State of Charge Estimation in Li-ion Batteries

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University of British Columbia
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Why Batteries?

- Portable
- No moving parts
- High power
- Environmentally friendly
  - no exhaust
  - quiet
  - no vibration
- High efficiency - of the order of 90% are more
- Low operating cost & minimal maintenance

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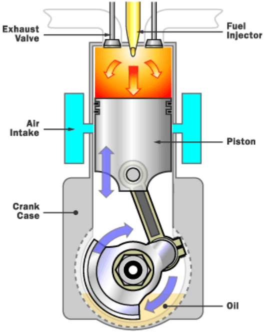

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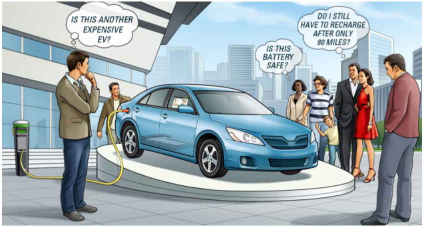
- High energy density
- Can provide high current
  - useful in high power tools
  - race cars
- Low maintenance
  - Minimal memory effect
  - Minimal self-discharge
- Environmentally friendly
  - no poisonous metals
  - little harm when disposed
- Aging
- Temperature has to be controlled
- Expensive to manufacture



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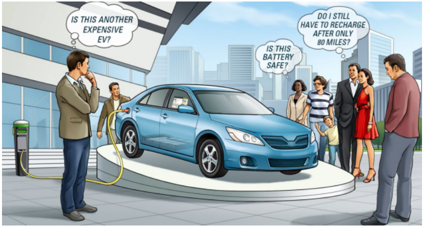

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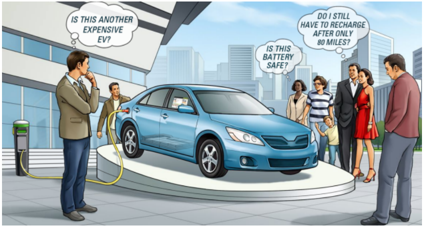

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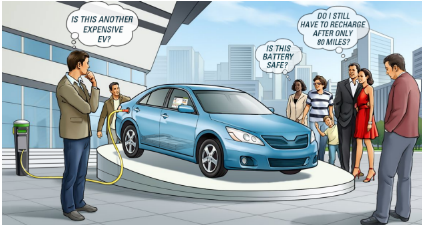

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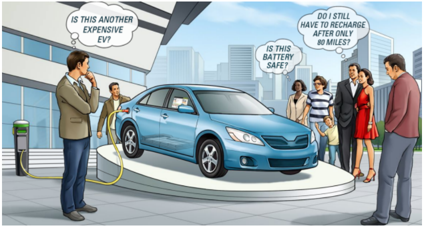

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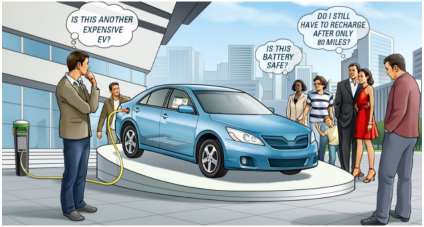

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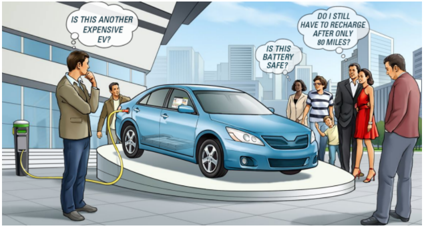
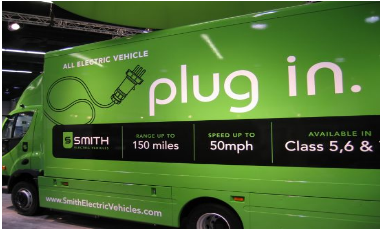


Li-ion Batteries: Challenges

- Predict battery life under diverse operating conditions

High C rate

Low C Rate



Cold weather

Hot weather

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New York Times Tesla S model test drive
"Stalled Out on Tesla's Electric Highway", NYT Feb 8, 2013

Quote by New York Times Reporter John Broder

As I crossed into New Jersey some 15 miles later, I noticed that the estimated range was falling faster than miles were accumulating. At 68 miles since recharging, the range had dropped by 85 miles, and a little mental math told me that reaching Milford would be a stretch.

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I discovered on a recent test drive of the company's high-performance Model S sedan, theory can be trumped by reality, especially when Northeast temperatures plunge.

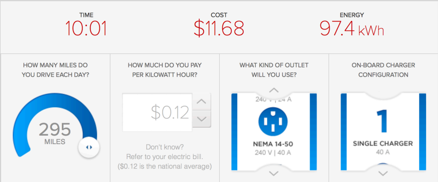
Li-ion Batteries: Challenges

- Ensure safe operation
  - Danger of explosion at high C rates or at high temperatures

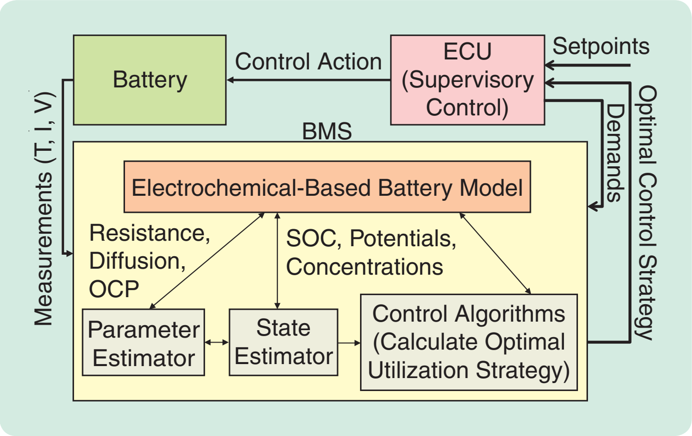
Laptop

Boeing dreamliner

- Fast charging



Battery Management System

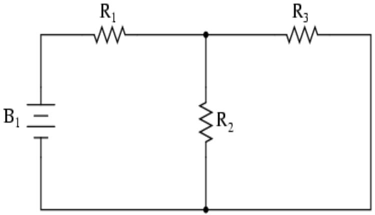


(Source: Chaturvedi et al, IEEE CSM, June 2010)

- Good mathematical models needed to meet these challenges
  - Physical models are complex
  - Limited data

Li-on Battery Models

- Electrical Circuit Models
- Single Particle Model
- Porous Electrode Pseudo Two Dimensional Model (P2D)
- 3D Thermal Model
- P2D Stress-Strain Model
- Population Balance Model
- Molecular Dynamics



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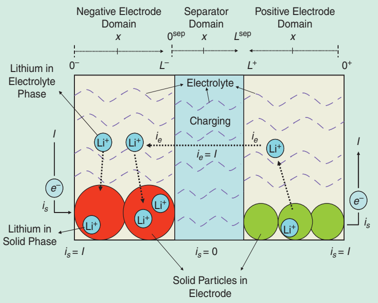

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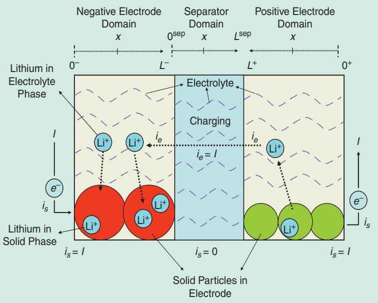

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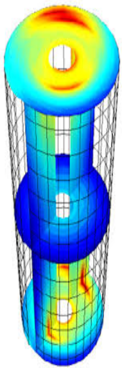

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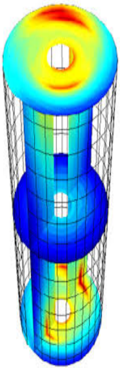

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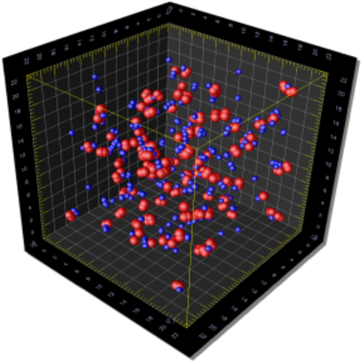

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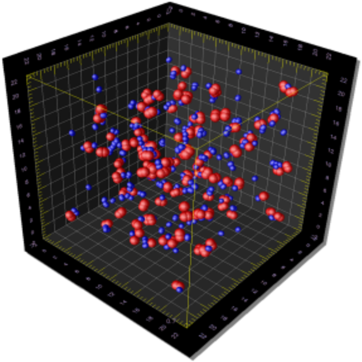

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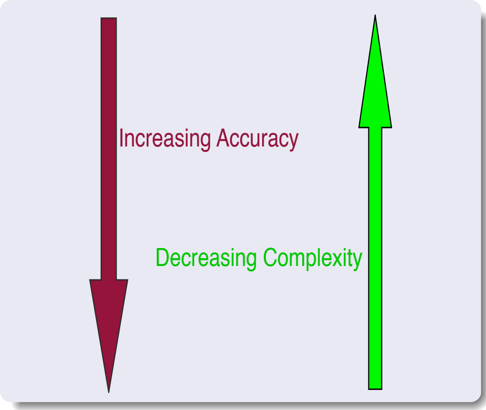

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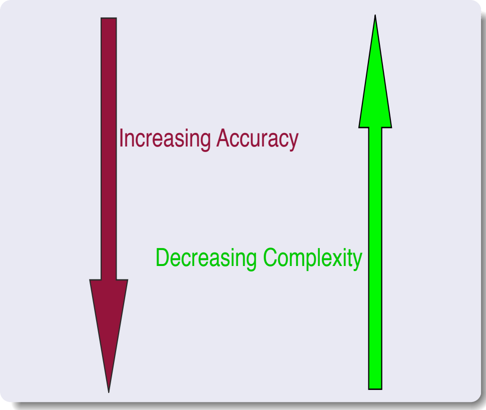

Pseudo 2D Model

Mass Conservation

(M1) $\epsilon_i \dfrac{\partial c_e}{\partial t} = \dfrac{\partial}{\partial x}\left(D_i \dfrac{\partial c_e}{\partial x}\right) + a_i(1-t_+)j_i$

(M2) $\dfrac{\partial \bar{c}_s}{\partial t} = -3\dfrac{j_i}{R_i}$

(M3) $c_s^* - \bar{c}_s = -\dfrac{R_i}{D_s}\dfrac{j_i}{5}$

Charge Conservation

(C1) $i_e = -\kappa_i \dfrac{\partial \Phi_e}{\partial x} + \dfrac{2\kappa_i RT}{F}(1-t_+)\dfrac{\partial \ln c_e}{\partial x}$

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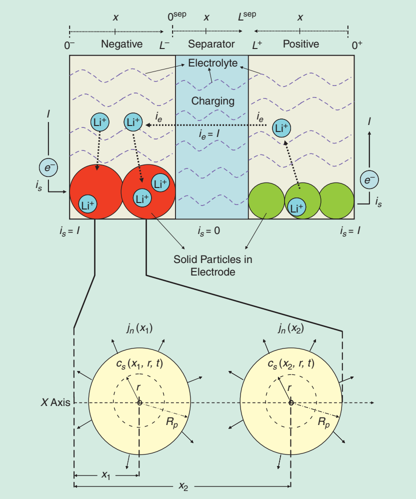

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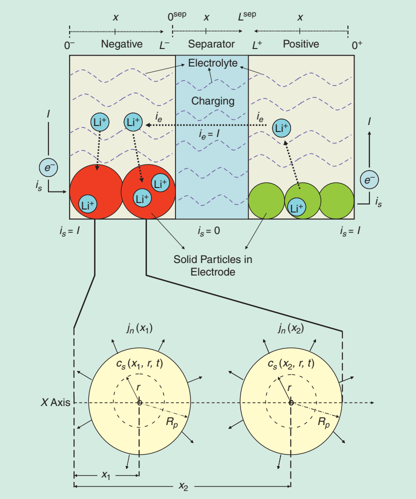

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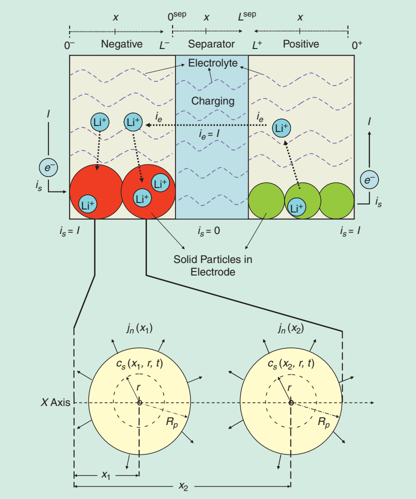

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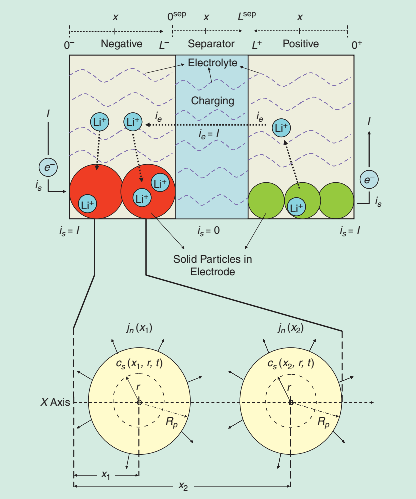

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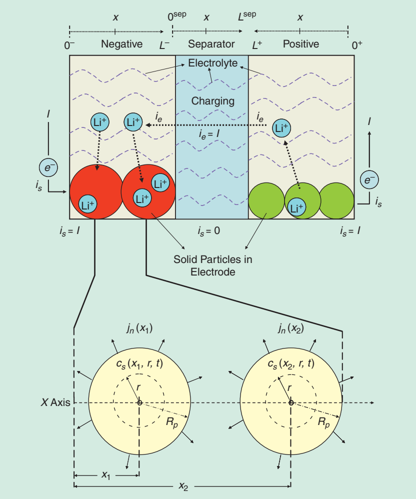

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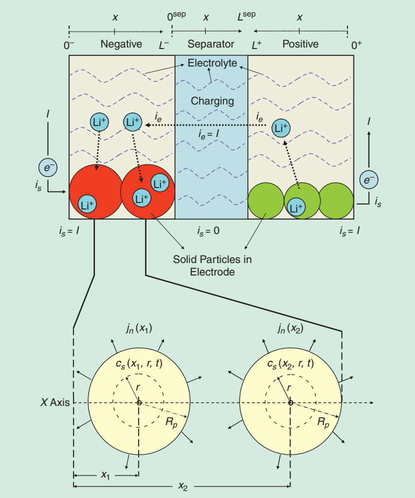

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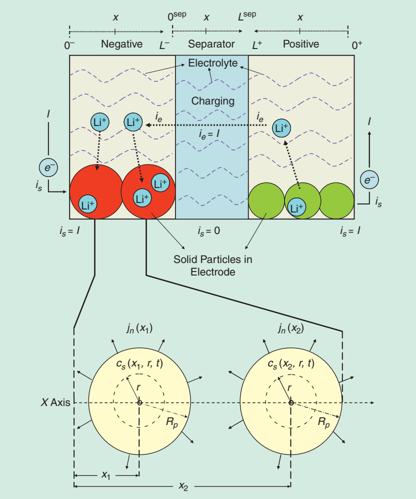

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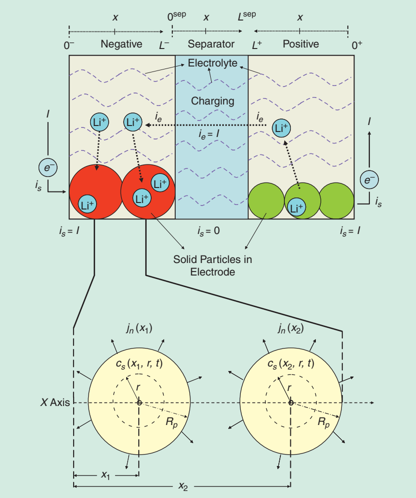

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Boundary Conditions

$\mathbf{x}$ = col.	$\mathbf{x}$ = sep./elec.
$\Rightarrow \frac{\partial c_e}{\partial x} = 0$	$-D_p \frac{\partial c_e}{\partial x} = -D_s \frac{\partial c_e}{\partial x}$
–	–
–	–

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$\Rightarrow i_e = 0$	$i_e = I$
–	–

Thermal Model

Energy Conservation: BCs - $\mathbf{x} = \text{col.}$ $\mathbf{x} = \text{sep./elec.}$

$$\rho_i C_{p,i} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda_i \frac{\partial T}{\partial x}\right) + Q_i \qquad \frac{\partial T}{\partial x} = 0 \qquad -\lambda_{cc}\frac{\partial T}{\partial x} = -\lambda_p \frac{\partial T}{\partial x}$$

Butler-Volmer Equation

$$j_i = 2k_i \left[c_e c_s^* (c_i^{max} - c_s^*)\right]^{0.5} \sinh\left(\frac{0.5}{F} RT(\Phi_s - \Phi_e - U_i)\right)$$

Challenges with the Model

- Including the electrodes, separator and collectors there are 19 PDEs.
- PDEs are highly coupled.
- Diffusion, reaction coefficients and other parameters are temperature dependent.
- The PDEs are stiff.

Thermal Model

Energy Conservation: BCs - $\mathbf{x}$ = col. $\mathbf{x}$ = sep./elec.

$$\rho_i C_{p,i} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda_i \frac{\partial T}{\partial x}\right) + Q_i \qquad \frac{\partial T}{\partial x} = 0 \qquad -\lambda_{cc}\frac{\partial T}{\partial x} = -\lambda_p \frac{\partial T}{\partial x}$$

Butler-Volmer Equation

$$j_i = 2k_i\left[c_e c_s^*(c_i^{max} - c_s^*)\right]^{0.5} \sinh\left(\frac{0.5}{F} RT(\Phi_s - \Phi_e - U_i)\right)$$

Challenges with the Model

- Including the electrodes, separator and collectors there are 19 PDEs.
- PDEs are highly coupled.
- Diffusion, reaction coefficients and other parameters are temperature dependent.
- The PDEs are stiff.

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Challenges with the Model

- Some PDEs don't have explicit boundary conditions.
- Model initialization is difficult.
- Stable in a narrow operating region.
- The model has to be solved within a few seconds for real time implementation.

An iterative fast solution

Observations

- Model is linear if flux j_i is known - Guess it!
- The PDE for current in the electrolyte has two boundary conditions

$$\boxed{\frac{\partial i_e}{\partial x} = a_i F j_i}$$

Guess the initial value and iterate using a shooting method.

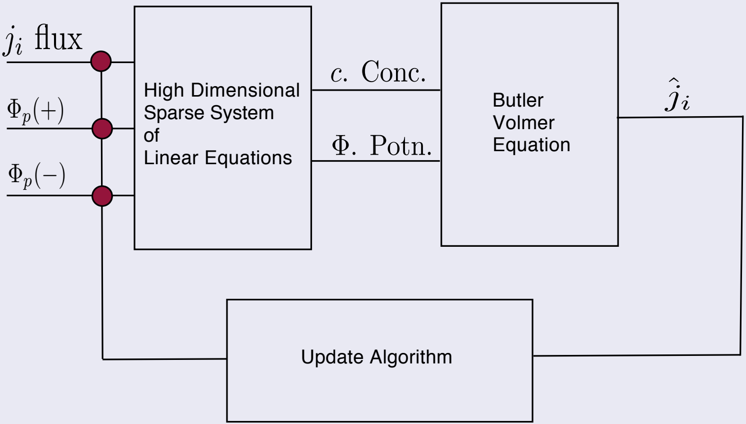
- The PDE for solid potential has no boundary conditions

$$\boxed{\frac{\partial \Phi_s}{\partial x} = \frac{i_e - I}{\sigma_i}}$$

Guess a boundary condition.

An iterative fast solution

The Algorithm



A state-space reformulation

Advantages

- The system is expressed as a "standard" state-space model.
- Simulating a discharge cycle of 1 hr takes about $2 \sim 15$ sec.

State-Space Model

$$\mathbf{x_m^{\ell}} = \begin{bmatrix} \mathbf{A_c}(\boldsymbol{\theta}) & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \mathbf{x_{m-1}^{\ell}} + \begin{bmatrix} \mathbf{B_c}(\boldsymbol{\theta}) \\ \bar{\mathbf{B}}(\boldsymbol{\theta}) \end{bmatrix} \otimes \mathbf{x_m^n},$$

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$$v(m) = \Phi_p(m, 0) - \Phi_p(m, N_n).$$ Measurements

Uncertainty Characterization

Types of Uncertainty

- Parametric uncertainty

$$p_{\boldsymbol{\theta}}(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}; \boldsymbol{\theta}, \Sigma_{\boldsymbol{\theta}})$$

- Structural uncertainty

$$\begin{aligned}
\mathbf{X}_{\mathbf{m}}^{\boldsymbol{\ell}} | \mathbf{x}_{\mathbf{m}}^{\boldsymbol{\ell}}(\boldsymbol{\theta}) &\sim \mathcal{N}(\mathbf{0}, \Sigma_\ell) \\
\mathbf{X}_{\mathbf{m}}^{\mathbf{a_i}} | \mathbf{x}_{\mathbf{m}}^{\mathbf{a_i}}(\boldsymbol{\theta}) &\sim \mathcal{N}(\mathbf{0}, \Sigma_i) \quad \text{for } i = 1 \text{ to } 3 \\
\mathbf{X}_{\mathbf{m}}^{\mathbf{n}} | \mathbf{x}_{\mathbf{m}}^{\mathbf{n}}(\boldsymbol{\theta}) &\sim \mathcal{N}(\mathbf{0}, \Sigma_n), \\
\mathbf{X}_{\mathbf{m}}^{\mathbf{T}} | \mathbf{x}_{\mathbf{m}}^{\mathbf{T}}(\boldsymbol{\theta}) &\sim \mathcal{N}(\mathbf{0}, \Sigma_T), \\
V_m | v_{m-1} &\sim \mathcal{N}(\mathbf{0}, \Sigma_v)
\end{aligned}$$

- Not necessary to assume Gaussian uncertainty - any probabilistic uncertainty fine.

Important Properties of Li-ion Battery

State of Charge (SOC)

A quantitative measure of expendable charge remaining in the battery.

$$\mathcal{S}(t) = \frac{1}{l_p} \int_0^{l_p} \frac{\bar{c}_s(x,t)}{c_{max}} dx$$

$$\mathbb{E}\left[\mathcal{S}(m)\right] \approx \frac{\Delta x}{l_p c_{max}} \sum_{n=1}^{N_p} \int \bar{c}_s(m,n) p_{\bar{c}_s}(\bar{c}_s(m,n)|v_{1:m}) dc_s.$$

State of Health (SOH)

A quantitative measure of the battery's ability to store and release energy at high efficiency. No unique measure.

Challenge

How do we estimate State of Charge in presence of uncertainty?

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State Estimator!

What is wrong with Standard Particle Filter?

High-Dimensionality and Particle Degeneracy

- The desired target density function is very high-dimensional. Defining the state vector

$$\mathbf{x_m} = \{\mathbf{x_m^\ell}, \mathbf{x_m^{a_1}}, \mathbf{x_m^{a_2}}, \mathbf{x_m^{a_3}}, \mathbf{x_m^{n}}, \mathbf{x_m^{T}}\}$$

  Target density function is $p_{x_m}(\mathbf{x_m}|v_{1:m})$. For N discretization points in the spatial direction, the dimensionality is $7N$.

Computational Complexity

- The model equations have to be solved as many times as the number of particles increasing the computational complexity.

Importance Density

- It is difficult to choose a large dimensional importance density function.

Marginalized and Tethered Particle Filter

Marginalized Particle Filter

- For SOC estimation, only the lower dimensional marginal density $p_{\bar{c}_c}(\bar{c}_s(m,n)|v_{1:m})$ is required.
- Dimensionality can be reduced by partitioning the states and splitting the filter density into a series of marginal density functions,

$$p_{x_m}(\mathbf{x_m}|v_{1:m}) = p_{x_m^\ell}(\mathbf{x_m^\ell}|v_{1:m},\mathbf{x_m^n})p_{x_m^{a_1}}(\mathbf{x_m^{a_1}}|v_{1:m},\mathbf{x_m^n})p_{x_m^{a_2}}(\mathbf{x_m^{a_2}}|v_{1:m},\mathbf{x_m^\ell},\mathbf{x_m^n}) \times p_{x_m^{a_3}}(\mathbf{x_m^{a_3}}|v_{1:m},\mathbf{x_m^\ell},\mathbf{x_m^n})p_{x_m^n}(\mathbf{x_m^n}|v_{1:m}).$$

- Some density functions corresponding to PDEs with spatial derivatives only can be further marginalized.

Tethered Particle Filter

- Kalman filter can be used if $\mathbf{x_m^n}$ is "known".
- A 'tether particle' is created by using the average of $\mathbf{x_m^n}$ particles in estimating other marginalized densities.

Marginalized and Tethered Particle Filter

Optimal Estimators

Density	Optimal Marginal Estimator	Dimension	
		Full	Marginal
(1) $p_{x_m^\ell}(\mathbf{x_m^\ell} \mid v_{1:m}, \mathbf{x_m^n})$	Temporal & Spatial Kalman filter	$2N$	2
(2) $p_{x_m^{a_1}}(\mathbf{x_m^{a_1}} \mid v_{1:m}, \mathbf{x_m^n})$	Spatial Kalman filter	$2N$	2
(3) $p_{x_m^{a_2}}(\mathbf{x_m^{a_2}} \mid v_{1:m}, \mathbf{x_m^\ell}, \mathbf{x_m^n})$	Spatial Kalman filter	N	1
(4) $p_{x_m^{a_3}}(\mathbf{x_m^{a_3}} \mid v_{1:m}, \mathbf{x_m^\ell}, \mathbf{x_m^n})$	Spatial Particle Filter	N	1
(5) $p_{x_m^n}(\mathbf{x_m^n} \mid v_{1:m})$	Spatial Particle Filter	N	1

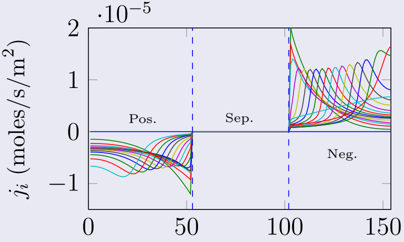
Some Observations

- Kalman filters can be implemented online very fast.
- One dimensional particle filters are also very fast.
- The marginal filter dimension is independent of fineness of discretization.

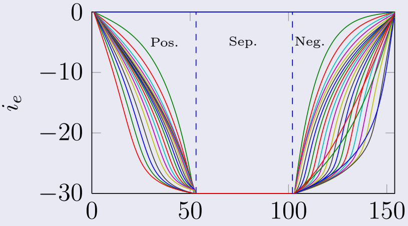
State of Charge Estimation - Simulations

Deterministic Model

- Model simulated at constant galvanostatic discharge current of $I = -30A/m^2$.
- Initial guesses for the solid potential at the collectors are 4.116 V and 0.074 V.
- Initial electrolyte concentration was 1000 mol/L.



(a) Flux



(b) Electrolyte current

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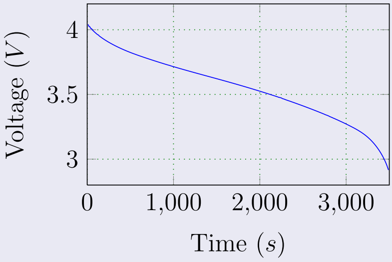
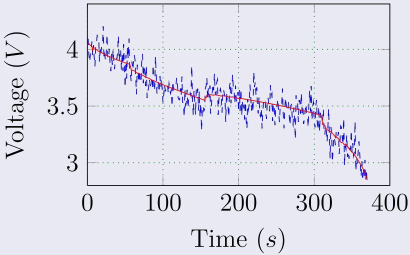


(a) Deterministic simulation.

State of Charge Estimation - Simulations

Stochastic Model

- Gaussian noise introduced in all the state equations.
- Applied current randomly switched between $-35A/m^2$ and $-25A/m^2$ (RBS).
- 2000 particles used.



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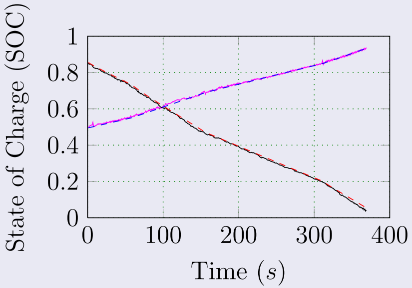
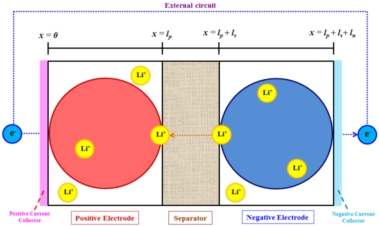


Acknowledgements

Prof. Richard Braatz
Yiting Tsai

www.apple.com;www.studyvilla.com;www.gettyimages.com;randomwire.com; savagechickens.com;green.autoblog.com;commons.wikimedia.org;www.ecofriend.com; www.motherearthnews.com;w7swall.com;www.techatplay.com;www.geek.com; www.jalopnik.com;Chaturvedi et al IEEE CSM June 2010; www.urel.gov;

Single Particle (SPM) Model



Cell Compartments:

- Positive Electrode (p)
- Separator (s)
- Negative Electrode (n)

Phases:

- Solid (s)
- Electrolyte (e)

State Variables:

- Voltage (V)
- Current (I)
- Li^+ Ion Concentration (C)
- State Of Charge (SOC)

Coordinate variables:

- Time (t)
- Radius (r)

Characteristics of SPM:

1. Assume spatial variations negligible
2. PDEs reduced to ODEs
3. Position coordinates (x),(y),(z) eliminated
4. State variables change only w.r.t (r),(t)

Single-Particle Model (SPM) in Detail

Approximate Potentials

$$\Phi_s(t) = \frac{2RT}{F} sinh^{-1}\left(\frac{I(t)}{2al\sqrt{(c_e c^*(t)(c_{max} - c^*))}}\right)$$

Fickian Mass Diffusion of Li$^+$

$$\frac{\partial}{\partial t} c_s(x, r, t) = \frac{1}{r^2} \frac{\partial}{\partial r} (D_s r^2 \frac{\partial}{\partial r} c_s(x, r, t))$$

Molar Flux of Li$^+$

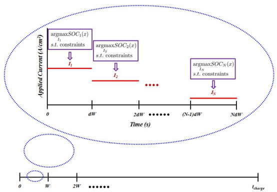
$$j_p = -\frac{I}{F a_p l_p} \qquad j^n = -\frac{I}{F a_n l_n}$$

Voltage

$$v = \Phi_p - \Phi_n$$

Algorithm for Optimal Charging

Moving Window Approach



Battery Properties:

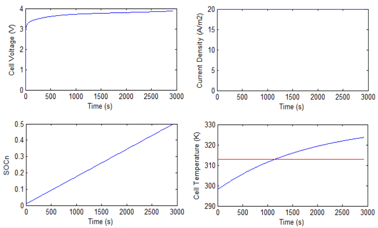
- Cell Temperature: $[T_p, T_n]^T$
- Li^+ Concentration: $[C_p, C_n]^T$
- State of Charge: $[SOC_p, SOC_n]^T$

Moving Horizon Approach:

- Total charge time $= t_{total}$
- Divide t_{total} into Windows W
- Divide W into N sub-windows: $dW = \frac{W}{N}$
- Time axis: $[0, dW, 2dW, \cdots, NdW]$
- Charge current profile: $[I_1, I_2, \cdots, I_N]$

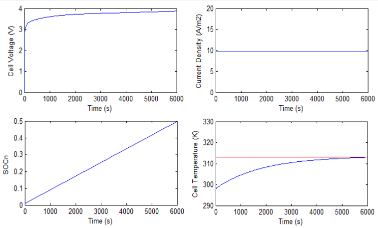
Results and Analyses

Case 1: Charging with No Constraints



- Charge at $I_{max} = 20\frac{A}{cm^2}$
- No constraints considered
- Full charge reached at 3000s
- Temp constraint violated at 1000s

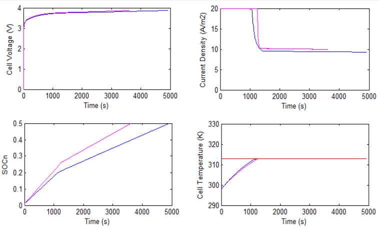
Case 2: Static Optimization



- Solve: $\underset{I}{\text{argmax}} SOC(x)$ s.t. constraints are satisfied
- Obtain $I_{opt} = 9.7\frac{A}{cm^2}$
- Full charge reached at 6000s
- Temp constraint respected

Results and Analyses Cont'd

Case 3: Moving Horizon Approach



- Window size: $W = 100s$ and $dW = 10s$
- $I_{opt} = 20\frac{A}{cm^2}$ for 1000s, drop to $I_{opt} = 9.3\frac{A}{cm^2}$ and hold.
- Total charge time reduced to 5000s.
- Reduce window size to $W = 20s$ and $dW = 2s$: reduce total charge time to 3600s.

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www.apple.com;www.studyvilla.com;www.gettyimages.com;randomwire.com; savagechickens.com;green.autoblog.com;commons.wikimedia.org;www.ecofriend.com; www.motherearthnews.com;w7swall.com;www.techatplay.com;www.geek.com; www.jalopnik.com;Chaturvedi et al IEEE CSM June 2010; www.urel.gov;