Comparison of a Particle Filter and Other State Estimation Methods for Prognostics of Lithium-ion Batteries

Eric A. Walker

Supervised by:
Professor Ralph E. White

Thesis Defense:
In partial fulfillment of the requirements for the degree of Master of Science in Chemical Engineering

August 14th 2013

Outline

- Introduction
  - Particle filtering previous work
  - Two models considered in this work
- He, et al model
  - Results with three methods
- Equivalent circuit model
- Single particle model
- Conclusions
- Acknowledgement

Introduction- He, et al

$Q_k = a \cdot \exp(b \cdot k) + c \cdot \exp(d \cdot k)$

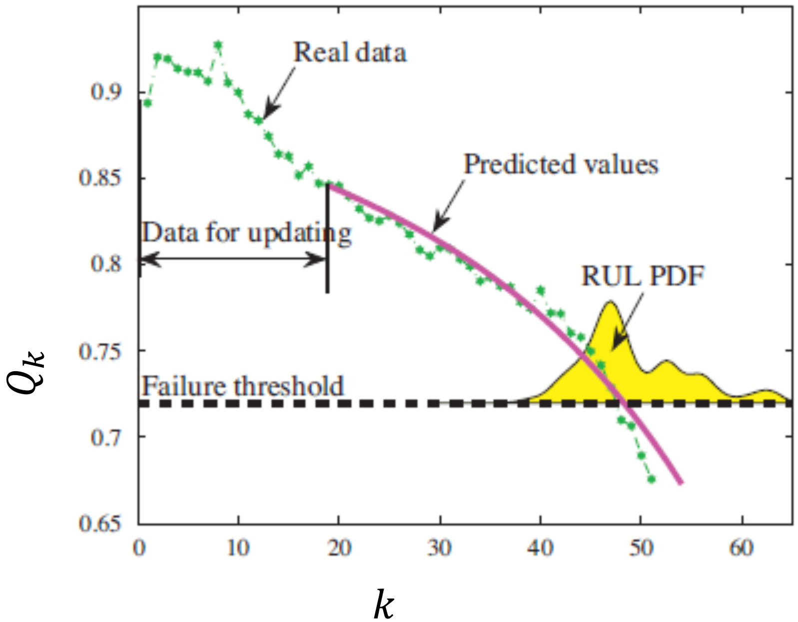
$\underline{x} = [a\ b\ c\ d]^T$

Failure threshold, Q_{EUL} is 80% of the rated capacity.

$a \cdot \exp(b \cdot k_{EUL}) + \cdots$
$c \cdot \exp(d \cdot k_{EUL}) = Q_{EUL}$

$RUL = k_{EUL} - k$

- $a(Ah), b\left(\frac{1}{cycle}\right), c(Ah), d\left(\frac{1}{cycle}\right)$ are states.
- $k(cycle)$ is the cycle index.
- $Q_k(Ah)$ is the capacity at cycle k.
- End of Useful Life (EUL), Remaining Useful Life(RUL) and Probability Density Function (PDF)



Center for Advanced Life Cycle Engineering (CALCE) Prognostics and Health Management (PHM) newsletter September 2012

A Saxena, B Bole, M Daigle, K Goebel, NASA Battery Workshop 2012 (images from private communication)

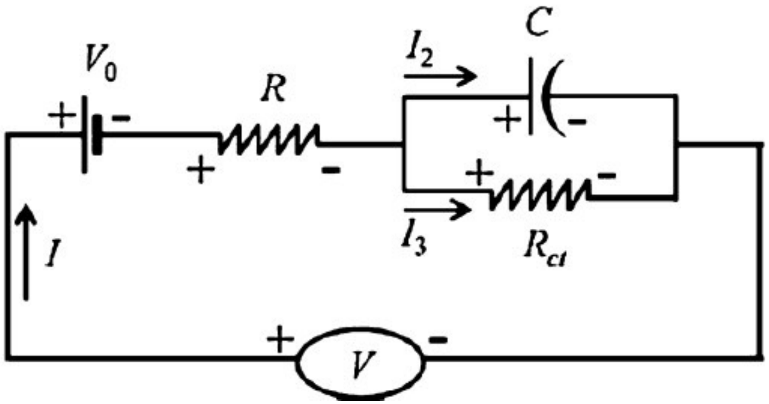
Introduction

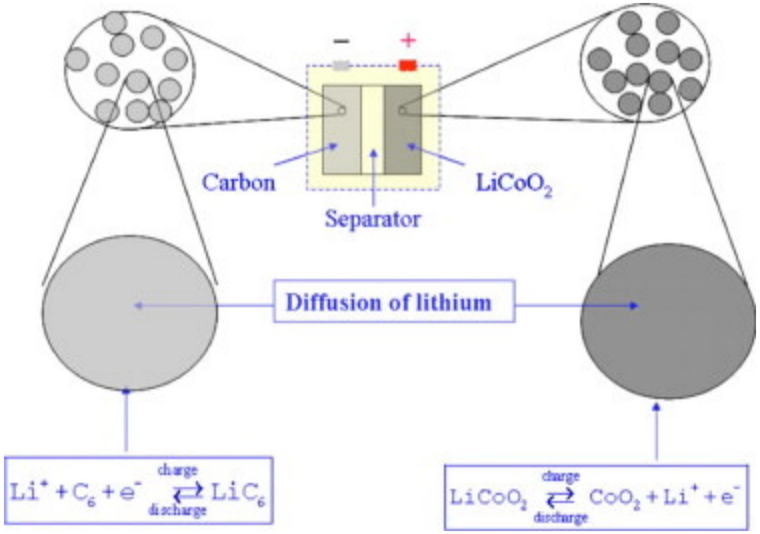
- **Other particle filtering works (reference handout)**
  - **Saha, et al**
  - **Jin, et al**
  - **Daigle, et al Cadini, et al An, et al**
- **No comparison of accuracy or comparison with a less than ideal method**
- **Data-driven models or empirical**

Xing, et al found $Q_k = p_1 k^2 + p_2 k + p_3$ less accurate.

Introduction

- **Rahimian, et al**
  - Physics-based single particle (SP) model more accurate than equivalent circuit model (ECM).
  - Both models are re-applied for predicting time until end of discharge voltage (EODV) in this work.
- **Unscented Kalman filter (UKF) performed better than extended Kalman filter (EKF) with SP.**





He, et al model

$$Q_k = g(\underline{x}, k) = a \cdot \exp(b \cdot k) + c \cdot \exp(d \cdot k)$$

$$\underline{x} = [a\ b\ c\ d]^T$$

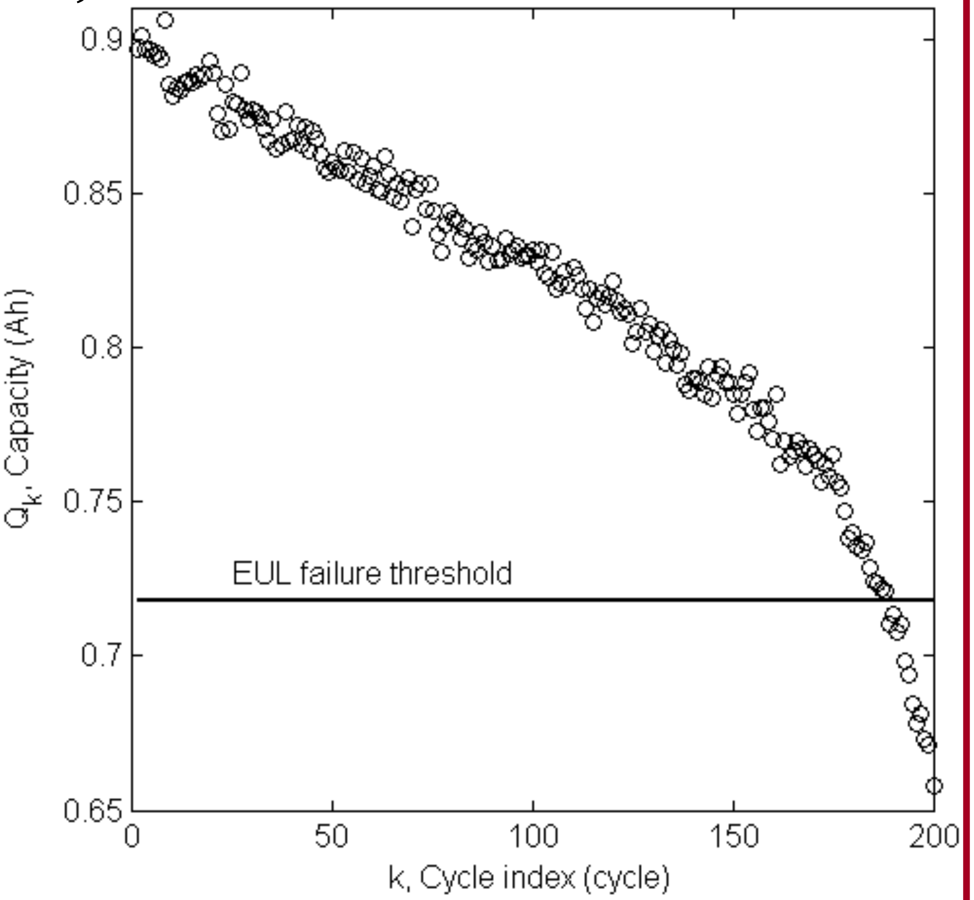
$$Q_{EUL} = 0.8Q_{k=1}$$

$$a \cdot \exp(b \cdot k_{EUL}) + \cdots$$
$$c \cdot \exp(d \cdot k_{EUL}) = 0.8Q_{k=1}$$

$$RUL = k_{EUL} - k$$

- $a(Ah), b\left(\frac{1}{cycle}\right), c(Ah), d\left(\frac{1}{cycle}\right)$ are states.
- $k(cycle)$ is the cycle index.
- $Q_k(Ah)$ is the capacity at cycle k.
- End of Useful Life (EUL) and Remaining Useful Life
- The error is reported by the magnitude of $k^*_{EUL} - k_{EUL}$ where $*$ indicates experiment.

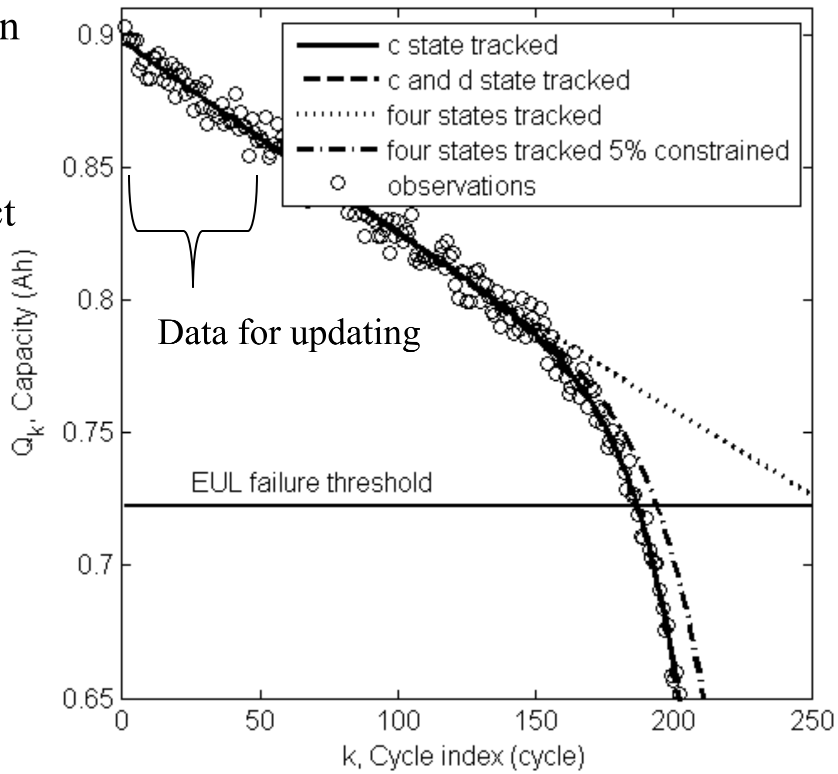
~.5% noise added to synthetic data



He, et al model

$$Q_k = g(\underline{\theta}, k) = a \cdot \exp(b \cdot k) + c \cdot \exp(d \cdot k)$$

- c state tracked with correct a, b, d fixed. c is given the correct initial guess.
- c, d state tracked with correct a, b fixed. The problem is now non-linear. c, d state given the correct initial guess.
- Four states tracked constrained to correct sign.
- Four states tracked constrained to 5% of the correct values (because PF will vary the particles within $\pm 5\%$ of the correct values).



NLLS four states error (cycles)
88

- The error is reported by the magnitude of $k^*_{EUL} - k_{EUL}$ where $*$ indicates experiment.

He, et al model- UKF

- UKF is a sample-based filter for non-linear models. $2n+1$ is the sampling scheme used in this work, where n is the number of states.
- $\underline{\hat{x}}$ state estimate vector
- P^x state covariance matrix
- X matrix containing samples
- W matrix containing weights
- P^{yy} measurement covariance matrix
- P^{xy} cross covariance matrix
- K_k Kalman gain matrix
- Q^* experimental capacity (Ah)
- κ tuning parameter

a,b,c,d correct IG

Initialize the state estimate, $\underline{\hat{x}}_0$, and its covariance matrix, P_0^x

Generate $2n+1$ samples and store them in X,

$$C = chol(P_{k-1}^x) \quad \mathrm{X}_{0,k-1} = \underline{\hat{x}}_{k-1}$$

$$\mathrm{X}_{i,k-1} = \underline{\hat{x}}_{k-1} + \sqrt{n+\kappa c_{jj}} \quad \mathrm{X}_{i+n,k-1} = \underline{\hat{x}}_{k-1} - \sqrt{n+\kappa c_{jj}}$$

C is the Cholesky decomposition of P_{k-1}^x, and c_{jj} are its diagonal entries.

Generate weights and store them in W,

$$W_0 = \kappa/\sqrt{n+\kappa} \quad W_i = 1/[2(n+\kappa)] \quad W_{i+n} = 1/[2(n+\kappa)]$$

Generate the prior state estimate at index, k,

$$[\underline{\hat{x}}_{k,-}, P_{k,-}^x] = UT(\underline{\hat{x}}_{k-1,+}, C_{k-1,+}, f(\cdot), \kappa)$$

Obtain necessary matrices,

$$Y_{i,k} = h_k(X_i, I_{app,k}) \quad \hat{y}_k^- = \sum_i^{2n} W_i Y_i$$

$$P_k^{yy} = \sum_{i=0}^{2n} W_i (Y_{i,k} - \hat{y}_k^-)(Y_{i,k} - \hat{y}_k^-)^T$$

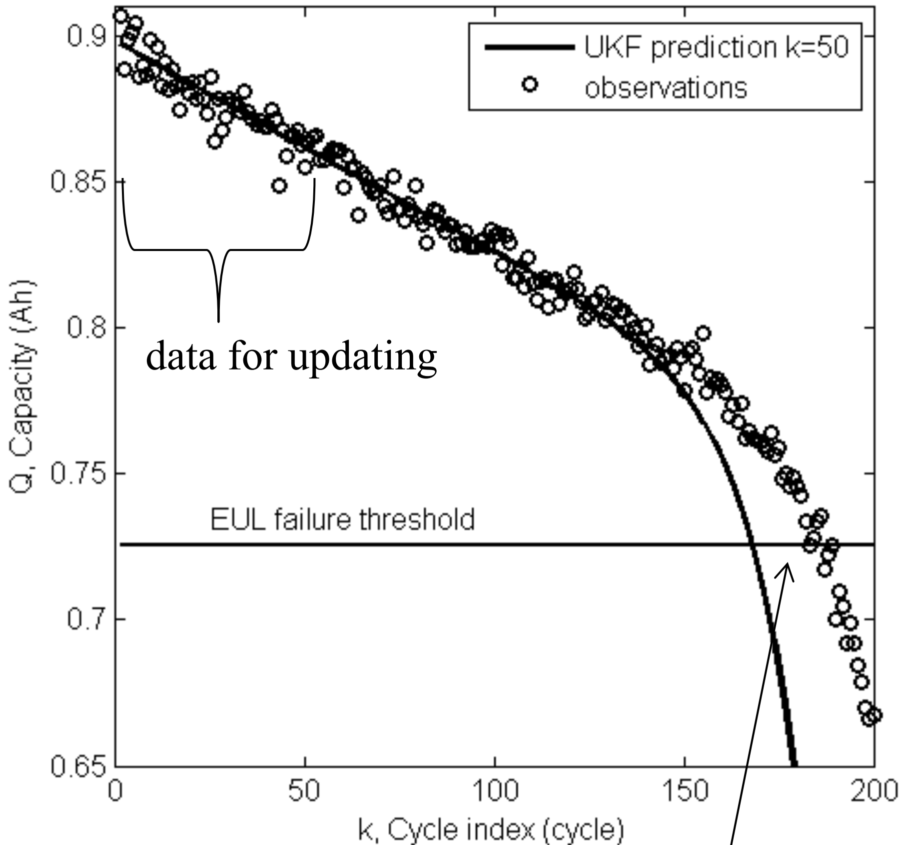
$$P_k^{xy} = \sum_{i=0}^{2n} W_i (\mathrm{X}_i - \underline{\hat{x}}_{k,-})(Y_{i,k} - \hat{y}_{k,-}) \quad K_k = P_k^{xy}(P_k^y)^{-1}$$

Complete the posterior estimate,

$$\underline{\hat{x}}_k^+ = \underline{\hat{x}}_k^- + K_k(Q_k^* - \hat{y}_k^-) \quad P_k^{x+} = P_k^{x-} - K_k P_k^y K_k^T$$

k=k+1

He, et al model- UKF prediction



Error is 19 cycles.

He, et al model- PF

$\underline{x}$ state vector

Q^* experimental capacity (Ah)

k (cycle) index

$p(\underline{x}_k|Q^*_{0:k-1})$ prior distribution

| "given"

w^i_k weight of particle i

$f(\cdot)$ state function

$p\left(Q^*_k|\underline{x}^i_k\right)$ posterior distribution

$g(\cdot)$ measurement function

$\delta(\cdot)$ Dirac delta

A set of particles are initialized.

$k = 1$

The prior distribution is obtained by

$$p(\underline{x}_k|Q^*_{0:k-1}) \approx \sum_{i=1}^{N} w^i_{k-1} f_{k-1}(\underline{x}^i_{k-1})$$

The weights of $\underline{x}^i_k$ are obtained by $\overline{w}^i_k = w^i_{k-1}\, p\left(Q^*_k|\underline{x}^i_k\right)$where

$$p\left(Q^*_k|\underline{x}^i_k\right) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\frac{\left(Q^*_k - g_k\left(\underline{x}^i_k, k\right)\right)^2}{\sigma^2}\right)$$

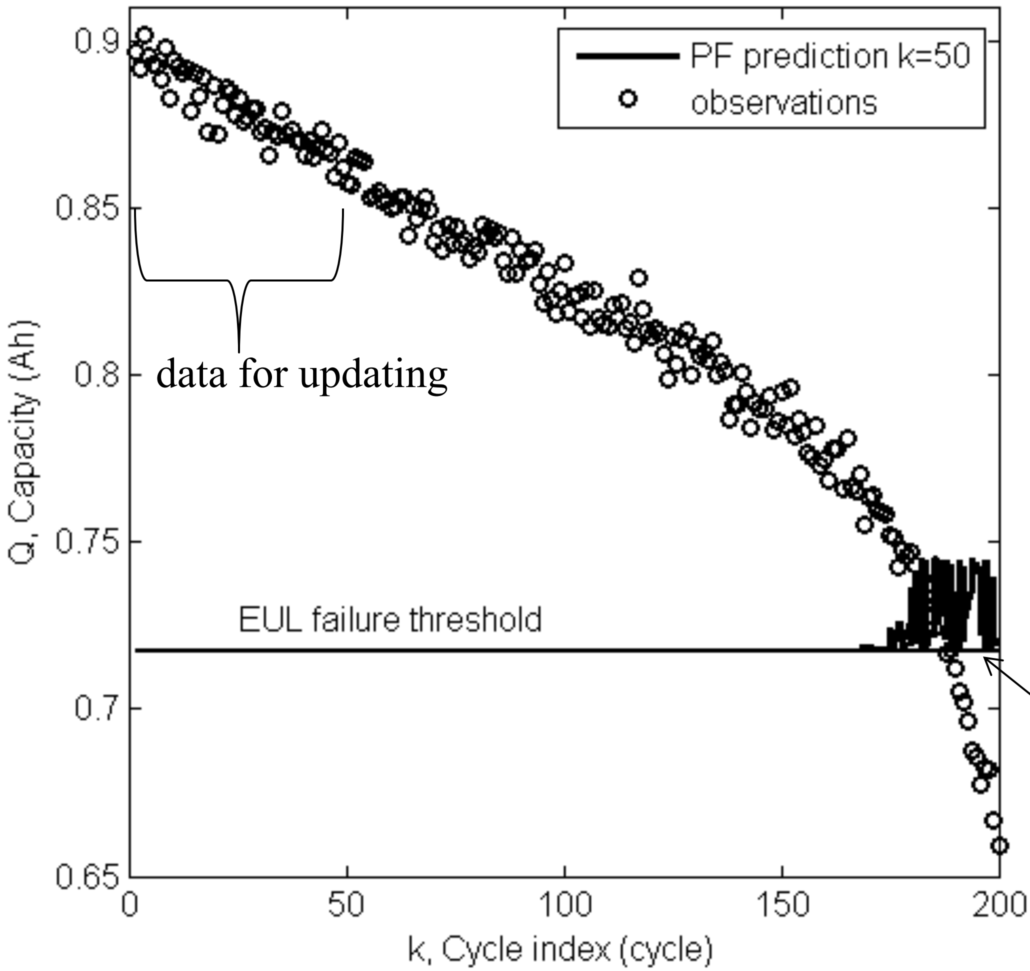
The posterior distribution is obtained by

$$p(\underline{x}_k|Q^*_{0:k}) \approx \sum_{i=1}^{N} w^i_k \delta(\underline{x}_k - \underline{x}^i_k)$$

The posterior distribution, $p\left(\underline{x}_k|Q^*_{0:k}\right)$, is used to calculate a prediction.

$k = k + 1$

He, et al model



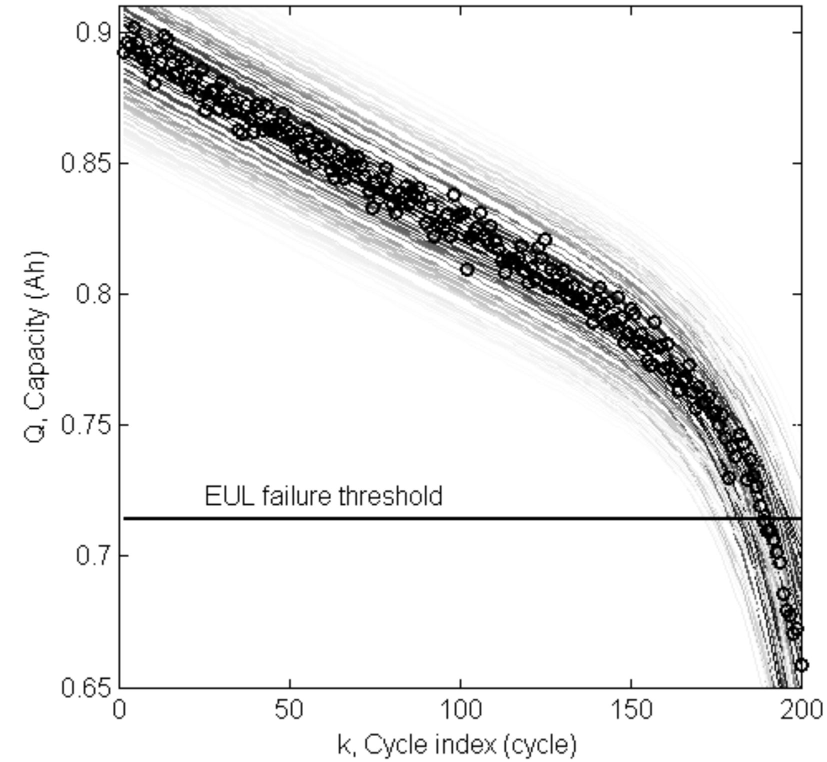
100 particles

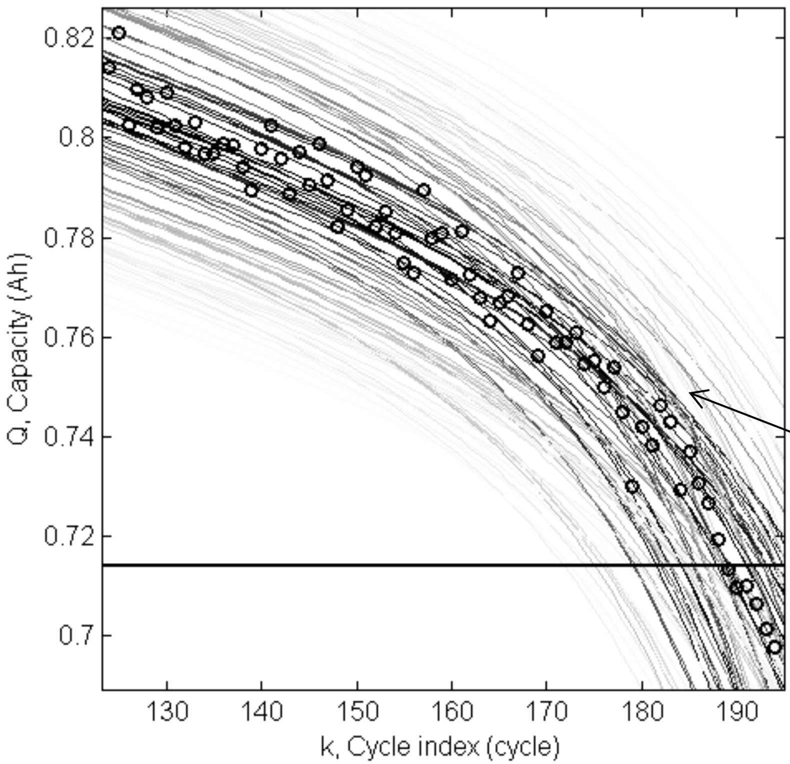
PDF by particles rough because…

He, et al model

100 particles

- Zoom in on PDF
- Particles close together in data for updating criss-cross near EUL for a rough PDF.
- Still, error by weighted average is ~ 1cycle, compared to the next method, NLLS 5% constrained, with an error on the order of ~10 cycles.

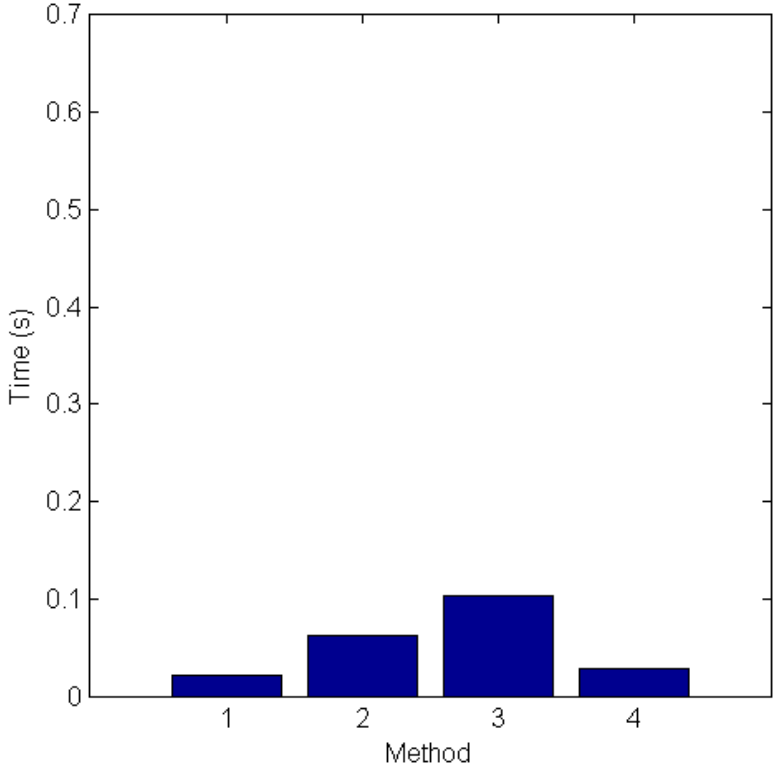




Particles criss-cross near EUL, yet the weighted average prediction is more accurate than deterministic methods.

Times for methods He, et al

	Time (seconds)
PF solve all particles for data set and find RUL for each particle	1.17e-2
PF time to update weights 200 cycles	9.34e-3
UKF solve for 200 data update states until 50 data	6.26e-2
NLLS estimate states	1.03e-1
NLLS find RUL	7.45e-4
NLLS 5% constrained estimate states	2.67e-2
NLLS 5% constrained find RUL	6.05e-4

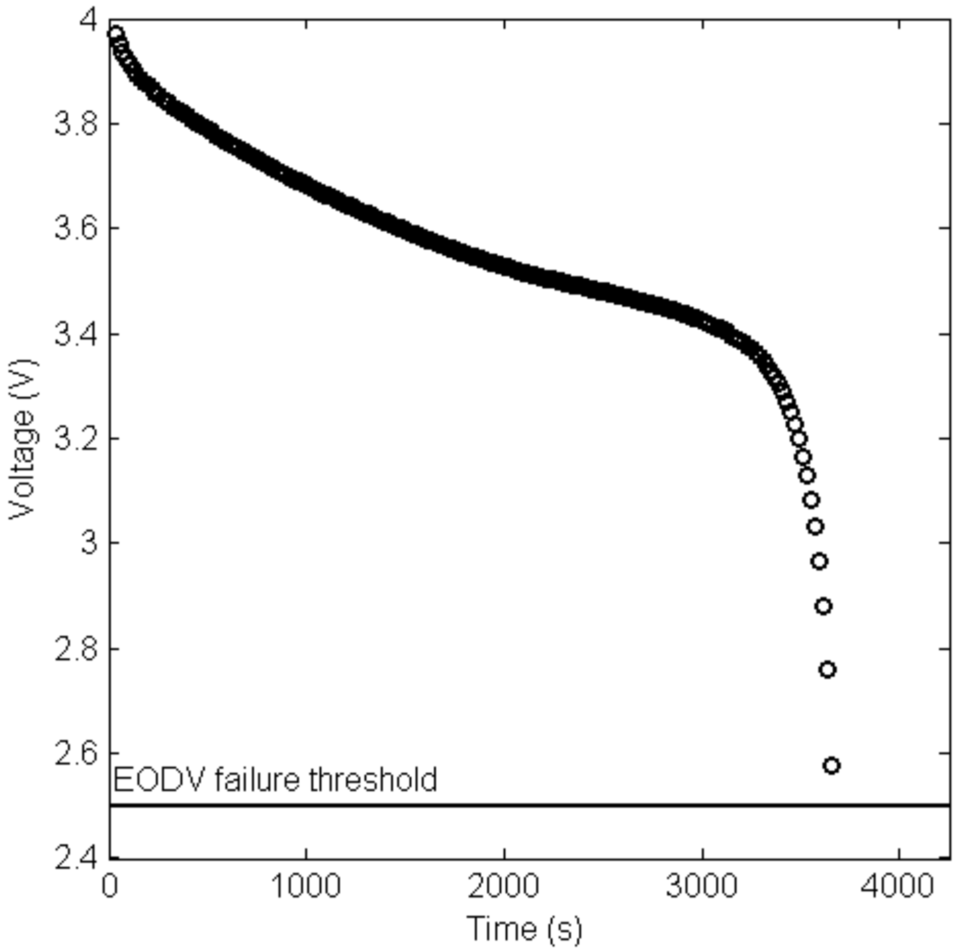


Outline

- Introduction
- He, et al model
  - Results with three methods
- **Equivalent circuit model**
- Single particle model
- Conclusions
- Acknowledgement

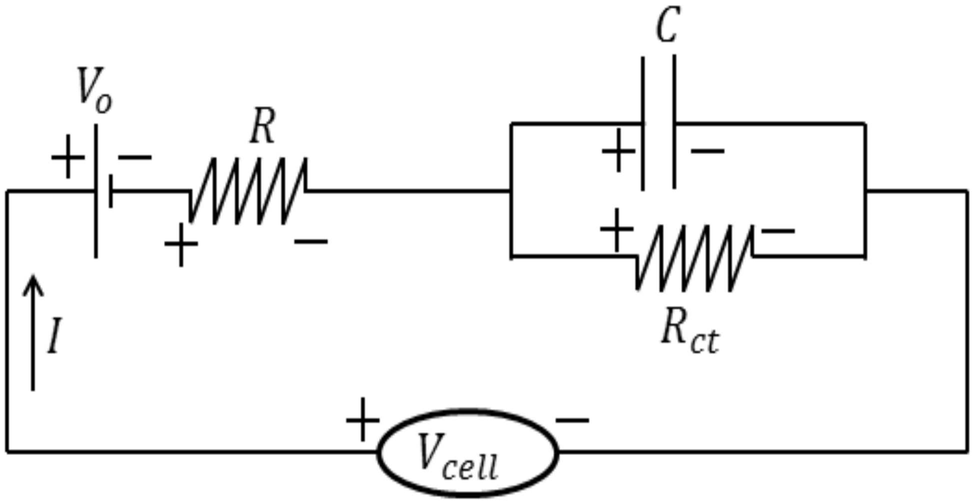
Equivalent circuit model- data set

- End of discharge voltage (EODV) is 2.5 (V).
- Fifty data points is 928.6 (s), the time of prediction.
- Prediction is time until EODV assuming constant-current discharge.
- Batteries are discharged at a constant current of 2 (A) from a fully charged 4.2 (V) to a EODV cutoff voltage of 2.5 (V).



Source: NASA Ames Prognostics Repository (reference handout)

Equivalent circuit model



$$V_{cell} = V_o + IR + \frac{Q}{C}\exp\left(-\frac{t}{R_{ct}C}\right) + IR_{ct}\left(1 - \exp\left(-\frac{t}{R_{ct}C}\right)\right)$$

$$V_o = U_p^\theta(SOC_p) - U_n^\theta(SOC_n)$$

$$SOC_{cell} = SOC_{0,cell} + \frac{I}{3600Q}t$$

$$SOC_n = 0.79SOC_{cell} + 0.01 \qquad SOC_p = 0.97 - 0.51SOC_{cell}$$

$V_{cell}(V)$ Cell voltage

$R(\Omega)$ Resistance

$R_{ct}(\Omega)$ Charge transfer resistance

$C(F)$ Capacitance

$Q(Ah)$ Capacity

$t(s)$ time

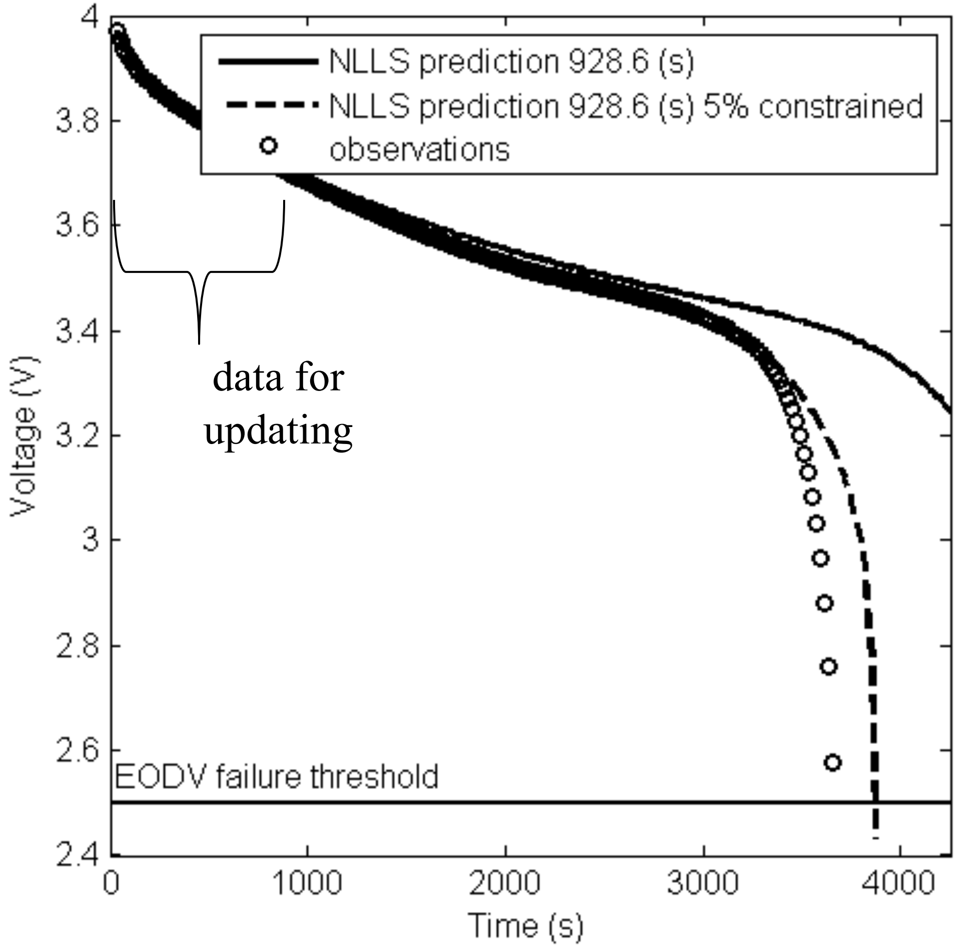
SOC_i State of charge

U_i^θ Open circuit potential

$I(A)$ Current

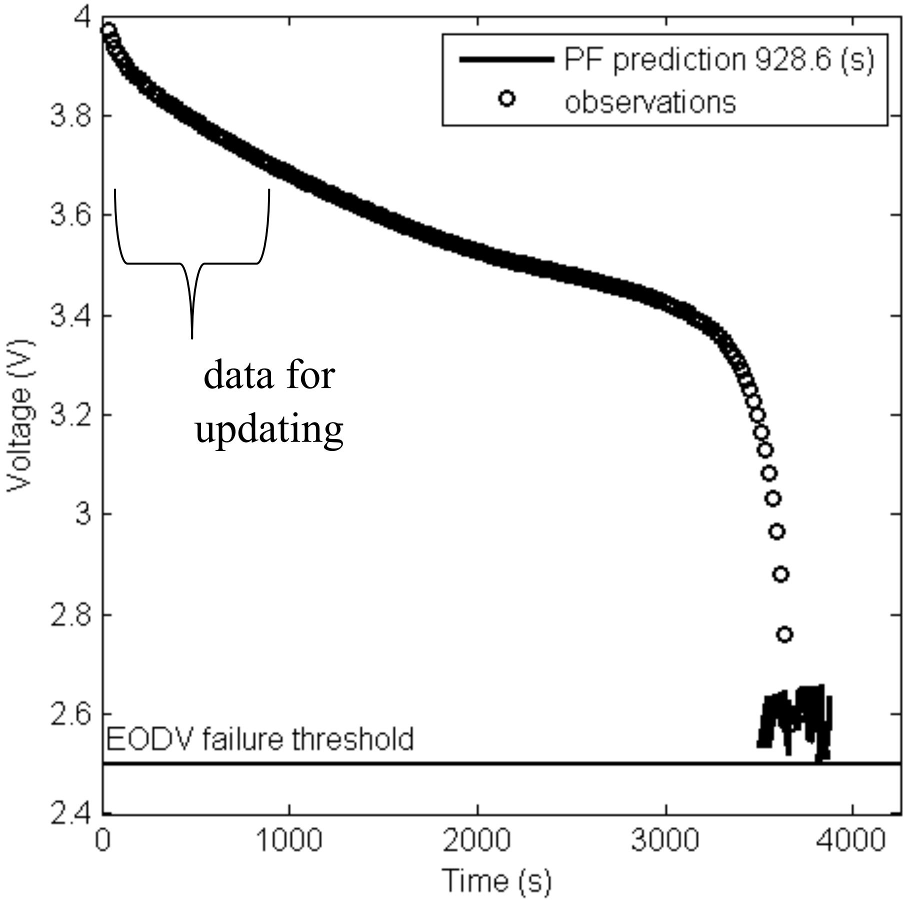
Equivalent circuit model

- Initial guesses are obtained by fitting a separate cycle of the same cell.
- NLLS predictions are inaccurate.
- $\underline{\hat{x}} \equiv [R, C, Q, R_{ct}]$



Equivalent circuit model-PF

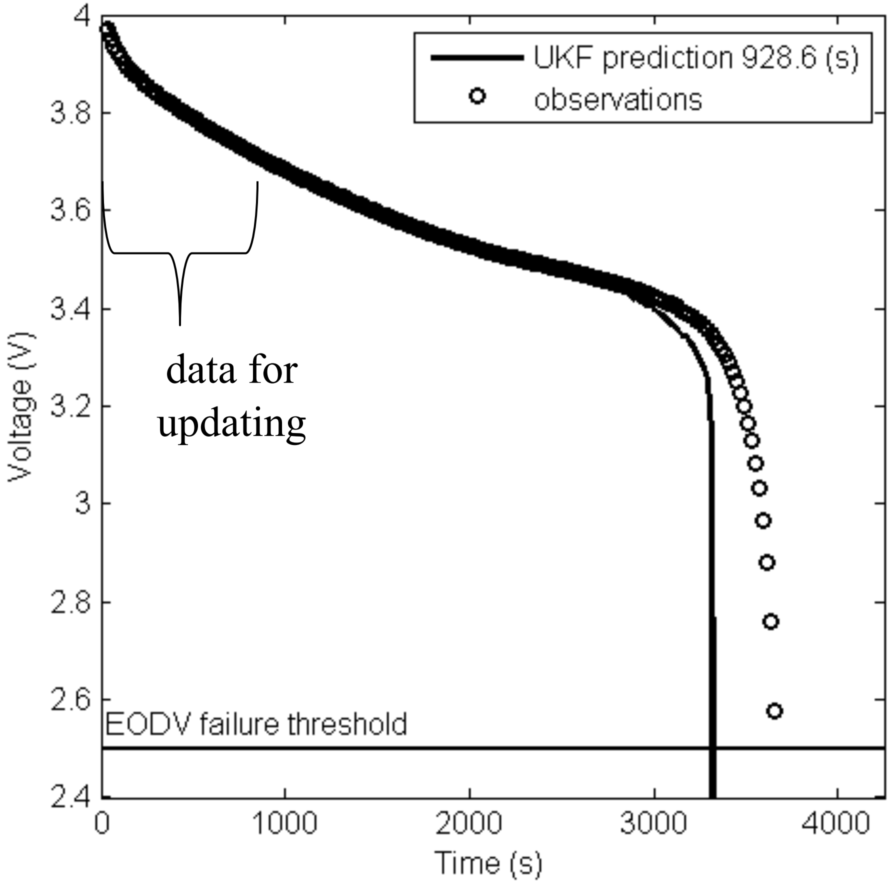
$\underline{\hat{x}} \equiv [R, C, Q, R_{ct}]$



The weighted average prediction error is on the order of ~26 seconds, more accurate than the next method, NLLS 5% constrained, with an error of 212 seconds.

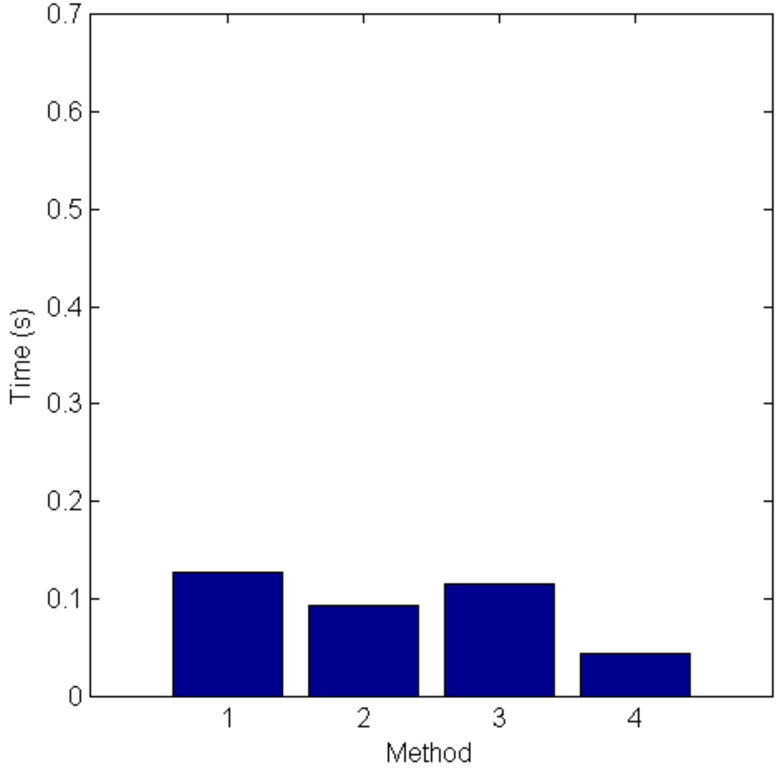
Equivalent circuit model-UKF

$\underline{\hat{x}} \equiv [R, C, Q, R_{ct}]$



Times for methods ECM

	Time (seconds)
PF solve all particles for data set and find time of EODV for each particle	1.17e-1
PF time to update weights 194 cycles	9.73e-3
UKF solve for 195 data update states until 50 data	9.21e-2
NLLS estimate states	1.15e-1
NLLS find RUL	9.5e-5
NLLS 5% constrained estimate states	4.37e-2
NLLS 5% constrained find RUL	7.8e-5



Outline

- Introduction
- He, et al model
  - Results with three methods
- Equivalent circuit model
- **Single particle model**
- Conclusions
- Acknowledgement

Single particle model

$$J_p = \frac{I_{app}}{S_p} \qquad J_n = -\frac{I_{app}}{S_n} \qquad \frac{dx_{i,avg}}{dt} = -\frac{3J_i}{FR_i c_{i,max}} \qquad x_{i,surf} - x_{i,avg} = -\frac{J_i R_i}{5FD_{s,i} c_{i,max}}$$

$$\frac{J_i}{F} = k_i\left(c_{i,max} - x_{i,surf} c_{i,max}\right)^{0.5}\left(x_{i,surf} c_{i,max}\right)^{0.5} c_e^{0.5}\left[\exp\left(\frac{\alpha_{a,i} F}{R_g T}\eta_i\right) - \exp\left(\frac{-\alpha_{c,i} F}{R_g T}\eta_i\right)\right]$$

$$\eta_i = \frac{R_g T}{0.5F}\ln\left(\frac{\left(J_i \pm \left(-4c_e F^2 c_{i,max}^2 k_i^2 x_{i,surf}^2 + 4c_e F^2 c_{i,max}^2 k_i^2 x_{i,surf} + J_i^2\right)^{0.5}\right)}{2Fc_e^{0.5} k_i\left(c_{i,max} x_{i,surf}\right)^{0.5}\left(c_{i,max} - c_{i,max} x_{i,surf}\right)^{0.5}}\right)$$

$$\eta_p = \phi_p - U_p^\theta \qquad \eta_n = \phi_n - U_n^\theta \qquad V_{cell} = \eta_p + U_p^\theta - \left(\eta_n + U_n^\theta\right)$$

In the cathode $i = p$ and in the anode $i = n$.

J_i is the exchange current density for each electrode $\left[\frac{A}{m^2}\right]$. $x_{i,avg}$ is the ratio of the solid bulk concentration to the maximum solid concentration of Lithium for each electrode. F is Faraday's constant, 96485 in $\left[\frac{C}{mol\ e^-}\right]$. $R_i[m]$ is the particle radius for each electrode. $c_{i,max}$ $\left[\frac{mol}{m^3}\right]$ is the maximum solid phase concentration of Lithium for each electrode. $S_i^0[m^2]$ is the electroactive surface area for each electrode. $x_{i,surf}$ is the ratio of the solid surface concentration to the maximum solid concentration for each electrode, $c_{i,surf}/c_{i,max}$. $D_{s,i}$ $\left[\frac{m^2}{s}\right]$ is the solid phase diffusion coefficient of Lithium for each electrode. Butler-Volmer kinetics are used to describe the intercalation and de-intercalation reactions of Lithium at the electrodes.

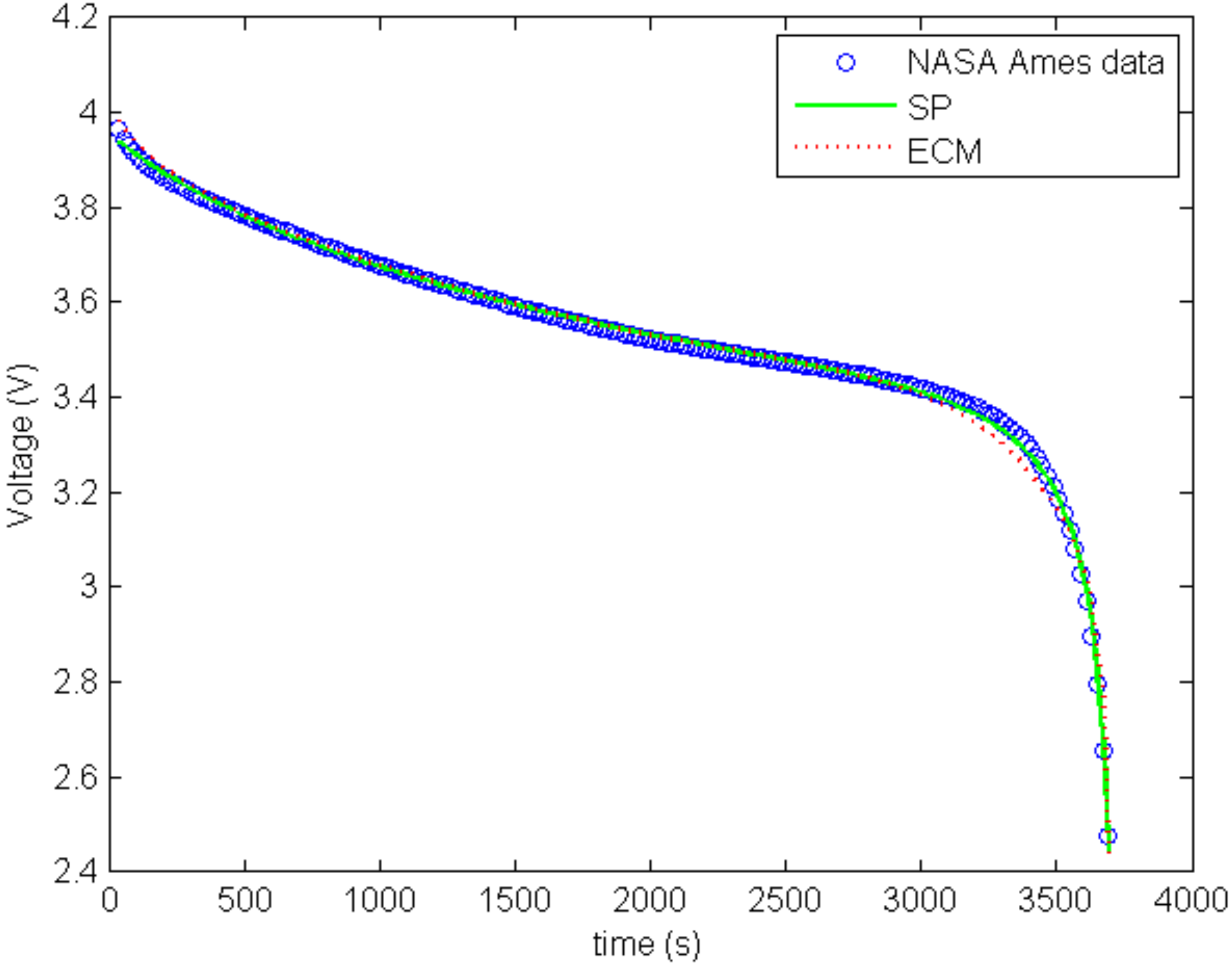
Single Particle model initial guesses

Two parameters in open circuit potentials are adjusted for SP fit.

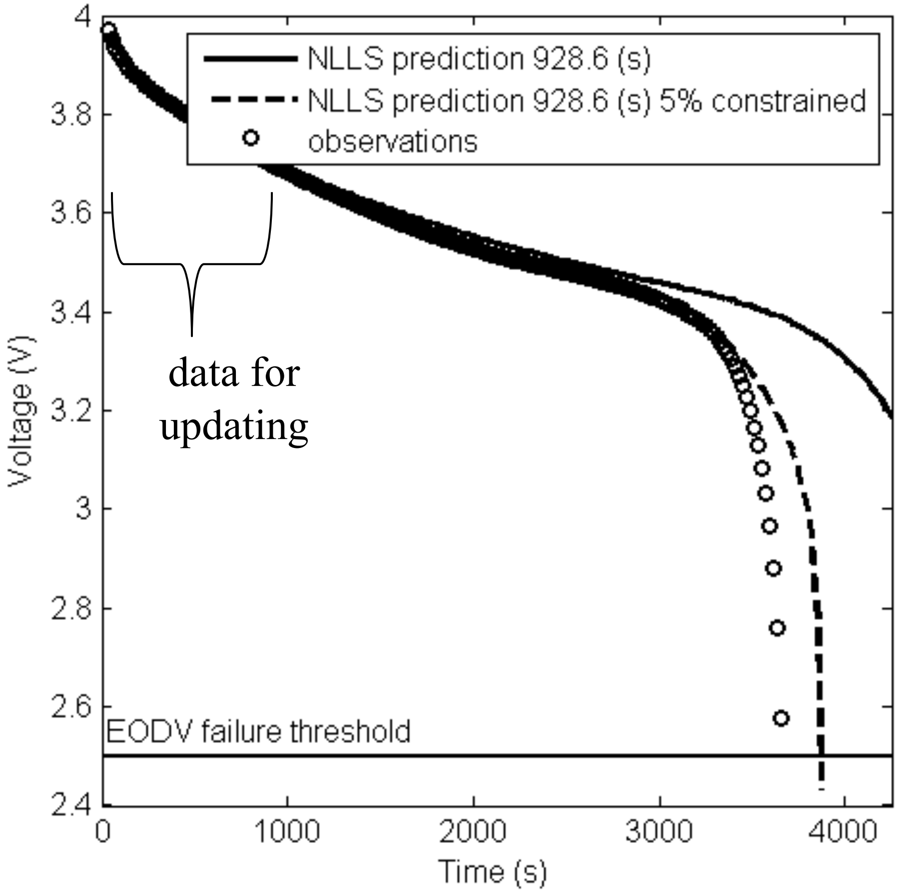
Norm of squared residuals:

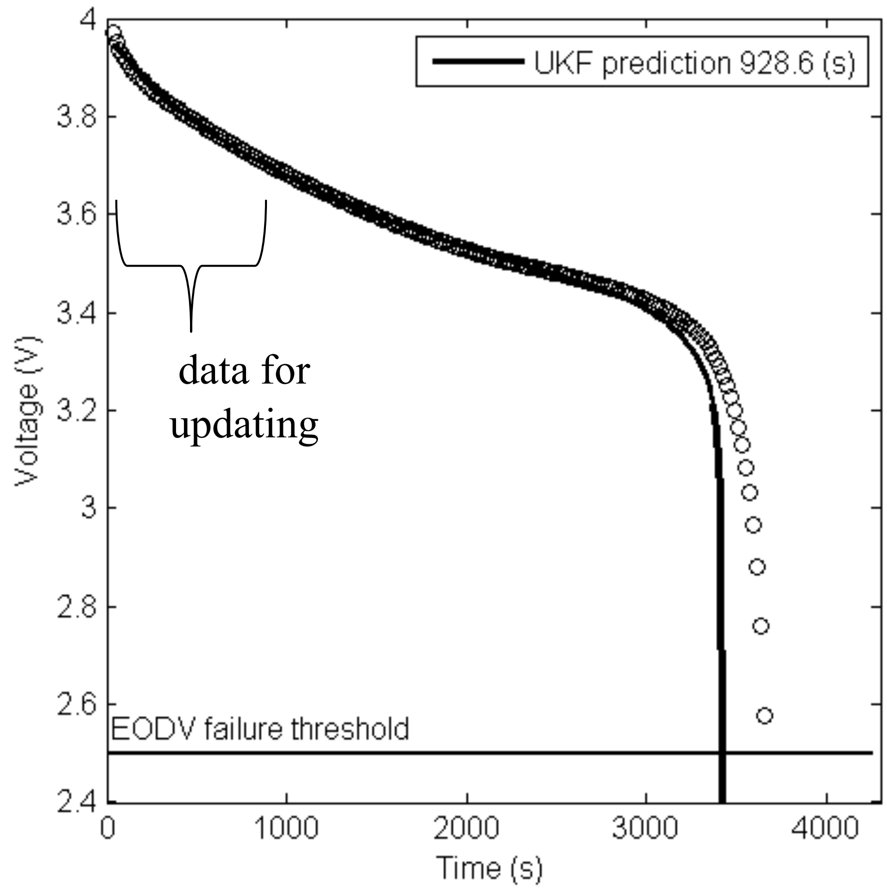
0.0145 for SP

0.0824 for ECM



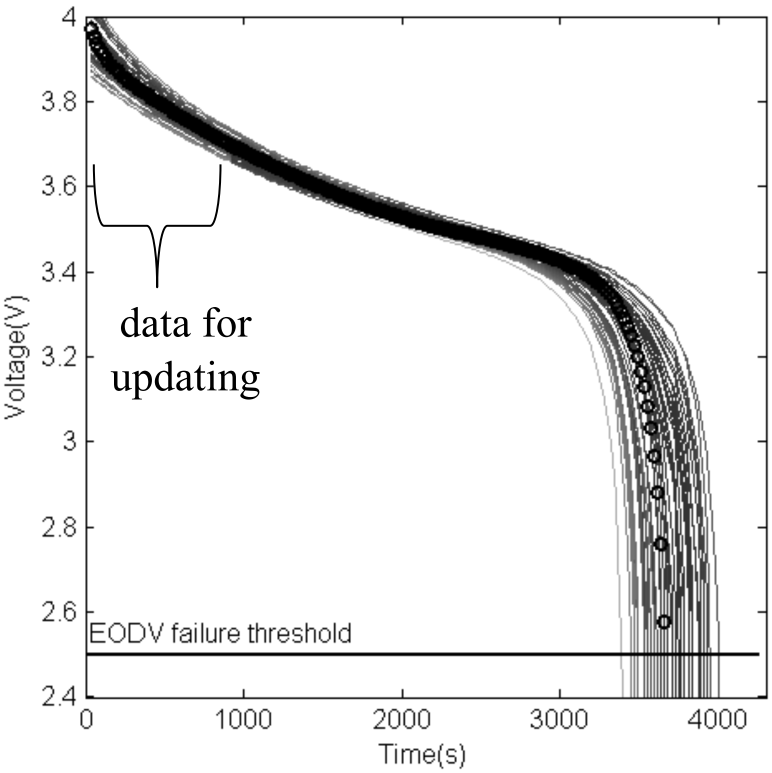
Single particle model NLLS and UKF

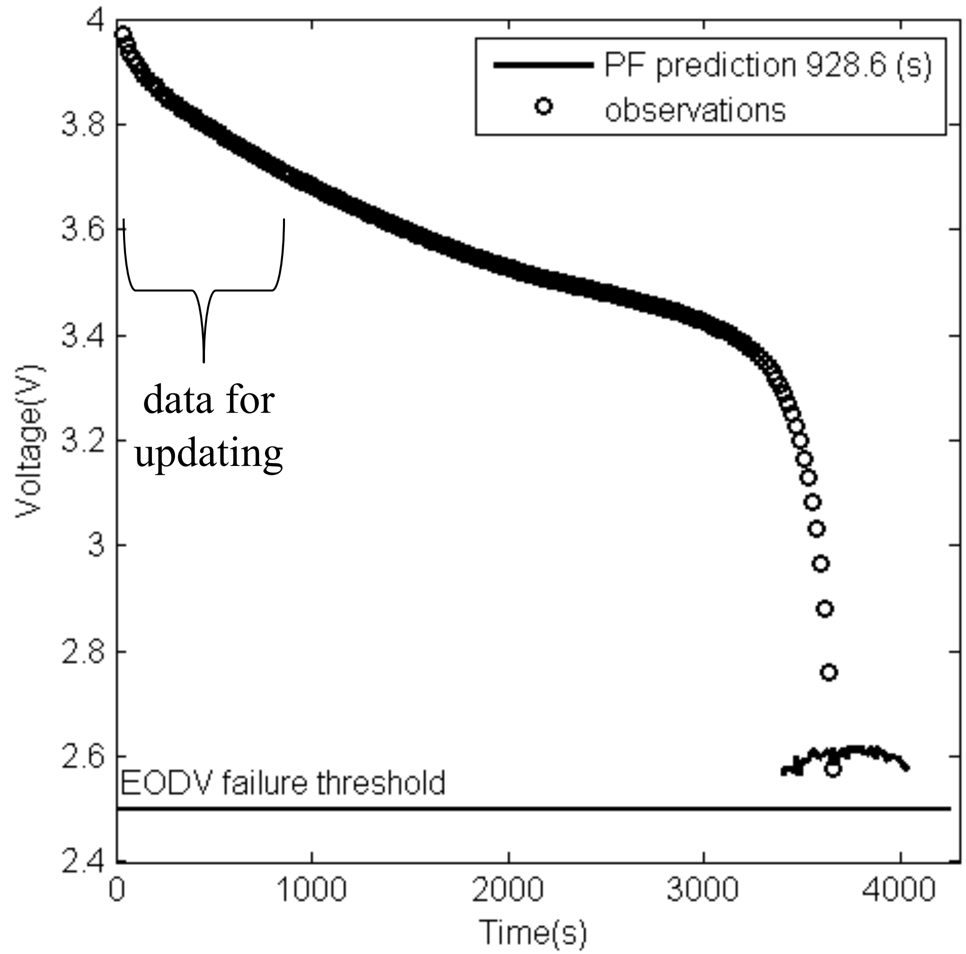




Single particle model PF

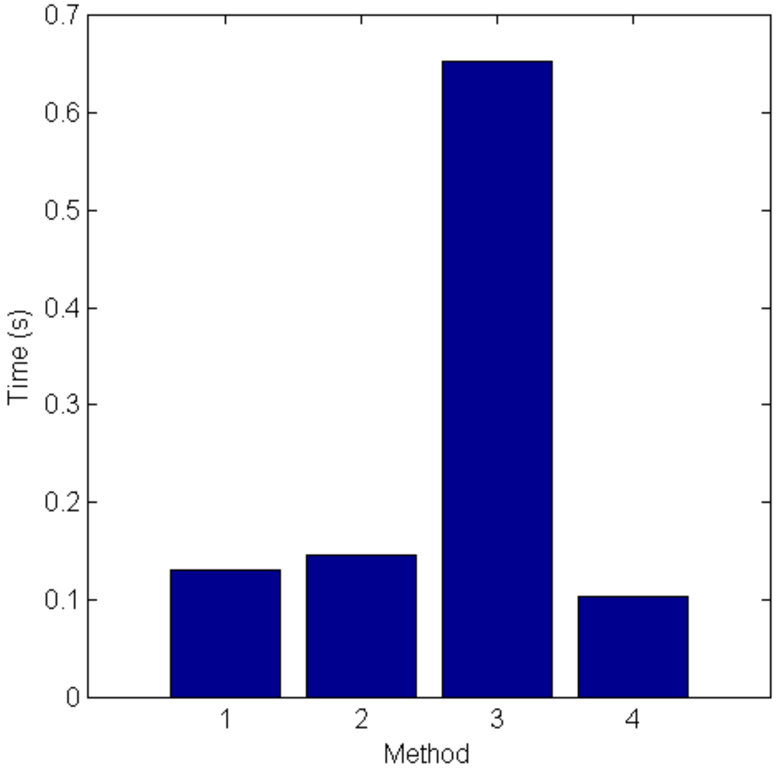
Weighted average prediction error of PF is on the order of ~8.5 seconds.





Times for methods SP

	Time (seconds)
PF solve all particles for data set and find time of EODV for each particle	1.24e-1
PF time to update weights 195 cycles	5.57e-3
UKF solve for 225 data update states until 50 data	1.46e-1
NLLS estimate states	5.25e-1
NLLS find RUL	1.29e-1
NLLS 5% constrained estimate states	4.47e-2
NLLS 5% constrained find RUL	5.80e-2



Conclusions

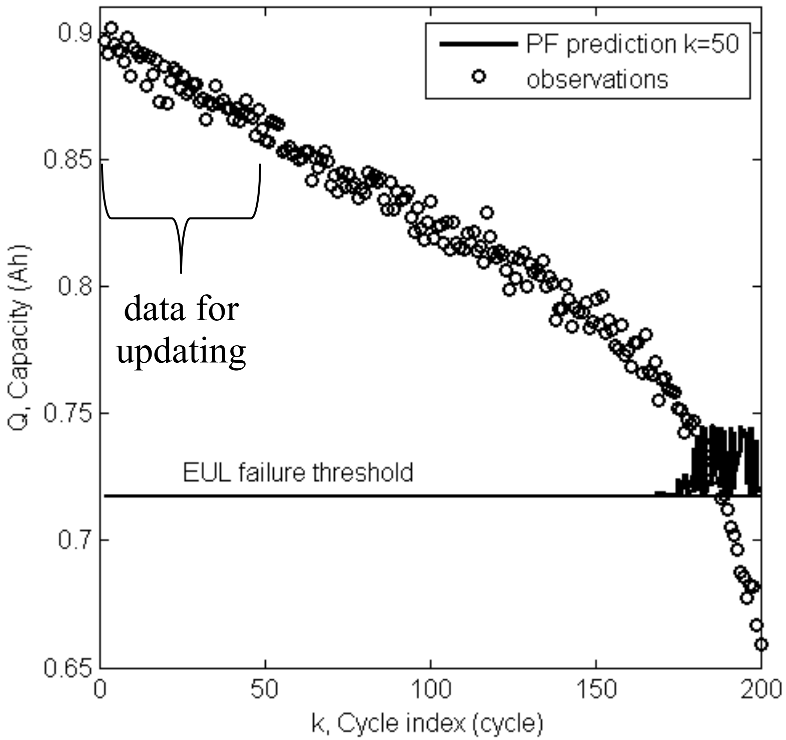
- **The particle filter is compared based on prediction error to NLLS and UKF, not performed in previous work.**
- **Three models are used for predictions.**
  - **He, et al's model predicts remaining useful life.**
  - **Equivalent circuit model predicts time until EODV.**
  - **Single particle model predicts time until EODV, not performed in previous work.**
- **PF makes the most accurate predictions regardless of model.**

Conclusions

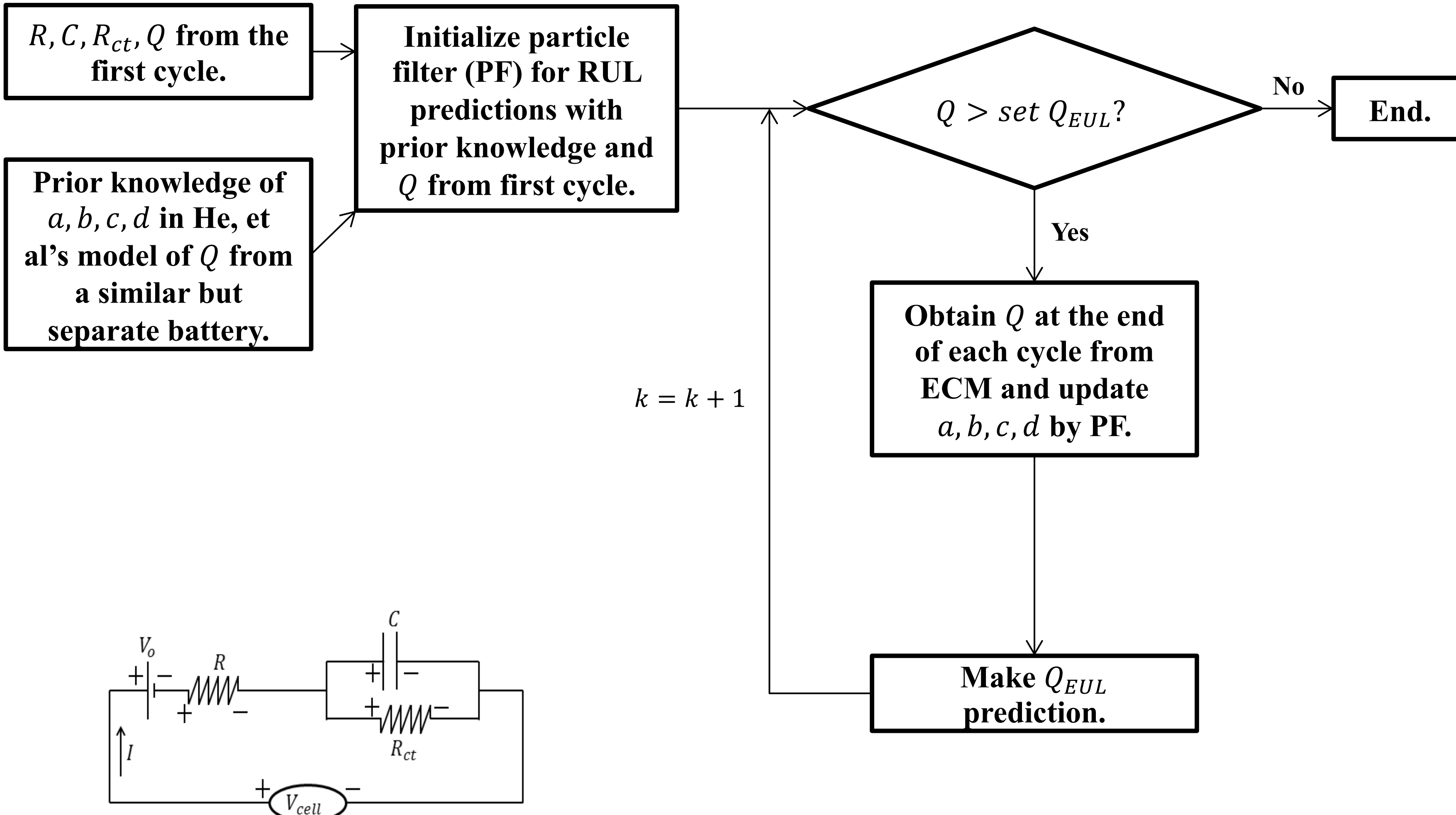
	He, et al	ECM	SP
NLLS	88 $(cycles)$	874 $(seconds)$	772 $(seconds)$
UKF	19 $(cycles)$	396 $(seconds)$	272 $(seconds)$
NLLS 5% constrained	10 $(cycles)$	212 $(seconds)$	127 $(seconds)$
PF (weighted average)	0.82 $(cycles)$	25.62 $(seconds)$	8.54 $(seconds)$

Future work

- Q has been used to make predictions amount remaining useful life.
- In future work, Q from an equivalent circuit model may be used to make predictions of remaining useful life.
- Likewise, S_n from a single particle model may be used to make predictions of remaining useful life.



Using equivalent circuit model for remaining useful life (RUL) predictions



Equivalent circuit

Using single particle (SP) model for RUL predictions

$x_{p,avg,0}$, $x_{n,avg,0}$, S_p, S_n from SP the first cycle.

Prior knowledge of a, b, c in polynomial model of S_n from a similar but separate battery.

Initialize particle filter (PF) for RUL predictions with prior knowledge and S_n from first cycle.

$S_n > set\ S_{n,EUL}$?

No

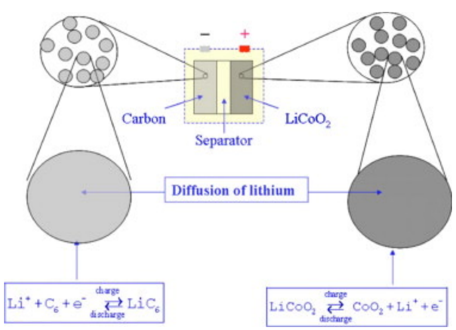
End.

Yes

Obtain S_n by SP and update a, b, c by PF.

Make $S_{n,EUL}$ prediction.

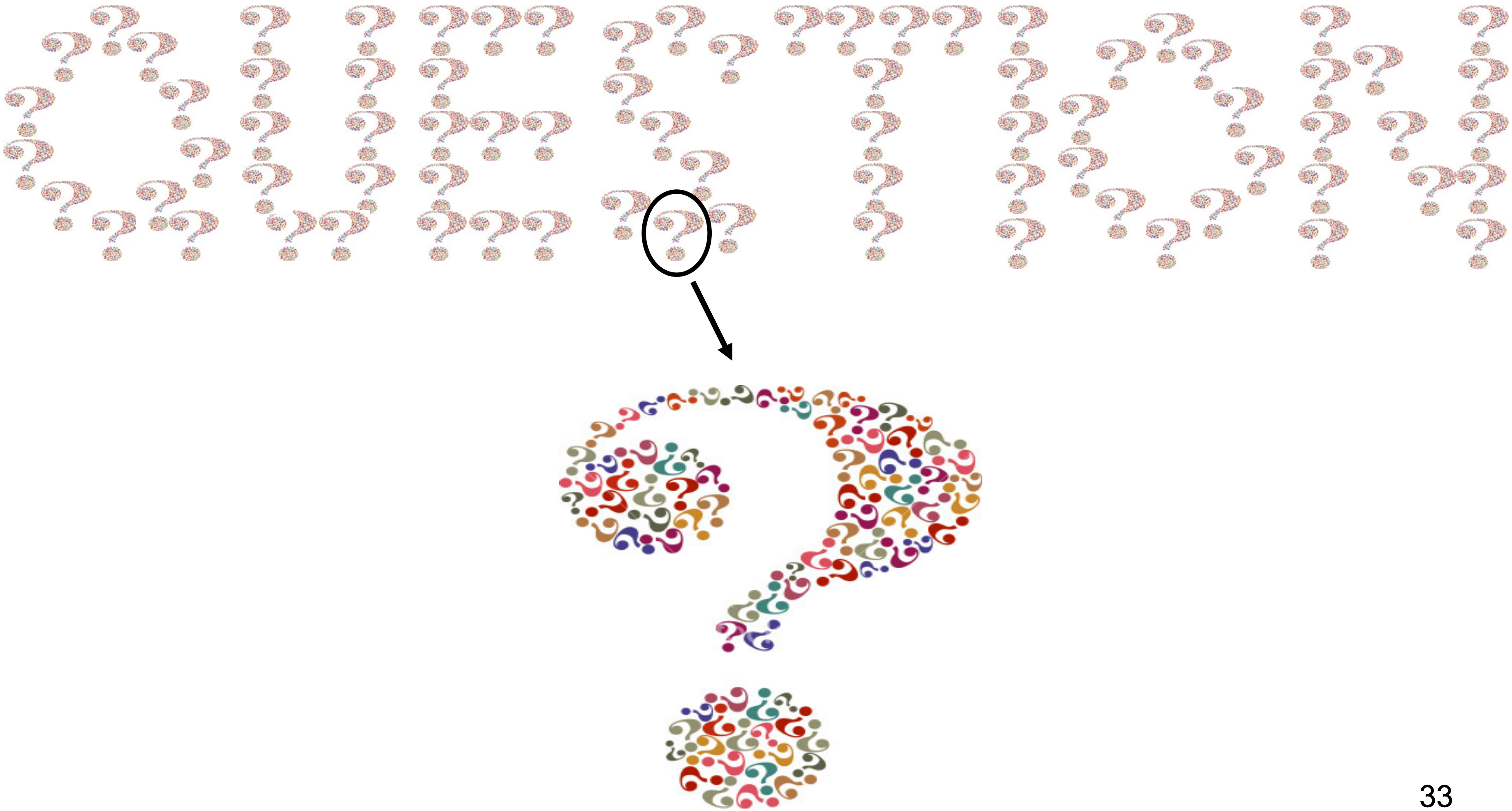
$k = k + 1$



S.K. Rahimian, S. Rayman, R.E. White, Journal of Power Sources 20 (2011) 8450-8462.

Acknowledgments

- **Advisor:** Dr. Ralph White
- **Committee:** Dr. Edward Gatzke, Dr. Sean Rayman, Dr. Gabriel Terejanu, Dr. John Weidner
- **Group Member:** Long, Meng, Yiling, Saeed
- **Friends**, roommate- Bryan, Elina
- **Parents**
- Presidential Fellows program, Toastmasters


QUESTION