State Estimation of Lithium-Ion Batteries with Phase Transition Materials

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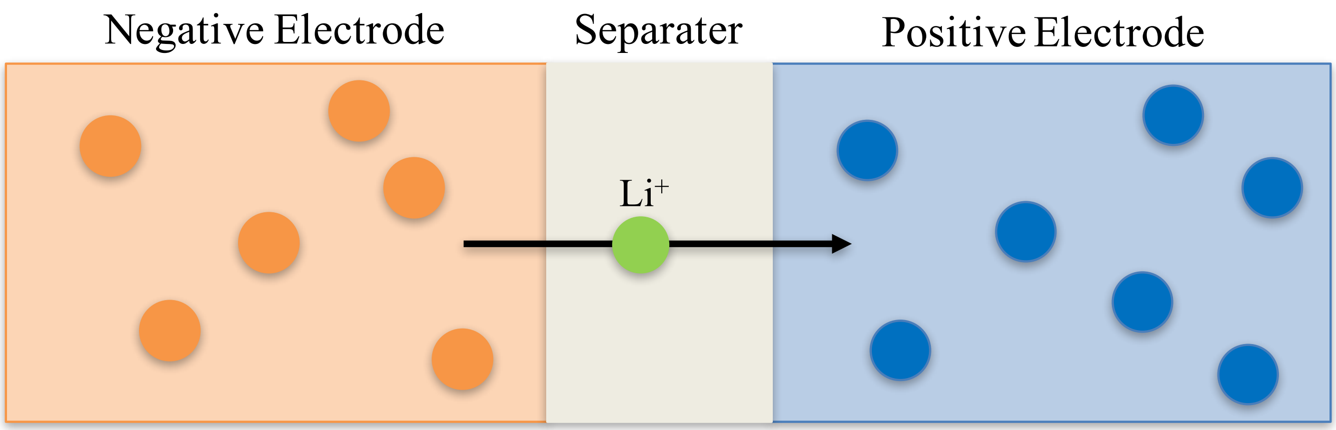
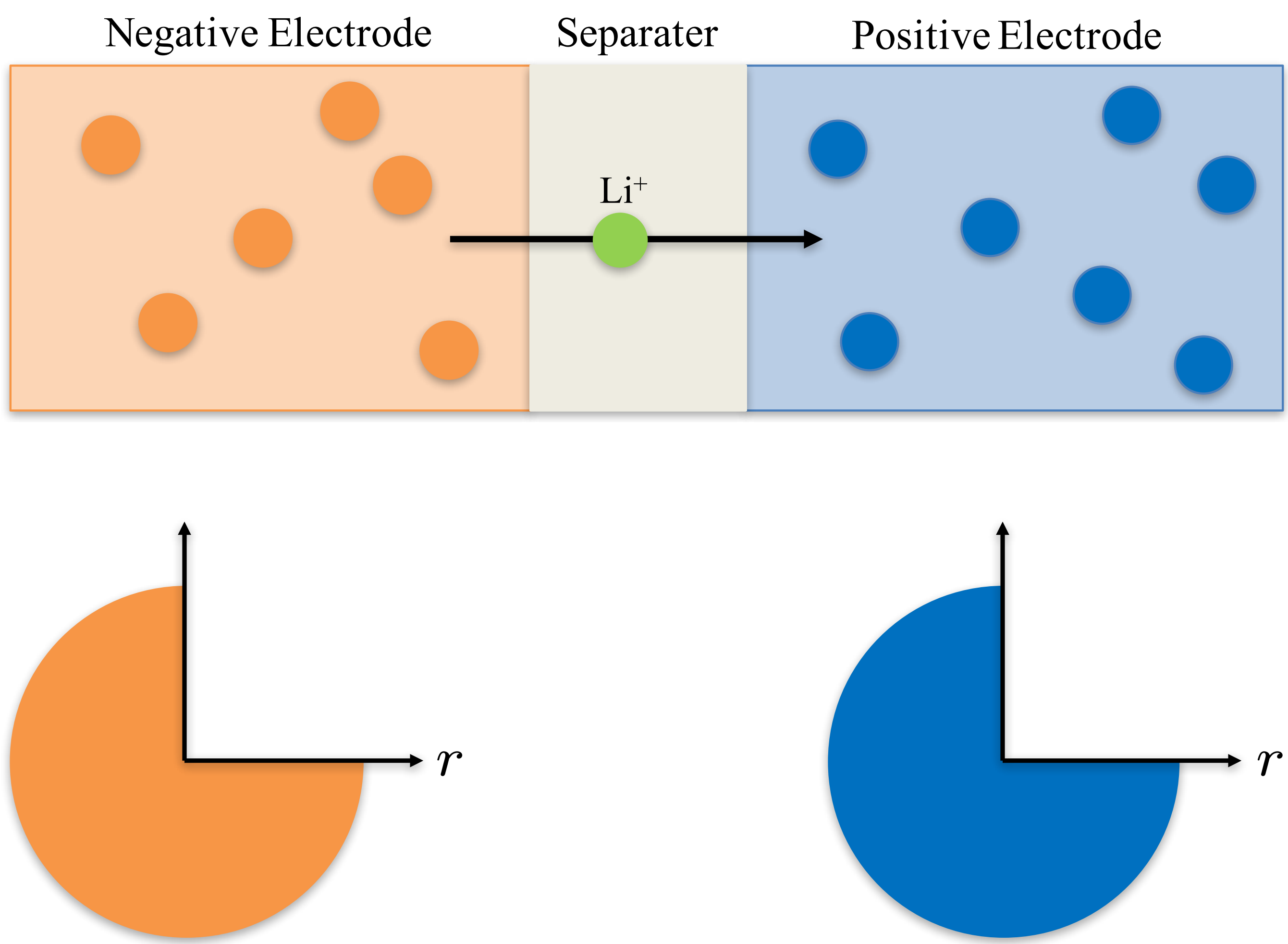
Lithium Ion Battery



Single Particle Model



Phase Transition Material

$LiFePO_4$ (LFP)

$\cdots$ strong candidate as positive electrode in lithium ion batteries

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(i) thermal stability

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(iii) long cycle life

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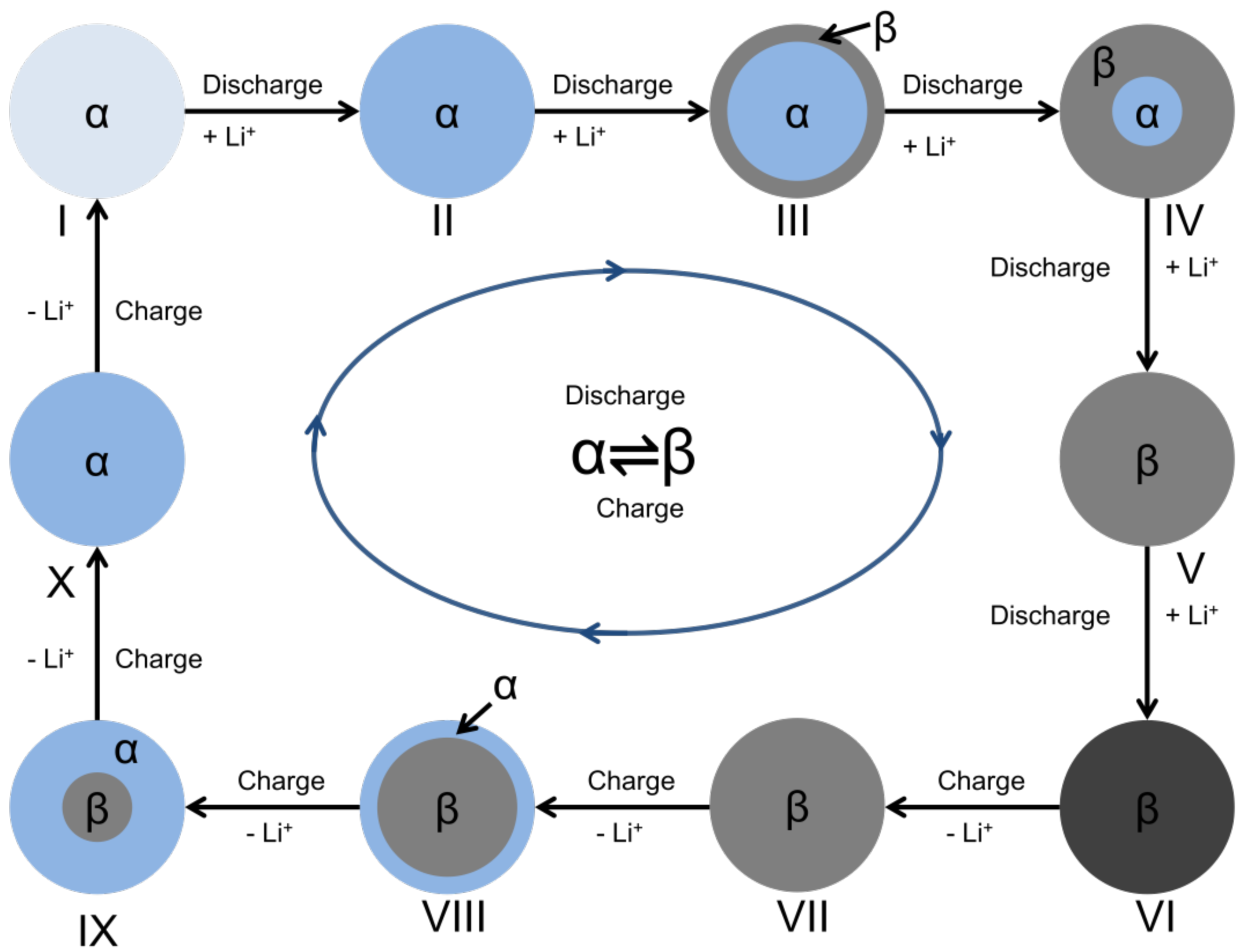
Structural phase transition is caused by lithium intercalation/extraction

$$FePO_4 + Li^+ + e^- \rightleftharpoons LiFePO_4$$

α-phase $\qquad\qquad$ β-phase

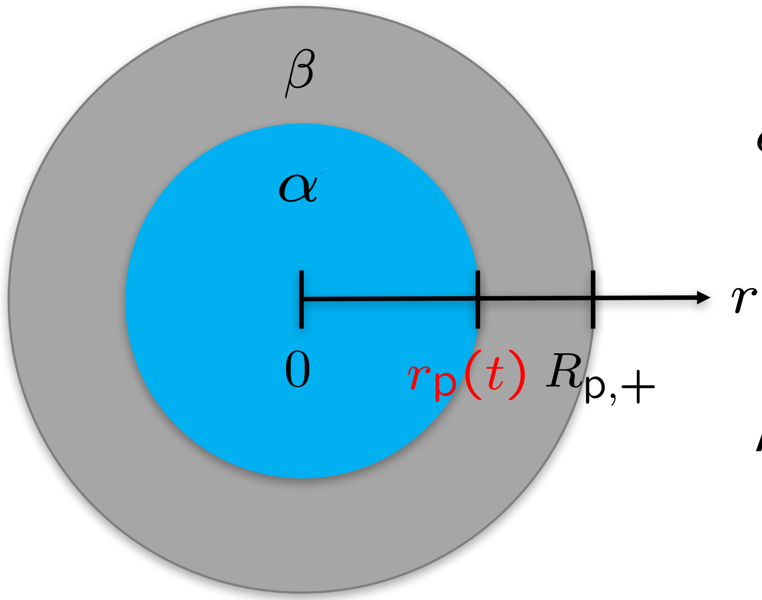
Charge-Discharge Cycle of LFP



α - Li poor phase
β – Li rich phase

Fig. by A. Khandelwal, et al, JPS 2014

Discharge Model of LFP (by Srinivasan and Newman 2004)



$c_{\mathrm{s},+}(r,t) \cdots$ concentration of lithium ion in positive electrode

Assumption : α-phase is equilibrium

$$c_{\mathrm{s},+}(r,t) = c_{\mathrm{s},\alpha} \text{ for } r \in (0, r_{\mathrm{p}}(t)).$$

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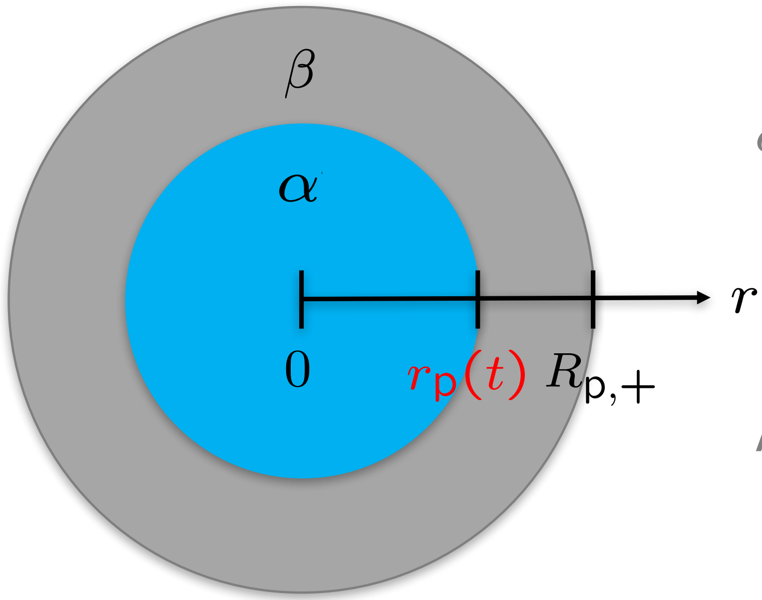

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Assumption : α-phase is equilibrium

$c_{\mathsf{s},+}(r,t) = c_{\mathsf{s},\alpha}$ for $r \in (0, r_{\mathsf{p}}(t))$.

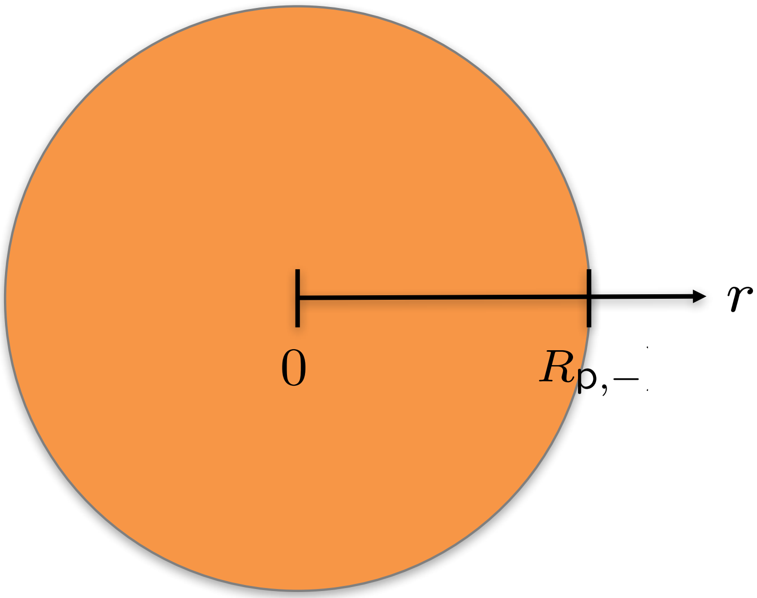
$$\frac{\partial c_{\mathsf{s},+}}{\partial t}(r,t) = \frac{D_{\mathsf{s},+}}{r^2}\frac{\partial}{\partial r}\left[r^2 \frac{\partial c_{\mathsf{s},+}}{\partial r}(r,t)\right], \quad r \in (r_{\mathsf{p}}(t), R_{\mathsf{p},+})$$

$$c_{\mathsf{s},+}(r_{\mathsf{p}}(t), t) = c_{\mathsf{s},\beta},$$

$$D_{\mathsf{s},+}\frac{\partial c_{\mathsf{s},+}}{\partial r}(R_{\mathsf{p},+}, t) = -j_{\mathsf{n},+}(t),$$

$$(c_{\mathsf{s},\beta} - c_{\mathsf{s},\alpha})\frac{d r_{\mathsf{p}}(t)}{dt} = -D_{\mathsf{s},+}\frac{\partial c_{\mathsf{s},+}}{\partial r}(r_{\mathsf{p}}(t), t).$$

Discharge Model of Negative Electrode



$c_{\mathsf{s},-}(r,t) \cdots$ concentration of lithium ion in negative electrode

$$\frac{\partial c_{\mathsf{s},-}}{\partial t}(r,t) = \frac{D_{\mathsf{s},-}}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial c_{\mathsf{s},-}}{\partial r}(r,t)\right], \quad r \in (0, R_{\mathsf{p},-})$$

$$\frac{\partial c_{\mathsf{s},-}}{\partial r}(0,t) = 0,$$

$$D_{\mathsf{s},-}\frac{\partial c_{\mathsf{s},-}}{\partial r}(R_{\mathsf{p},-},t) = -j_{\mathsf{n},-}(t),$$

Mass Conservation of Total Lithium

Lemma

Total amount of lithium-ion

$$n_{\mathsf{Li}}(t) = A_{-}\int_{0}^{R_{\mathsf{p},-}} c_{\mathsf{s},-}(r,t)r^{2}dr + A_{+}\int_{0}^{R_{\mathsf{p},+}} c_{\mathsf{s},+}(r,t)r^{2}dr,$$

where $A_i = \frac{3\epsilon_{\mathsf{s,i}} L_i}{R_{\mathsf{p,i}}^3}$ for $i \in \{-,+\}$, is conserved, i.e., $\frac{d}{dt}n_{\mathsf{Li}}(t) = 0$.

State Estimation for Phase Transition Positive Electrode

Measurements $\cdots \quad c_{\mathsf{ss},+}(t) := c_{\mathsf{s},+}(R_{\mathsf{p},+}, t), \quad r_{\mathsf{p}}(t),$

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Observer

$$\frac{\partial \widehat{c_{\mathsf{s},+}}}{\partial t}(r,t) = \frac{D_{\mathsf{s},+}}{r^2}\frac{\partial}{\partial r}\left[r^2 \frac{\partial \widehat{c_{\mathsf{s},+}}}{\partial r}(r,t)\right] + P(r_{\mathsf{p}}(t), r)\left[c_{\mathsf{ss},+}(t) - \widehat{c_{\mathsf{s},+}}(R_{\mathsf{p},+}, t)\right],$$

$$\widehat{c_{\mathsf{s},+}}(r_{\mathsf{p}}(t), t) = c_\beta,$$

$$D_{\mathsf{s},+}\frac{\partial \widehat{c_{\mathsf{s},+}}}{\partial r}(R_{\mathsf{p},+}, t) = -j_{\mathsf{n},+}(t) + Q(r_{\mathsf{p}}(t))\left[c_{\mathsf{ss},+}(t) - \widehat{c_{\mathsf{s},+}}(R_{\mathsf{p},+}, t)\right],$$

State Estimation for Phase Transition Positive Electrode

Measurements $\cdots \quad c_{\mathsf{ss},+}(t) := c_{\mathsf{s},+}(R_{\mathsf{p},+}, t), \quad r_{\mathsf{p}}(t),$

Observer

$$
\begin{aligned}
\frac{\partial \widehat{c_{\mathsf{s},+}}}{\partial t}(r,t) =& \frac{D_{\mathsf{s},+}}{r^2}\frac{\partial}{\partial r}\left[r^2 \frac{\partial \widehat{c_{\mathsf{s},+}}}{\partial r}(r,t)\right] \\
&+ P(r_{\mathsf{p}}(t), r)\left[c_{\mathsf{ss},+}(t) - \widehat{c_{\mathsf{s},+}}(R_{\mathsf{p},+}, t)\right], \\
\widehat{c_{\mathsf{s},+}}(r_{\mathsf{p}}(t), t) =& c_\beta, \\
D_{\mathsf{s},+}\frac{\partial \widehat{c_{\mathsf{s},+}}}{\partial r}(R_{\mathsf{p},+}, t) =& -j_{\mathsf{n},+}(t) \\
&+ Q(r_{\mathsf{p}}(t))\left[c_{\mathsf{ss},+}(t) - \widehat{c_{\mathsf{s},+}}(R_{\mathsf{p},+}, t)\right],
\end{aligned}
$$

The gains P, Q are derived via backstepping design for *moving boundary PDEs*.

Theorem The observer with gains

$$P(r_{\mathsf{p}}(t), r) = D_{s,+}\overline{\lambda}^2 \frac{R_{\mathsf{p},+}}{r} l(t) s(t) \frac{I_2\left(z(t)\right)}{z(t)},$$

$$Q(r_{\mathsf{p}}(t)) = \frac{D_{s,+}}{R_{\mathsf{p},+}} \left(\frac{\overline{\lambda}}{2} s(t) + 1 \right),$$

where

$$\overline{\lambda} = \frac{\lambda}{D_{s,+}},$$

$$s(t) = R_{\mathsf{p},+} - r_{\mathsf{p}}(t), \quad l(t) = r - r_{\mathsf{p}}(t),$$

$$z(t) = \sqrt{\overline{\lambda}\left[s(t)^2 - l(t)^2\right]}.$$

makes the observer error system glo. exp. stable in

$$\int_{r_{\mathsf{p}}(t)}^{R_{\mathsf{p},+}} r^2 \left(c_{\mathsf{s},+}(r,t) - \widehat{c_{\mathsf{s},+}}(r,t) \right)^2 dr.$$

State Estimation for Negative Electrode

Measurements $\cdots \quad c_{\mathsf{s},+}(R_{\mathsf{p},+}, t), \quad r_{\mathsf{p}}(t), \quad \frac{\partial c_{\mathsf{s},+}}{\partial r}(r_{\mathsf{p}}(t), t)$

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Observer

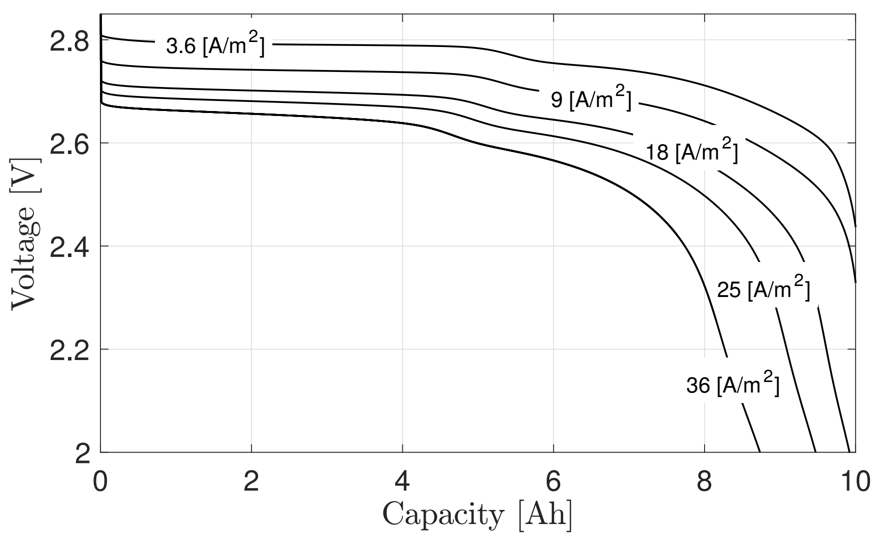
$$\frac{\partial \widehat{c_{\mathsf{s},-}}}{\partial t}(r,t) = \frac{D_{\mathsf{s},-}}{r^2}\frac{\partial}{\partial r}\left[r^2 \frac{\partial \widehat{c_{\mathsf{s},-}}}{\partial r}(r,t)\right] + P_-(r_{\mathsf{p}}(t))\widetilde{c_{\mathsf{s},+}}(R_{\mathsf{p},+},t) + F\left(r_{\mathsf{p}}(t)\right)\frac{\partial \widetilde{c_{\mathsf{s},+}}}{\partial r}(r_{\mathsf{p}}(t),t),$$

$$\frac{\partial \widehat{c_{\mathsf{s},-}}}{\partial r}(0,t) = 0,$$

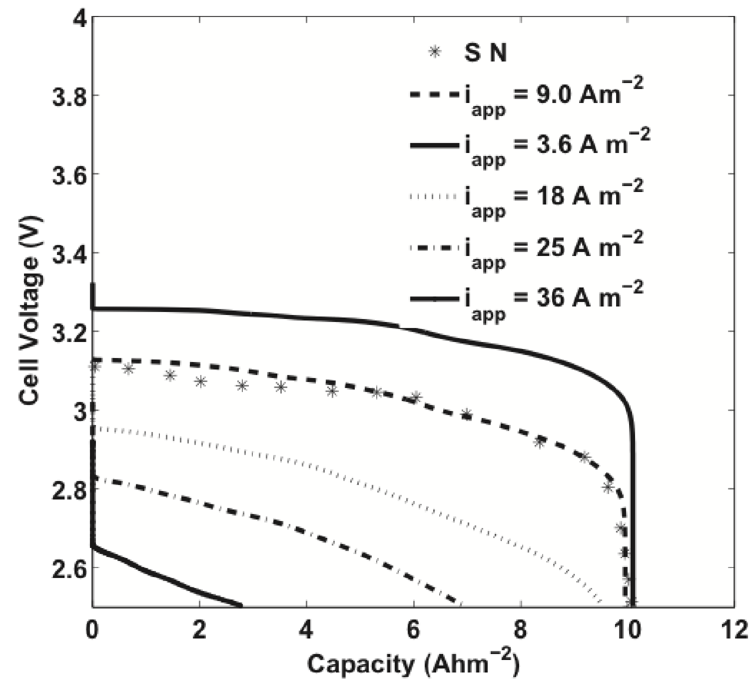
$$D_{\mathsf{s},-}\frac{\partial \widehat{c_{\mathsf{s},-}}}{\partial r}(R_{\mathsf{p},-},t) = -j_{\mathsf{n},-}(t) + Q_-(r_{\mathsf{p}}(t))\widetilde{c_{\mathsf{s},+}}(R_{\mathsf{p},+},t).$$

with the gains (P_-, F, Q_-) designed to conserve $\hat{n}_{\mathsf{Li}}(t)$ achieves $\widehat{c_{\mathsf{s},-}} \to c_{\mathsf{s},-}$

Simulation Test of Voltage Plot

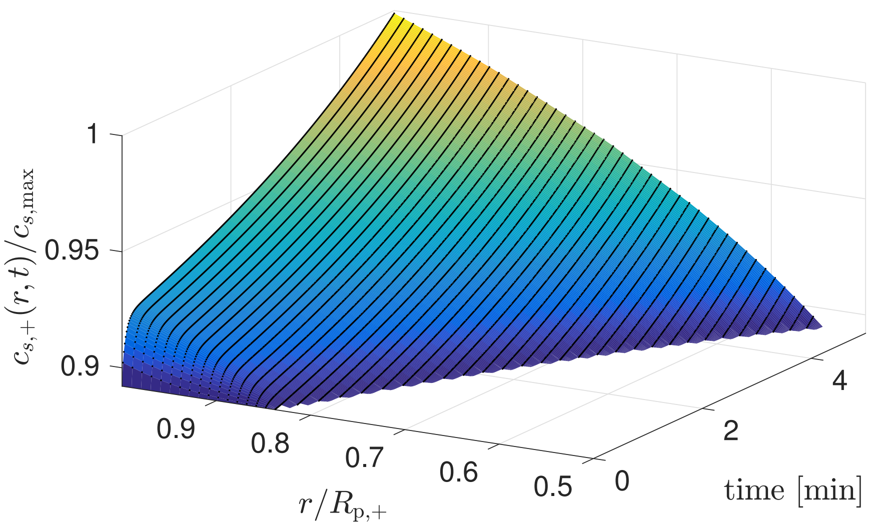


Our simulation

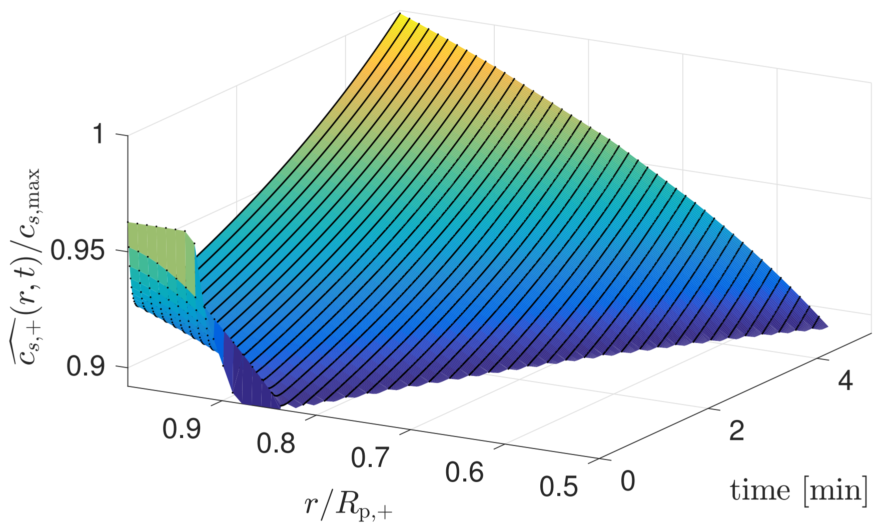


A. Khandelwal, et al, JPS 2014

Simulation of SoC (State-of-Charge) Estimation



True profile



Estimate profile

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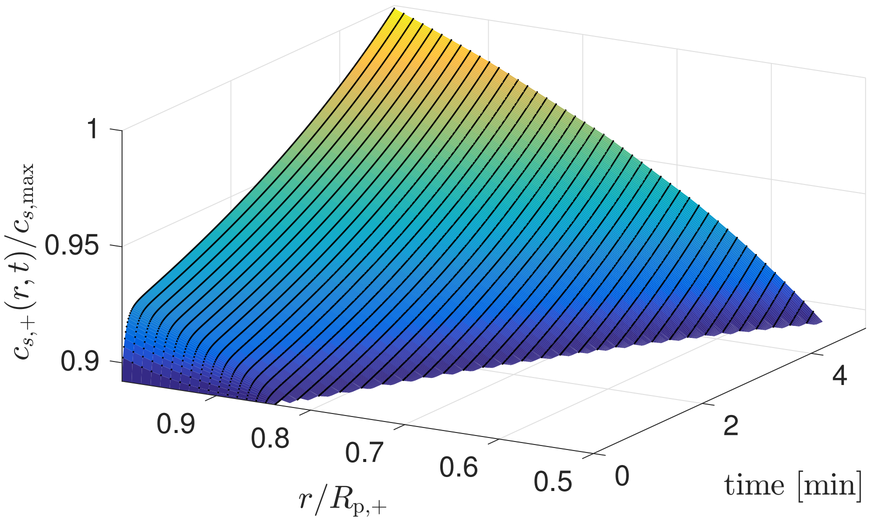

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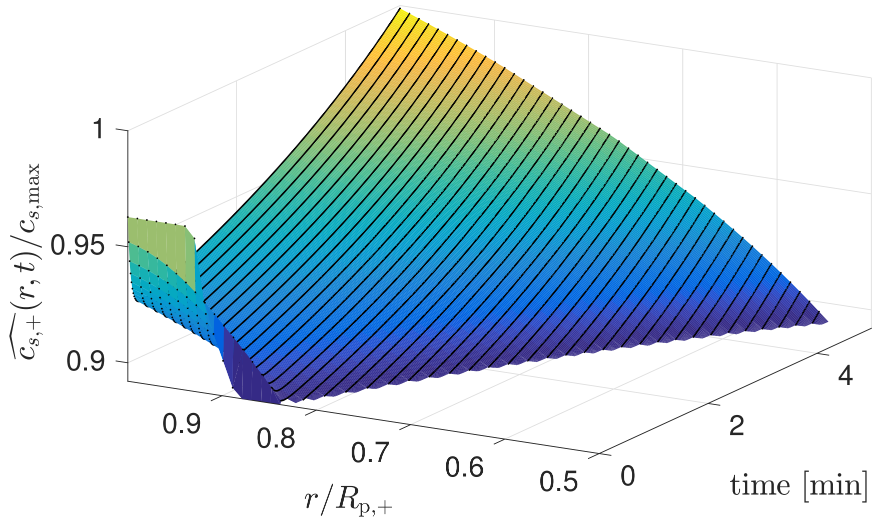

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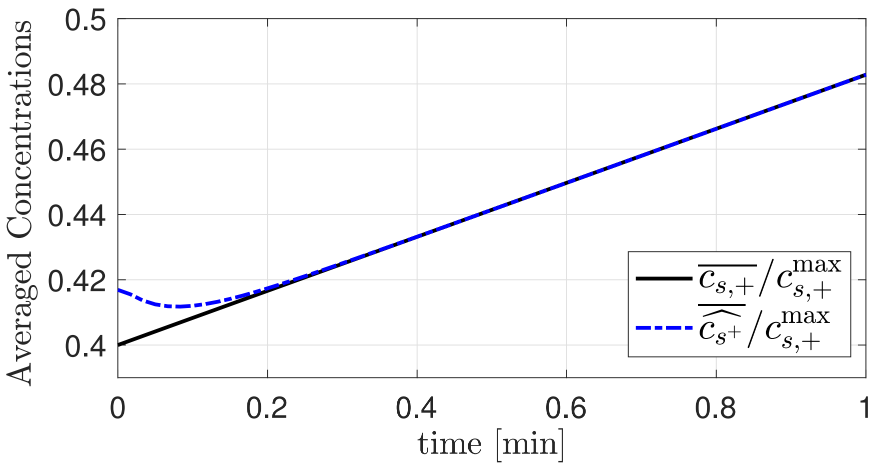

✓ SoC is accurately estimated

Future Work

- State estimation of two-phase (i.e., α phase is dynamic)
- State estimation without $r_{\mathrm{p}}(t)$ (phase boundary radius)
- State and parameter estimation