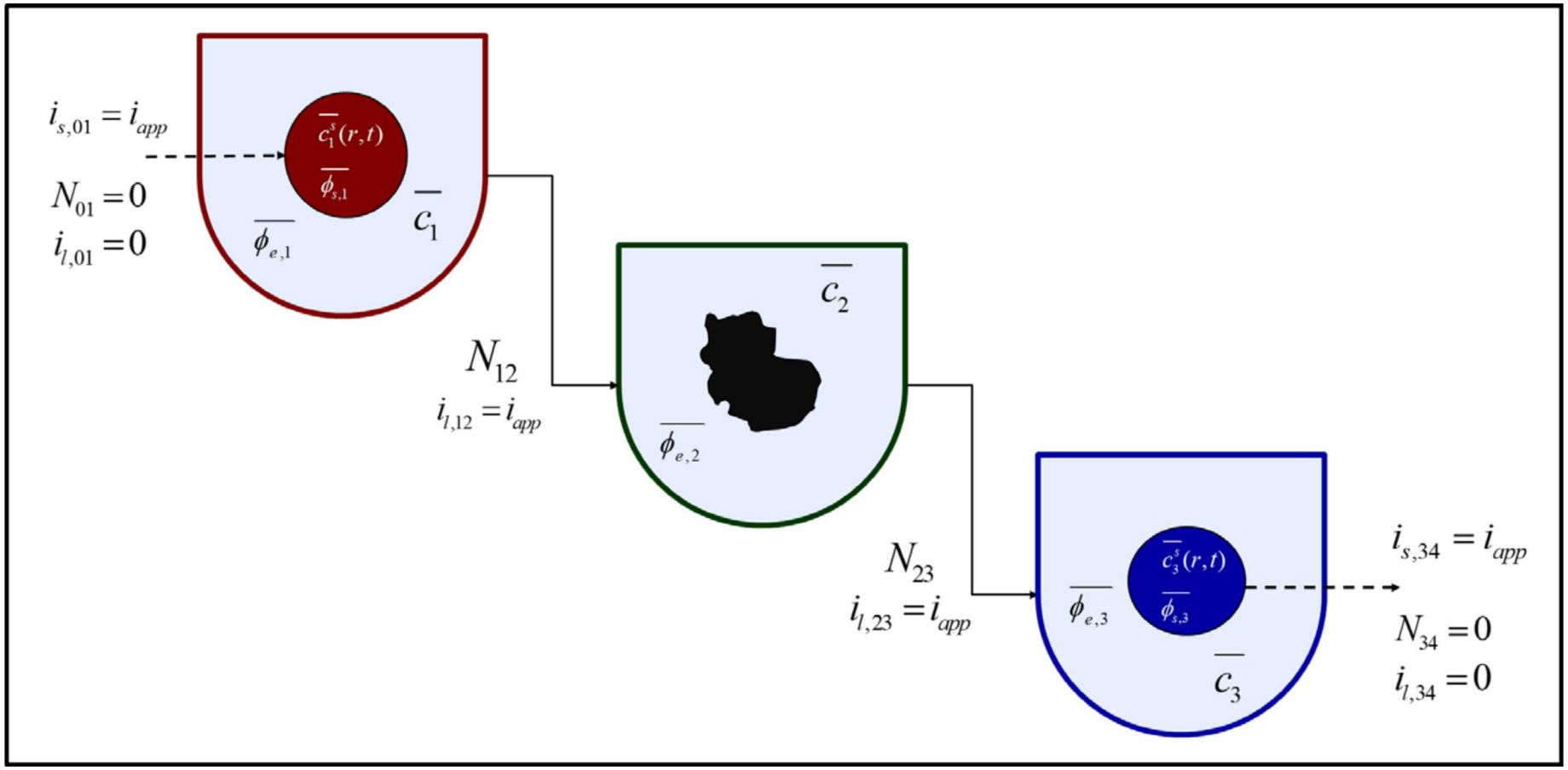
$$\frac{\partial \int_{x=0}^{x=l_1} c_1^s dx}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D_1^s \frac{\partial \int_{x=0}^{x=l_1} c_1^s dx}{\partial r} \right)$$

$$\frac{\partial \overline{c_1^s}}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D_1^s \frac{\partial \overline{c_1^s}}{\partial r} \right)$$



Restricted to moderate current scenarios, where liquid phase polarizations aren't significant

Lithium-ion Battery as Tanks in Series



Can we incorporate average electrolyte dynamics by a similar volume-averaging approach?

Ref: Subramaniam, A. et. al. (2020). JES, 167(1), 013534.

Generating the Tank Model

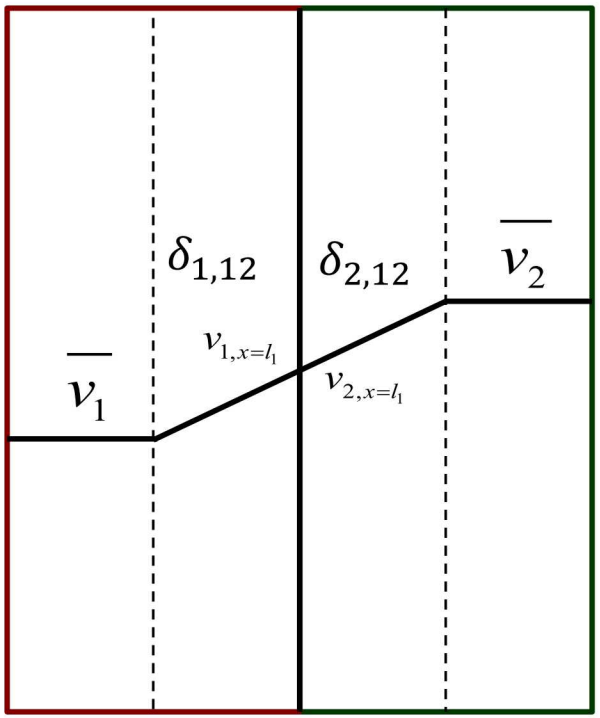
Example Conservation Equation:

$$\varepsilon_1 \frac{\partial c_1}{\partial t} = -\frac{\partial N_1}{\partial x} + a_1\left(1 - t_+^0\right) j_1$$

$$\frac{d\int_{V_1} \varepsilon_1 c_1 dV}{dt} = -\int_{V_1} \frac{\partial N_1}{\partial x} dV + \int_{V_1} a_1\left(1 - t_+^0\right) j_1 dV$$

$$\varepsilon_1 \frac{d\overline{c_1}}{dt} = -\frac{\int_{x=0}^{x=l_1} \frac{\partial N_1}{\partial x} dx}{l_1} + a_1\left(1 - t_+\right)\overline{j_1} = \frac{N_{1,x=0} - N_{1,x=l_1}}{l_1} + a_1\left(1 - t_+\right)\overline{j_1}$$

Approximating Interfacial Fluxes



$$N_{1,x=l_1} = -D(c_{1,x=l_1})\varepsilon_1^{b_1}\left.\frac{\partial c_1}{\partial x}\right|_{x=l_1} \approx D(c_{1,x=l_1})\varepsilon_1^{b_1}\left(\frac{\Delta c_1}{\delta_{1,12}}\right) = D(c_{1,x=l_1})\varepsilon_1^{b_1}\left(\frac{\overline{c_1} - c_{1,x=l_1}}{\frac{l_1}{2}}\right)$$

$$N_{2,x=l_1} = -D(c_{2,x=l_1})\varepsilon_2^{b_2}\left.\frac{\partial c_2}{\partial x}\right|_{x=l_2} \approx D(c_{2,x=l_1})\varepsilon_2^{b_2}\left(\frac{\Delta c_2}{\delta_{2,12}}\right) = D(c_{2,x=l_1})\varepsilon_2^{b_2}\left(\frac{-\overline{c_2} + c_{2,x=l_1}}{\frac{l_2}{2}}\right)$$

$$D(c_{1,x=l_1})\varepsilon_1^{b_1}\left(\frac{\overline{c_1} - c_{1,x=l_1}}{\frac{l_1}{2}}\right) = D(c_{2,x=l_1})\varepsilon_2^{b_2}\left(\frac{-\overline{c_2} + c_{2,x=l_1}}{\frac{l_2}{2}}\right)$$

Naive assumptions of 'film thickness', can be regarded an adjustable parameter

Tank Model DAE System

Electronic Charge :

$$\overline{j_1} = \frac{i_{app}}{a_1 F l_1} \qquad \overline{j_3} = -\frac{i_{app}}{a_3 F l_3}$$

Electrolyte Mass:

$$\varepsilon_1 \frac{d\overline{c_1}}{dt} = \frac{\dfrac{2D(c_{12})(\overline{c_2} - \overline{c_1})}{\dfrac{l_1}{\varepsilon_1^{b_1}} + \dfrac{l_2}{\varepsilon_2^{b_2}}}}{l_1} + a_1(1 - t_+)\overline{j_1}$$

$$\varepsilon_2 \frac{d\overline{c_2}}{dt} = \frac{\dfrac{-2D(c_{12})(\overline{c_2} - \overline{c_1})}{\dfrac{l_1}{\varepsilon_1^{b_1}} + \dfrac{l_2}{\varepsilon_2^{b_2}}} + \dfrac{2D(c_{23})(\overline{c_3} - \overline{c_2})}{\dfrac{l_2}{\varepsilon_2^{b_2}} + \dfrac{l_3}{\varepsilon_3^{b_3}}}}{l_2}$$

$$\varepsilon_3 \frac{d\overline{c_3}}{dt} = \frac{\dfrac{-2D(c_{23})(\overline{c_3} - \overline{c_2})}{\dfrac{l_2}{\varepsilon_2^{b_2}} + \dfrac{l_3}{\varepsilon_3^{b_3}}}}{l_3} + a_3(1 - t_+)\overline{j_3}$$

Liquid Charge (plus reference) :

$$i_{l,1,x=l_1} = -2\kappa(c_{12})\left(\frac{\overline{\phi_{l,2}} - \overline{\phi_{l,1}}}{\dfrac{l_1}{\varepsilon_1^{b_1}} + \dfrac{l_2}{\varepsilon_2^{b_2}}}\right) + \frac{4RT(1 - t_+^0)}{F}\kappa(c_{12})\frac{1}{c_{12}}\left(\frac{\overline{c_2} - \overline{c_1}}{\dfrac{l_1}{\varepsilon_1^{b_1}} + \dfrac{l_2}{\varepsilon_2^{b_2}}}\right) = i_{app}$$

$$i_{l,3,x=l_1+l_2} = -2\kappa(c_{23})\left(\frac{\overline{\phi_{l,3}} - \overline{\phi_{l,2}}}{\dfrac{l_3}{\varepsilon_3^{b_3}} + \dfrac{l_2}{\varepsilon_2^{b_2}}}\right) + \frac{4RT(1 - t_+^0)}{F}\kappa(c_{23})\frac{1}{c_{23}}\left(\frac{\overline{c_3} - \overline{c_2}}{\dfrac{l_2}{\varepsilon_2^{b_2}} + \dfrac{l_3}{\varepsilon_3^{b_3}}}\right) = i_{app}$$

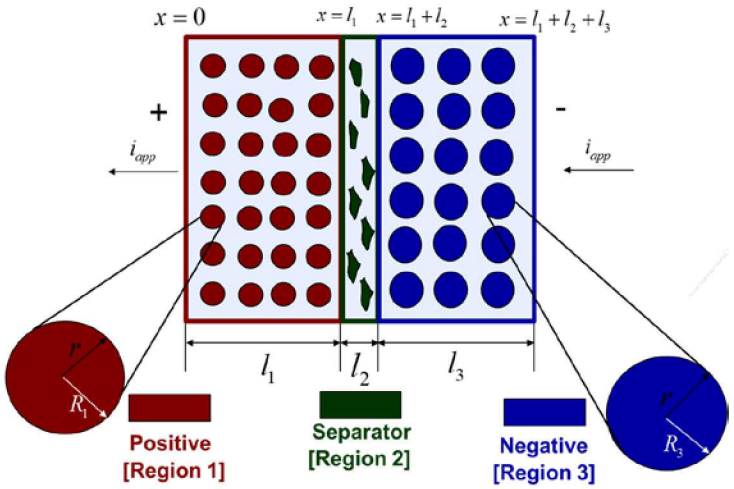
$$\phi_{l,12} = \left(\frac{\dfrac{\varepsilon_1^{b_1}}{l_1}\overline{\phi_{l,1}} + \dfrac{\varepsilon_2^{b_2}}{l_2}\overline{\phi_{l,2}}}{\dfrac{\varepsilon_1^{b_1}}{l_1} + \dfrac{\varepsilon_2^{b_2}}{l_2}}\right) = 0$$

Solid Phase Mass (SPM):

$$\frac{\partial \overline{c_1^s}}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D_1^s \frac{\partial \overline{c_1^s}}{\partial r}\right)$$

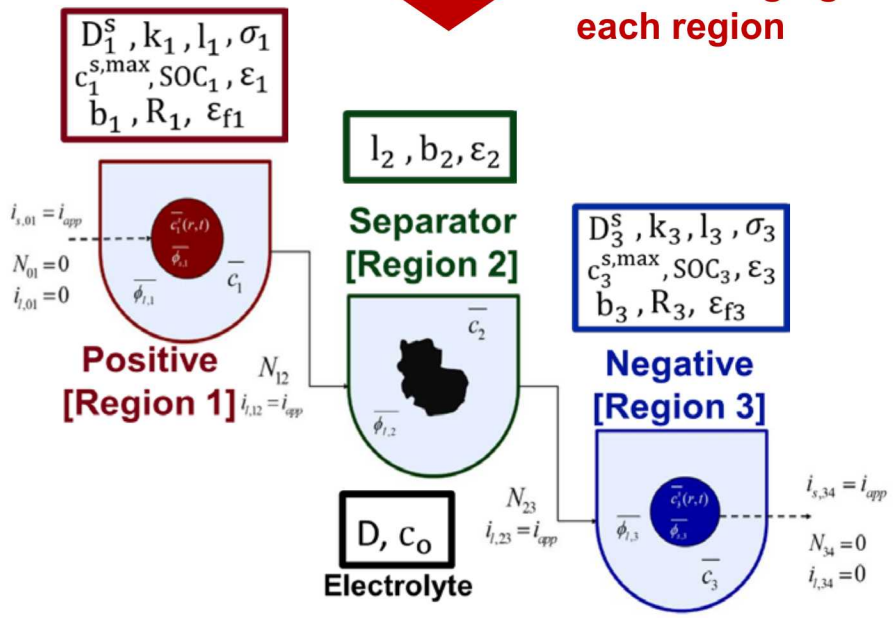
PDE Model is thus reduced to simplified DAE system for liquid phase.

Novel Tanks-in-Series Model



p2D model > 1000 DAEs (complex)
(Computation time, C++: 1493ms)

Volume averaging each region

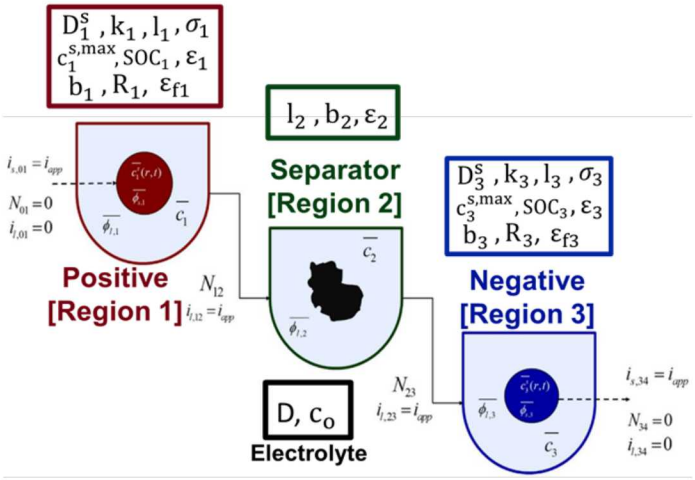


Tanks-in-Series model ~10 DAEs
(Computation time, C++: 2.1ms)

<1% error observed as compared to existing physics-based battery models (SPM, P2D, etc.)

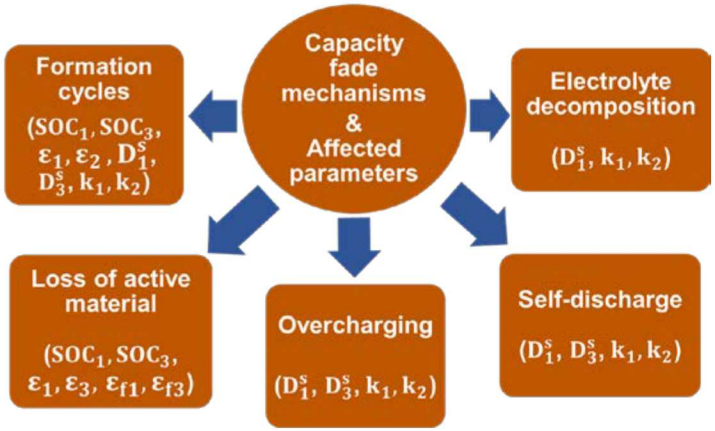
Ref: Subramaniam, A. et. al. (2020). JES, 167(1), 013534.

Novel Tanks-in-Series Model



List of Tanks-in-Series model parameters	
Parameter	**Symbol**
Electrolyte Diffusivity	D
Solid Phase Diffusivity	D_1^s, D_3^s
Reaction Rate Constant	k_1, k_3
Solid Phase Conductivity	σ_1, σ_3
Electrolyte Conductivity	κ
Electrolyte Concentration	c_o
Maximum Solid Phase Concentration	$c_1^{s,max}, c_3^{s,max}$
Initial SOC	SOC_1, SOC_3
Transference Number	t_+^0
Porosity	$\varepsilon_1, \varepsilon_2$
Filler Fraction	$\varepsilon_{f1}, \varepsilon_{f3}$
Bruggeman Constant	b_1, b_2, b_3
Thickness	l_1, l_2, l_3
Particle Size	R_1, R_3
index: 1 (+ve electrode), 2 (separator), 3 (-ve electrode)	

Parameters to be estimated to model Battery aging



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Optimization Formulation

Objective:

$$\min \sqrt{\frac{\left[\sum_{t_0=0}^{t_n=t_f}\left(V_{exp}(t_i) - V_{model}(t_i)\right)^2\right]}{N_{exp}}}$$

where, V_{exp}: experimental voltage profile

V_{model}: Tanks − in − Series model voltage profile

Subject to:

$$\frac{\partial}{\partial x} g_j(\bar{x}) = 0, \qquad j = 1, \ldots, J$$

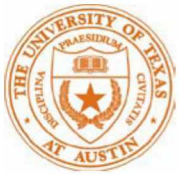
Ordinary differential equations (ODEs)

$$h_k(\bar{x}) = 0, \qquad k = 1, \ldots, K$$

Algebraic equations (AEs)

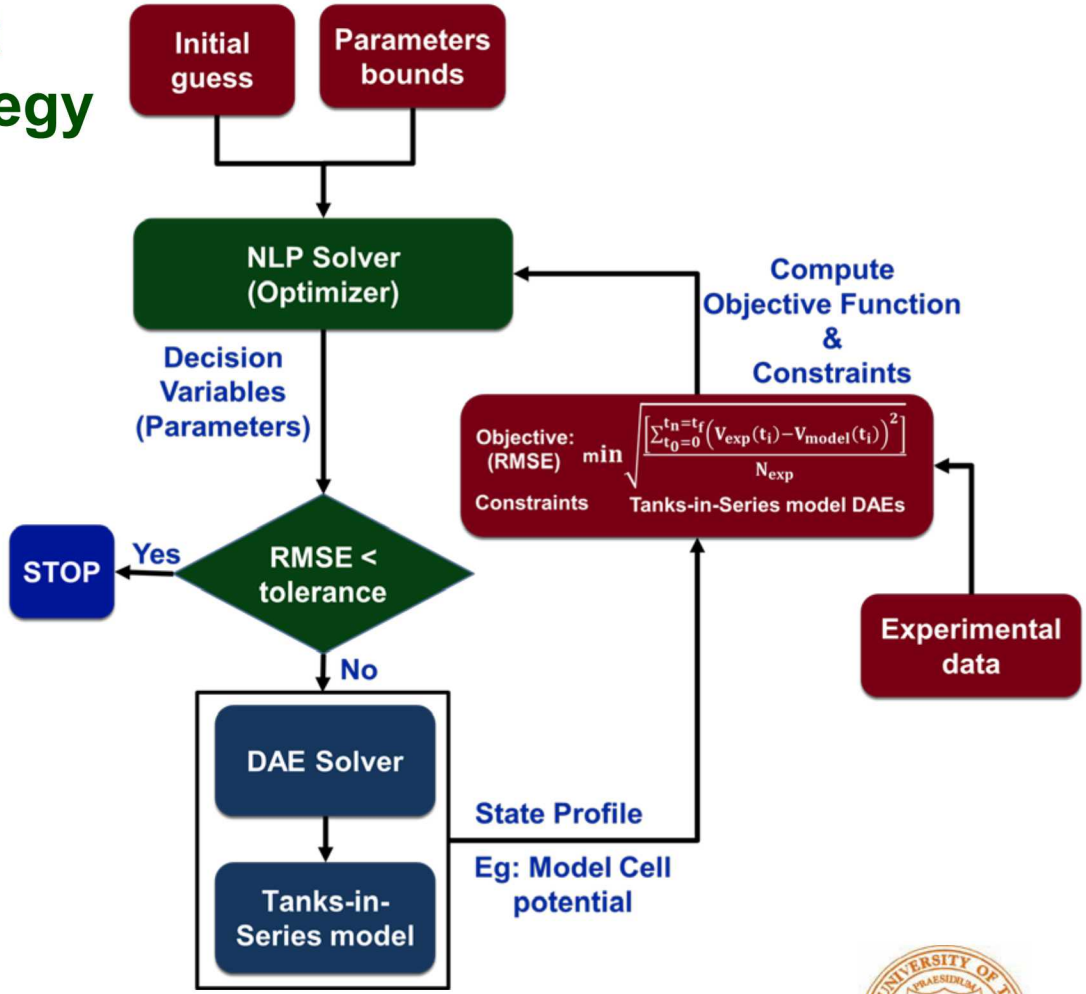
} Differential algebraic equations (DAEs)

Variables: $\bar{x} \in \Omega$ $\qquad lb \leq \bar{x} \leq ub$

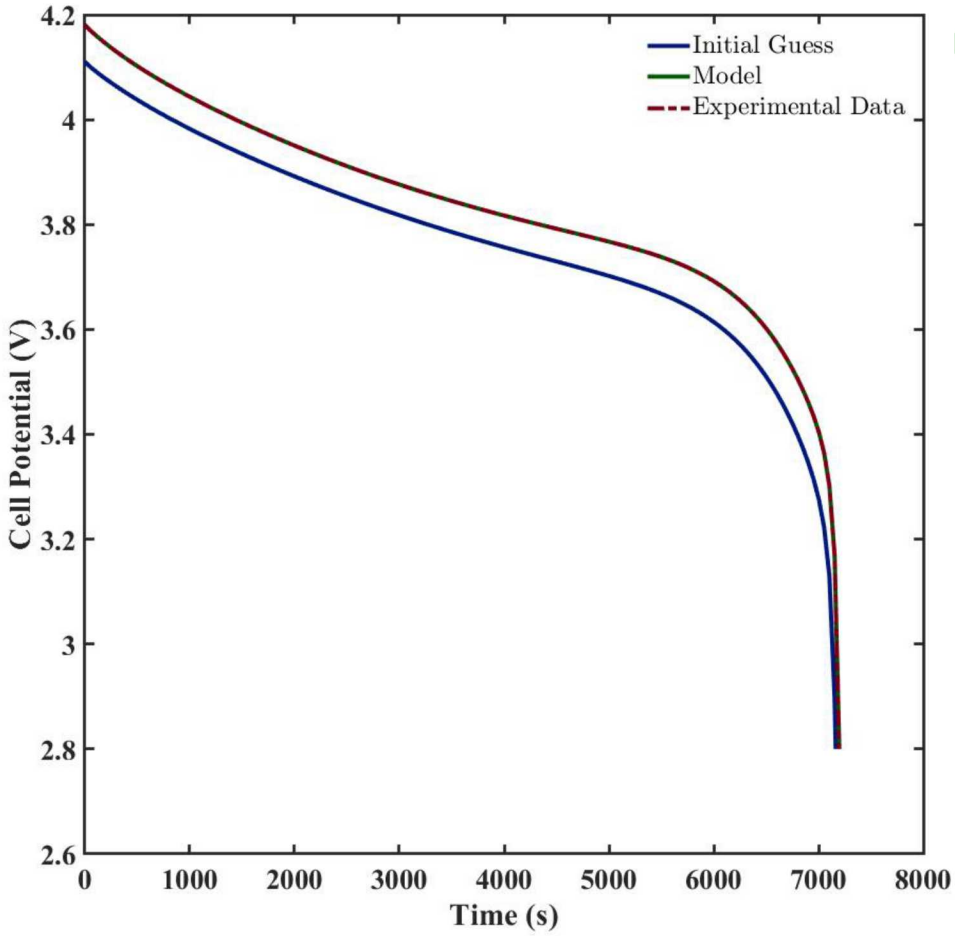


Proposed Methodology

Sequential parameter estimation using robust dynamic optimization strategy



Fast Computation

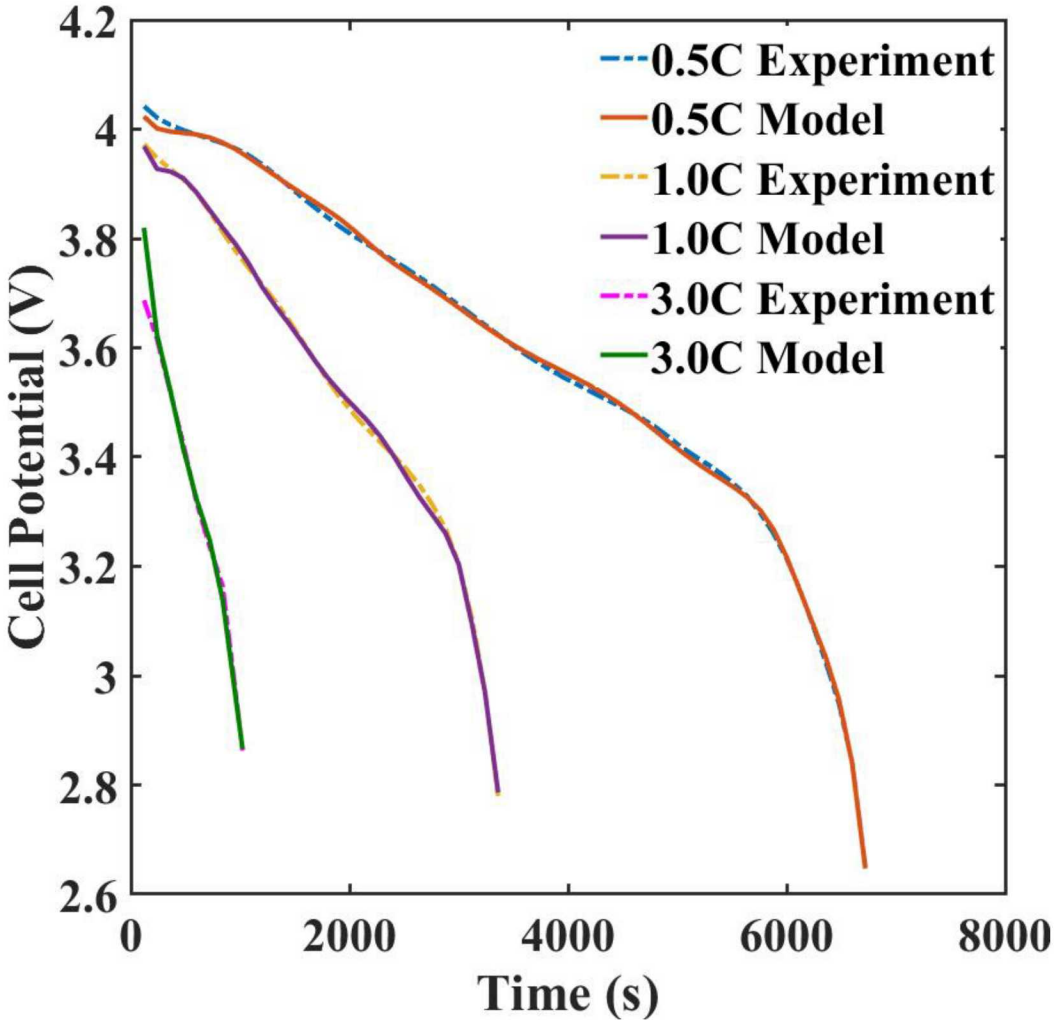


- **Tanks-in-Series model enables Fast Computation in MATLAB**

Battery Model	Total Estimation Time (s)
SPM	~40
Tanks-in-Series	~45
p2D	~900

Comparison plot between Initial Guess and Optimal parameters of Tanks-in-Series model for 0.5C synthetic discharge data.

Results and Discussions



RMSE error values (in mV)

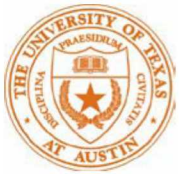
Crate	RMSE (mV)
0.5	7.22
1.0	10.13
3.0	11.64

Note: Experiments are performed on 3Ah 18650 cylindrical cell (Cathode: NMC811 and Anode: Si-C) at different discharge rates (C/2,1C and 3C) at Sandia National Laboratories.

* All reported simulations are performed on Intel® Core™ i5-8265U CPU @ 1.6GHz 8 GB RAM machine

Conclusions

- Novel Tanks-in-Series approach is adopted to model the cell behavior at different discharge rates (0.5C, 1C, and 3C).
- The adopted model competes with SPM (in terms of simulation time) and complies with the synthetic experimental data within 15 mV error.
- A robust sequential optimization approach is proposed to estimate the parameters of the battery model with <12 mV error.



Acknowledgements

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THANK YOU!

Any Questions?