Sensitivity-Based Interval PDE Observer for Battery SOC Estimation

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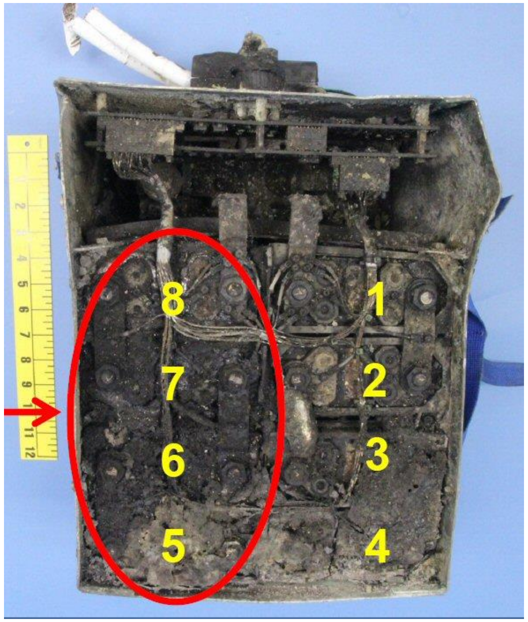
Agenda

- Motivation
- Lithium Ion Battery Operation
- Single Particle Model
- Reduced Single Particle Model
- Backstepping PDE Observer
- PDE Observer Sensitivity Analysis
- Sensitivity Based Interval PDE Observer
- Results
- Conclusion

Motivation

- Need for renewable energy systems adoption is apparent
- Electric vehicle sales rising (596k sold in 2013 (US))
- Smart phones everywhere (5.2B around the globe)
- Need cost effective, high energy/power/life batteries
- Can make better batteries or get more out of current batteries



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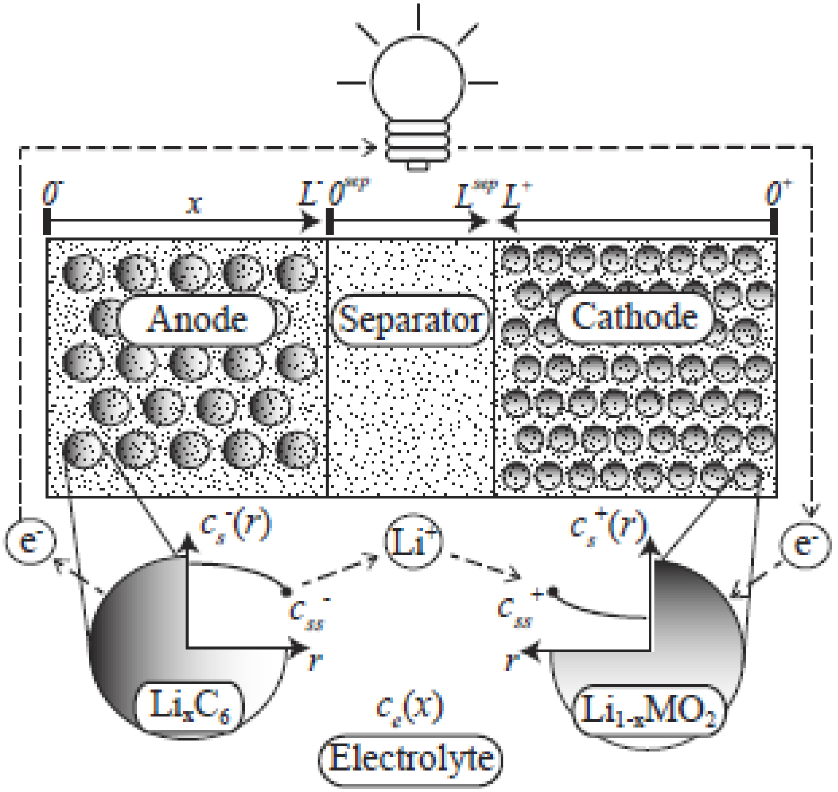
Lithium Ion Battery Operation

- Discharge:
  - Lithium ions flow internally from anode to cathode
  - Electrons flow externally from anode to cathode
  - Current flows externally from cathode to anode



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Electrochemical Single Particle Model

Diffusion of Li in Solid Phase (Anode/Cathode):

$$\frac{\partial c_s^-}{\partial t}(r,t) = D_s^- \left[\frac{2}{r}\frac{\partial c_s^-}{\partial r}(r,t) + \frac{\partial^2 c_s^-}{\partial r^2}(r,t)\right]$$

$$\frac{\partial c_s^+}{\partial t}(r,t) = D_s^+ \left[\frac{2}{r}\frac{\partial c_s^+}{\partial r}(r,t) + \frac{\partial^2 c_s^+}{\partial r^2}(r,t)\right]$$

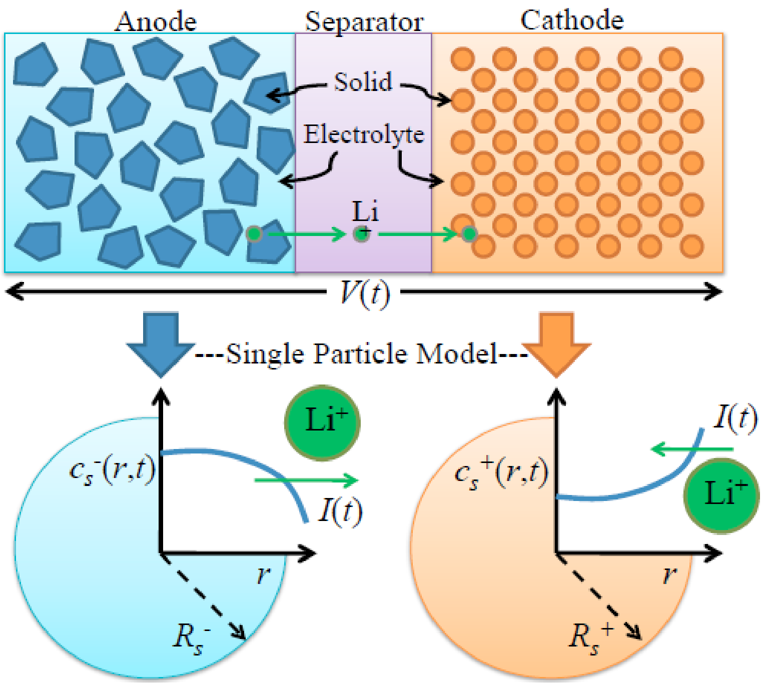
Boundary Conditions:

$$\frac{\partial c_s^-}{\partial r}(0,t) = 0, \quad \frac{\partial c_s^-}{\partial r}(R_s^-,t) = \frac{I(t)}{D_s^- F a^- A L^-},$$

$$\frac{\partial c_s^+}{\partial r}(0,t) = 0, \quad \frac{\partial c_s^+}{\partial r}(R_s^+,t) = -\frac{I(t)}{D_s^+ F a^+ A L^+}$$

Output Voltage:

$$V(t) = \frac{RT}{\alpha F}\sinh^{-1}\left(\frac{I(t)}{2a^+AL^+i_0^+(c_{ss}^+(t))}\right) - \frac{RT}{\alpha F}\sinh^{-1}\left(\frac{I(t)}{2a^-AL^-i_0^-(c_{ss}^-(t))}\right) + U^+(c_{ss}^+(t)) - U^-(c_{ss}^-(t)) + R_f I(t)$$



State of Charge (Bulk Anode):

$$SOC(t) = \frac{3}{c_{s,max}^-}\int_0^{R_s^-} r^2 c_s^-(r,t)\,dr$$

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Reduced Single Particle Model

- Model Simplification:
  - Achieve Model Observability
    - Approximate Cathode Diffusion by Equilibrium
  - Normalize in Space and Time
  - State Transformation

Reduced Single Particle Model

Space and Time Normalization:

$$\bar{r} = \frac{r}{R_s^-}, \qquad \bar{t} = \frac{D_s^-}{(R_s^-)^2} t.$$

State Transformation:

$$c(r,t) = r c_s^-(r,t)$$

Diffusion of Li in Solid Phase (Reduced):

$$\frac{\partial c}{\partial t}(r,t) = \varepsilon \frac{\partial^2 c}{\partial r^2}(r,t)$$

Boundary Conditions:

$$c(0,t) = 0$$

$$\frac{\partial c}{\partial r}(1,t) - c(1,t) = -q\rho I(t)$$

Where:

$$\rho = R_s^- / (D_s^- F a^- A L^-)$$

Output Voltage:

$$\begin{aligned} V(t) = {} & \frac{RT}{\alpha^+ F} \sinh^{-1}\left(\frac{I(t)}{2a^+ A L^+ i_0^+ (\alpha c_{ss}^-(t) + \beta)}\right) \\ & - \frac{RT}{\alpha^- F} \sinh^{-1}\left(\frac{I(t)}{2a^- A L^- i_0^- (c_{ss}^-(t))}\right) \\ & + U^+(\alpha c_{ss}^-(t) + \beta) - U^-(c_{ss}^-(t)) - R_f I(t) \end{aligned}$$

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Backstepping PDE Observer

Nominal State Estimator plus Boundary State Error Injection:

$$\frac{\partial \hat{c}}{\partial t}(r,t) = \varepsilon_0 \frac{\partial^2 \hat{c}}{\partial r^2}(r,t) + p_1(r)\left[\gamma_0 \varphi(V(t),I(t)) - \hat{c}(1,t)\right]$$

Initial Condition and Boundary Conditions:

$$\hat{c}(r,0) = \hat{c}_0(r)$$

$$\hat{c}(0,t) = 0$$

$$\frac{\partial \hat{c}}{\partial r}(1,t) - \hat{c}(1,t) = -q_0 \rho I(t) + p_{10}\left[\gamma_0 \varphi(V(t),I(t)) - \hat{c}(1,t)\right]$$

Observer Gains:

$$p_1(r) = \frac{-\lambda r}{2x}\left[I_1(x) - \frac{2\lambda}{x} I_2(x)\right], \text{where} \quad x = \sqrt{\lambda(r^2-1)}, \quad p_{10} = \frac{3-\lambda}{x} \quad \text{where} \quad x = \sqrt{\lambda(r^2-1)}.$$

Nominal Parameters:

$$\theta_0 = [\varepsilon_0, q_0, \gamma_0]^T = [1,1,1]^T$$

Output Function Inversion:

$$c_{ss}^{-}(t) = \varphi(V(t),I(t))$$

Nominal Solution:

$$\hat{c}(r,t;\theta_0)$$

Wish to study variations in nominal solution via Sensitivity Analysis

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PDE Observer Sensitivity Analysis

PDE Observer in Partio-Integro Differential Equation (PIDE) Form:

$$\hat{c}(r,t) \quad = \quad \hat{c}_0(r) + \int_{t_0}^{t} [\varepsilon \hat{c}_{rr}(r,s;\theta) + p_1(r)(\gamma\varphi(V(t),I(t)) - \hat{c}(1,s;\theta))]ds.$$

Boundary Conditions and Initial Condition:

$$\hat{c}(r,t_0) \quad = \quad \hat{c}_0(r)$$

$$\hat{c}(0,t) \quad = \quad 0$$

$$\hat{c}_r(1,t) - \hat{c}(1,t) \quad = \quad -q\rho I(t) + p_{10}[\gamma\varphi(V(t),I(t)) - \hat{c}(1,t)]$$

Where:

$$\hat{c}_{rr} = \partial^2 \hat{c} / \partial r^2$$

PDE Observer Sensitivity Analysis

Take Partial Derivative wrt. ε on both sides:

$$\frac{\partial \hat{c}}{\partial \varepsilon}(r,t) = \int_{t_0}^{t} [\varepsilon \frac{\partial \hat{c}_{rr}}{\partial \varepsilon}(r,s;\theta) + \hat{c}_{rr}(r,s;\theta) - p_1(r)\frac{\partial \hat{c}}{\partial \varepsilon}(1,s;\theta)]ds$$

Initial Condition and Boundary Conditions:

$$\frac{\partial \hat{c}}{\partial \varepsilon}(r,t_0) = \frac{\partial \hat{c}}{\partial \varepsilon}(0,t) = 0$$

$$\frac{\partial \hat{c}_r}{\partial \varepsilon}(1,t) - \frac{\partial \hat{c}}{\partial \varepsilon}(1,t) = -p_{10}\frac{\partial \hat{c}}{\partial \varepsilon}$$

Where:

$$\hat{c}_r = \partial \hat{c}/\partial r$$

PDE Observer Sensitivity Analysis

Let:

$$\hat{c}_\varepsilon = \partial \hat{c} / \partial \varepsilon$$

Change Order of Differentiation on RHS (first term):

$$\hat{c}_\varepsilon(r,t) = \int_{t_0}^{t} [\varepsilon \frac{\partial^2 \hat{c}_\varepsilon}{\partial r^2}(r,s;\theta) + \hat{c}_{rr}(r,s;\theta) - p_1(r)\hat{c}_\varepsilon(1,s;\theta)] ds$$

Initial Condition and Boundary Conditions:

$$\hat{c}_\varepsilon(r,t_0) \quad = \quad \hat{c}_\varepsilon(0,t) = 0$$

$$\frac{\partial \hat{c}_\varepsilon}{\partial r}(1,t) - \hat{c}_\varepsilon(1,t) \quad = \quad -p_{10}\hat{c}_\varepsilon(1,t)$$

PDE Observer Sensitivity Analysis

Differentiate wrt. Time:

$$\frac{\partial}{\partial t} c_{\varepsilon}(r,t) = \varepsilon \frac{\partial^2}{\partial r^2} \hat{c}_{\varepsilon}(r,t;\theta) + \hat{c}_{rr}(r,t;\theta) - p_1(r)\hat{c}_{\varepsilon}(1,t;\theta)$$

Initial Condition and Boundary Conditions:

$$\hat{c}_{\varepsilon}(r,t_0) = \hat{c}_{\varepsilon}(0,t) = 0$$

$$\frac{\partial \hat{c}_{\varepsilon}}{\partial r}(1,t) - \hat{c}_{\varepsilon}(1,t) = -p_{10}\hat{c}_{\varepsilon}(1,t)$$

Solution:

$$\hat{c}_{\varepsilon}(r,t)$$

PDE Observer Sensitivity Analysis

When:

$$\theta = \theta_0$$

Then RHS depends only on nominal solution:

$$\hat{c}(r,t;\theta_0)$$

Define the Sensitivity Function as:

$$S_1(r,t) = \hat{c}_\varepsilon(r,t;\theta_0)$$

The Sensitivity PDE is:

$$S_{1_t}(r,t) = \varepsilon_0 S_{1_{rr}}(r,t;\theta_0) + \hat{c}_{rr}(r,t;\theta_0) - p_1(r) S_1(1,t;\theta_0)$$

Initial Condition and Boundary Conditions:

$$S_1(r,t_0) = S_1(0,t) = 0$$

$$S_{1_r}(1,t) - S_1(1,t) = -p_{10} S_1(1,t)$$

PDE Observer Sensitivity Analysis

Similarly, define the next Sensitivity Function as:

$$S_2(r,t) = \hat{c}_q(r,t;\theta_0)$$

The Sensitivity PDE is:

$$S_{2_t}(r,t) = \varepsilon_0 S_{2_{rr}}(r,t;\theta_0) + p_1(r) S_2(1,t)$$

Initial Condition and Boundary Conditions:

$$S_2(r,t_0) = S_2(0,t) = 0$$

$$S_{2_r}(1,t) - S_2(1,t) = -\rho I(t) - p_{10} S_2(1,t).$$

PDE Observer Sensitivity Analysis

Similarly, define the next Sensitivity Function as:

$$S_3(r,t) = \hat{c}_\gamma(r,t;\theta_0)$$

The Sensitivity PDE is:

$$S_{3_t}(r,t) = \varepsilon_0 S_{3_{rr}}(r,t;\theta_0) + p_1(r)\varphi(V(t),I(t)) - p_1(r)S_3(1,t)$$

Initial Condition and Boundary Conditions:

$$S_3(r,t_0) = S_3(0,t) = 0$$

$$S_{3_r}(1,t) - S_3(1,t) = p_{10}\varphi(V(t),I(t)) - p_{10}S_3(1,t)$$

PDE Observer Sensitivity Analysis

Note that:

$$S_1(r,t) = \hat{c}_\varepsilon(r,t;\theta_0)$$

$$S_2(r,t) = \hat{c}_q(r,t;\theta_0)$$

$$S_3(r,t) = \hat{c}_\gamma(r,t;\theta_0)$$

Quantify sensitivity of the estimated states to variations in the uncertain parameter values

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Sensitivity-Based Interval PDE Observer

When the parameters are close to their nominal values, we approximate the solution to the Observer PDE around the nominal solution to first order accuracy as:

$$\hat{c}(r,t;\theta) \quad \approx \quad \hat{c}(r,t;\theta_0) + S_1(r,t)(\varepsilon - \varepsilon_0) + S_2(r,t)(q - q_0) + S_3(r,t)(\gamma - \gamma_0)$$

Assume parameters are bounded:

$$\underline{\varepsilon} \leq \varepsilon \leq \overline{\varepsilon}, \quad \underline{q} \leq q \leq \overline{q}, \quad \underline{\gamma} \leq \gamma \leq \overline{\gamma}, \qquad \underline{\theta} = [0.9, 0.9, 0.9]^T \quad \overline{\theta} = [1.1, 1.1, 1.1]^T$$

Define the interval estimates as:

$$\underline{\hat{c}}(r,t) = \hat{c}(r,t) + S_1(r,t)(\underline{\varepsilon} - \varepsilon_0) + S_2(r,t)(\underline{q} - q_0) + S_3(r,t)(\underline{\gamma} - \gamma_0)$$

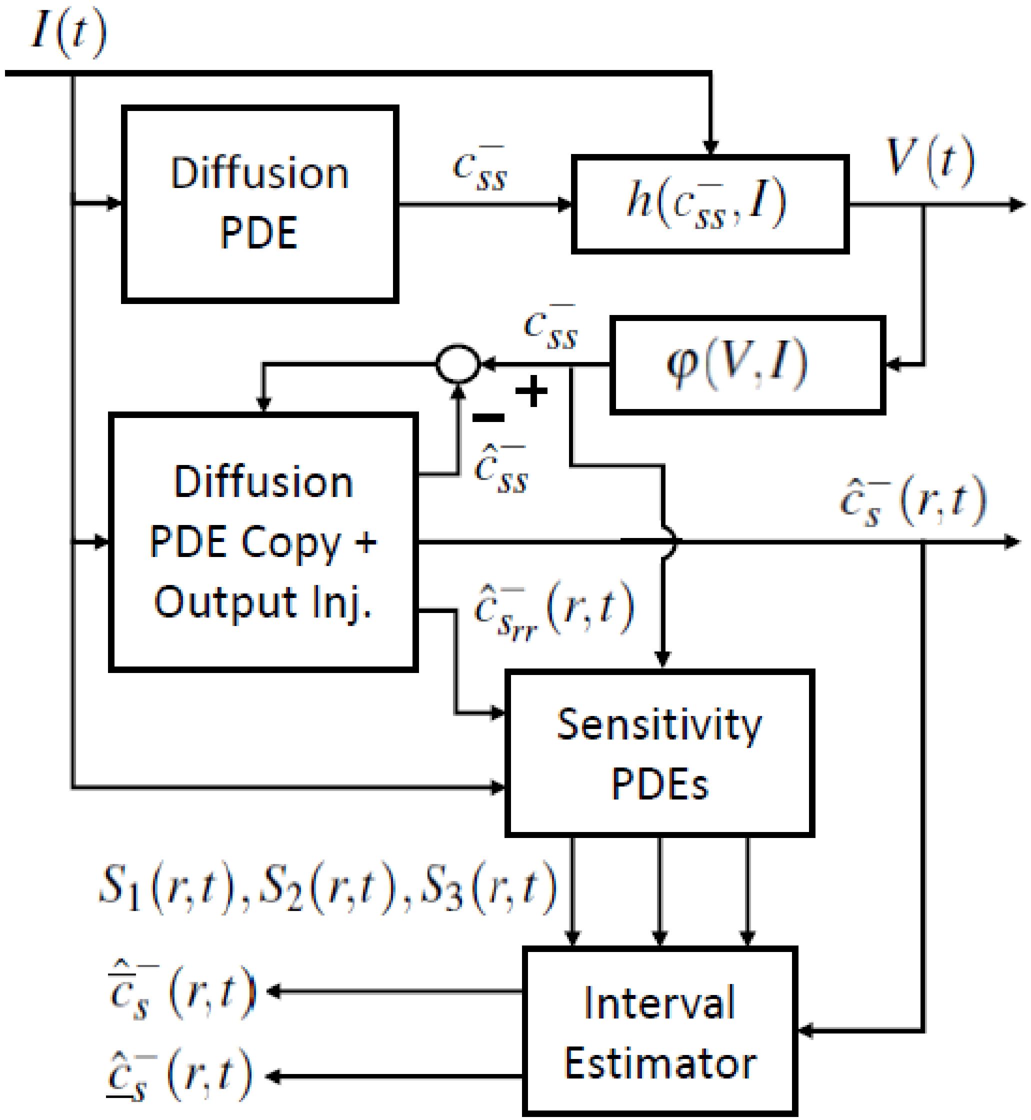
$$\overline{\hat{c}}(r,t) = \hat{c}(r,t) + S_1(r,t)(\overline{\varepsilon} - \varepsilon_0) + S_2(r,t)(\overline{q} - q_0) + S_3(r,t)(\overline{\gamma} - \gamma_0)$$

Interval estimates used to give interval estimates of:

$$\left(\underline{S\hat{O}C}(t), \overline{S\hat{O}C}(t)\right)$$

$$\left(\underline{\hat{V}}(t), \overline{\hat{V}}(t)\right)$$

Sensitivity-Based Interval PDE Observer



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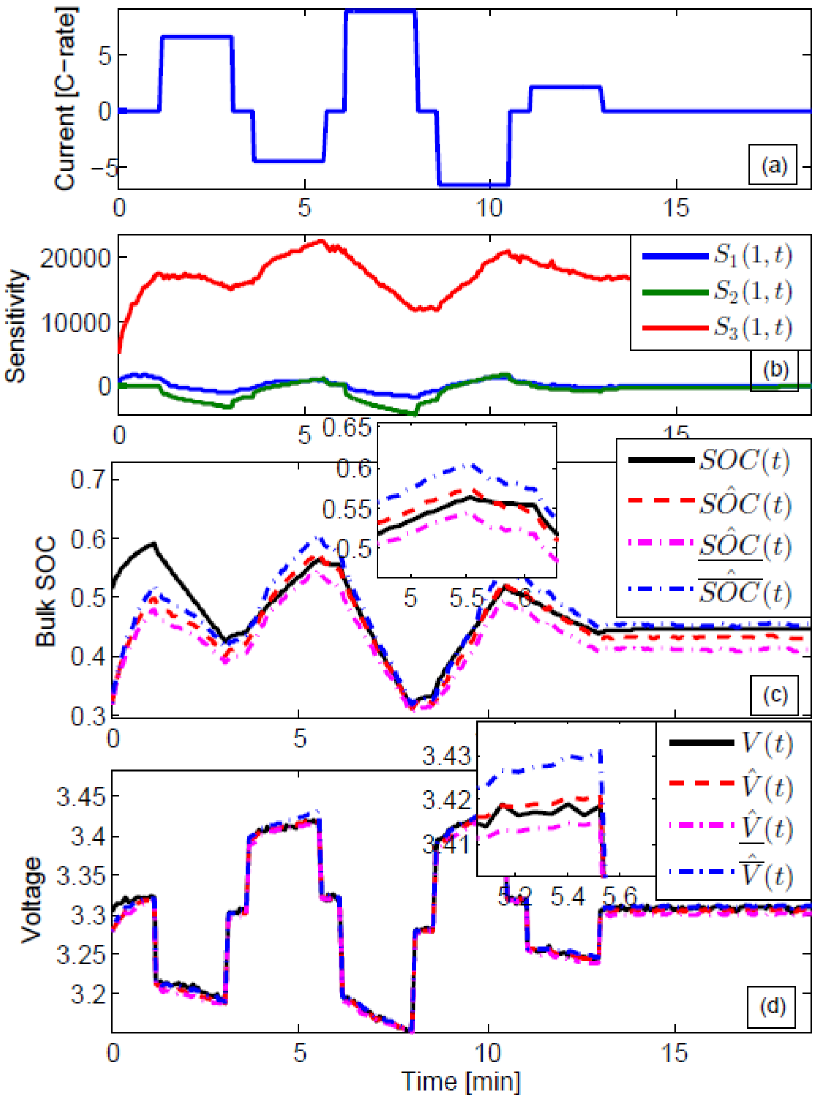
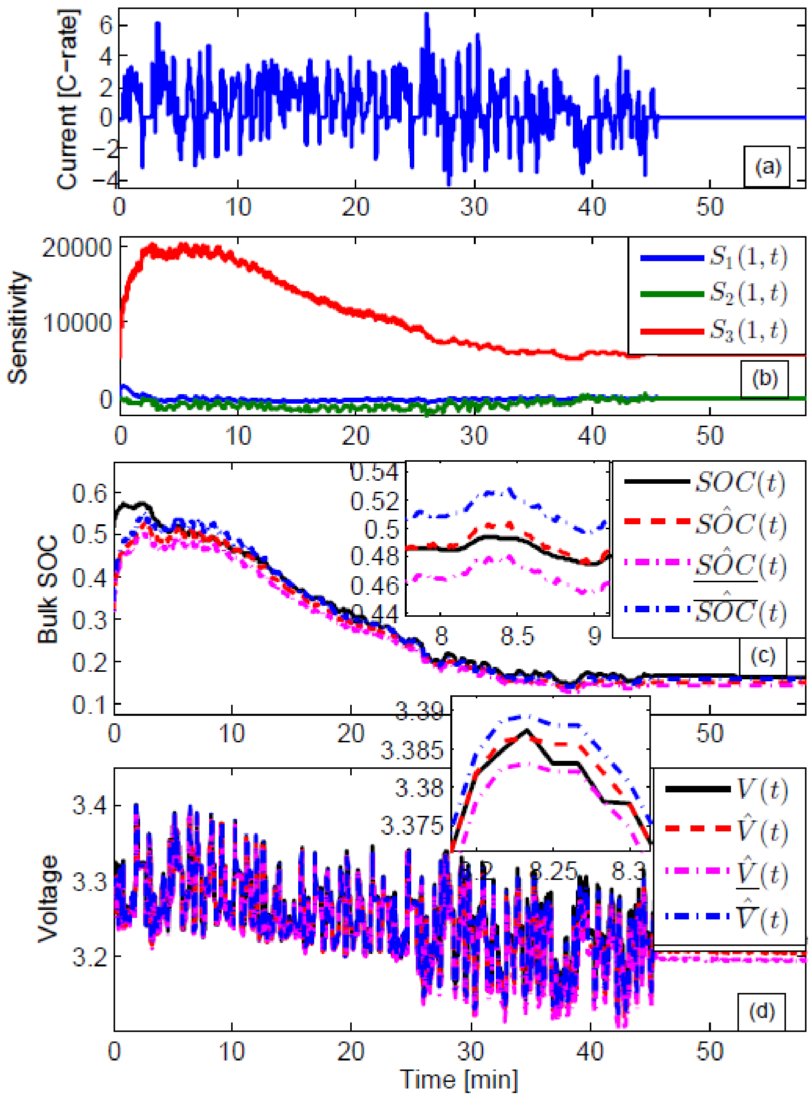
Results

- Pulse Charge/Discharge Cycle
- Observer system is most sensitive to perturbations in γ (S_3), followed by q (S_2), and finally ε (S_1)
- Interval estimates encapsulate real values



Results

- UDDS Charge/Discharge Cycle
- Observer system is most sensitive to perturbations in γ (S_3), followed by q (S_2), and finally ε (S_1)
- Interval estimates encapsulate real values

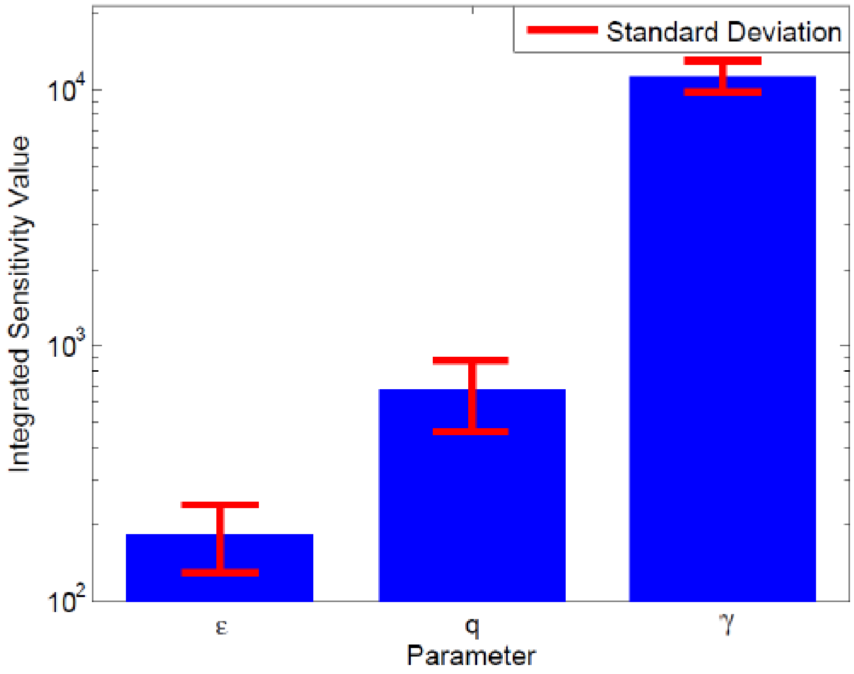


Results

- UDDS/US06/SC04/LA92/ DC1/DC2 Charge/Discharge Cycles
- Rank Parameters

$$S_{rank_i} = \frac{1}{T}\int_0^T |S_i(s)|\,ds$$

- Verifies observer system is most sensitive to perturbations in γ (S_3), followed by q (S_2), and finally ε (S_1)



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Conclusions

- Sensitivity analysis showed the effect of the parameters on state estimates
- Parameter ranking useful for system identification purposes
- Sensitivities used for interval estimates on battery SOC and voltage
- Interval estimates encapsulate real values

References

[1] T. Ahonen, Tomi Ahonen Almanac 2012- Mobile Telecoms Industry Review. Lulu.com, 2012.

[2] Electric Drive Transportation Association. (2012) Electric drive vehicle sales figures (U.S. Market) - EV sales. [Online]. Available: http://electricdrive.org/index.php?ht=d/sp/i/20952/pid/20952

[3] N. A. Chaturvedi, R. Klein, J. Christensen, J. Ahmed, and A. Kojic, “Algorithms for advanced battery-management systems,” IEEE Control Systems Magazine, vol. 30, no. 3, pp. 49 – 68, 2010.

[4] K. Thomas, J. Newman, and R. Darling, Advances in Lithium-Ion Batteries. New York, NY USA: Kluwer Academic/Plenum Publishers, 2002, ch. 12: Mathematical modeling of lithium batteries, pp. 345–392.

[5] K. A. Smith, C. D. Rahn, and C.-Y. Wang, “Model-based electrochemical estimation and constraint management for pulse operation of lithium ion batteries,” IEEE Transactions on Control Systems Technology, vol. 18, no. 3, pp. 654 – 663, 2010.

[6] D. D. Domenico, A. Stefanopoulou, and G. Fiengo, “Lithium-Ion Battery State of Charge and Critical Surface Charge Estimation Using an Electrochemical Model-Based Extended Kalman Filter,” Journal of Dynamic Systems, Measurement, and Control, vol. 132, no. 6, p. 061302, 2010.

[7] R. Klein, N. A. Chaturvedi, J. Christensen, J. Ahmed, R. Findeisen, and A. Kojic, “Electrochemical Model Based Observer Design for a Lithium-Ion Battery,” IEEE Transactions on Control Systems Technology, vol. 21, no. 2, pp. 289–301, March 2013.

[8] S. J. Moura, N. Chaturvedi, and M. Krstic, “Adaptive PDE Observer for Battery SOC/SOH Estimation via an Electrochemical Model,” ASME Journal of Dynamic Systems, Measurement, and Control, to appear, 2013.

[9] J. C. Forman, S. J. Moura, J. L. Stein, and H. K. Fathy, “Genetic identification and Fisher identifiability analysis of the Doyle-Fuller-Newman model from experimental cycling of a LiFePO4 cells,” Journal of Power, vol. 210, pp. 263–275, 2012.

[10] C. Combastel, “A state bounding observer for uncertain non-linear continuous-time systems based on zonotopes,” in Decision and Control, 2005 and 2005 European Control Conference. CDC-ECC ’05. 44th IEEE Conference on, Dec 2005, pp. 7228–7234.

[11] T. Raissi, D. Efimov, and A. Zolghadri, “Interval state estimation for a class of nonlinear systems,” Automatic Control, IEEE Transactions on, vol. 57, no. 1, pp. 260–265, Jan 2012.

[12] H. K. Khalil, Nonlinear Systems, 3rd ed. Prentice Hall, 2002.

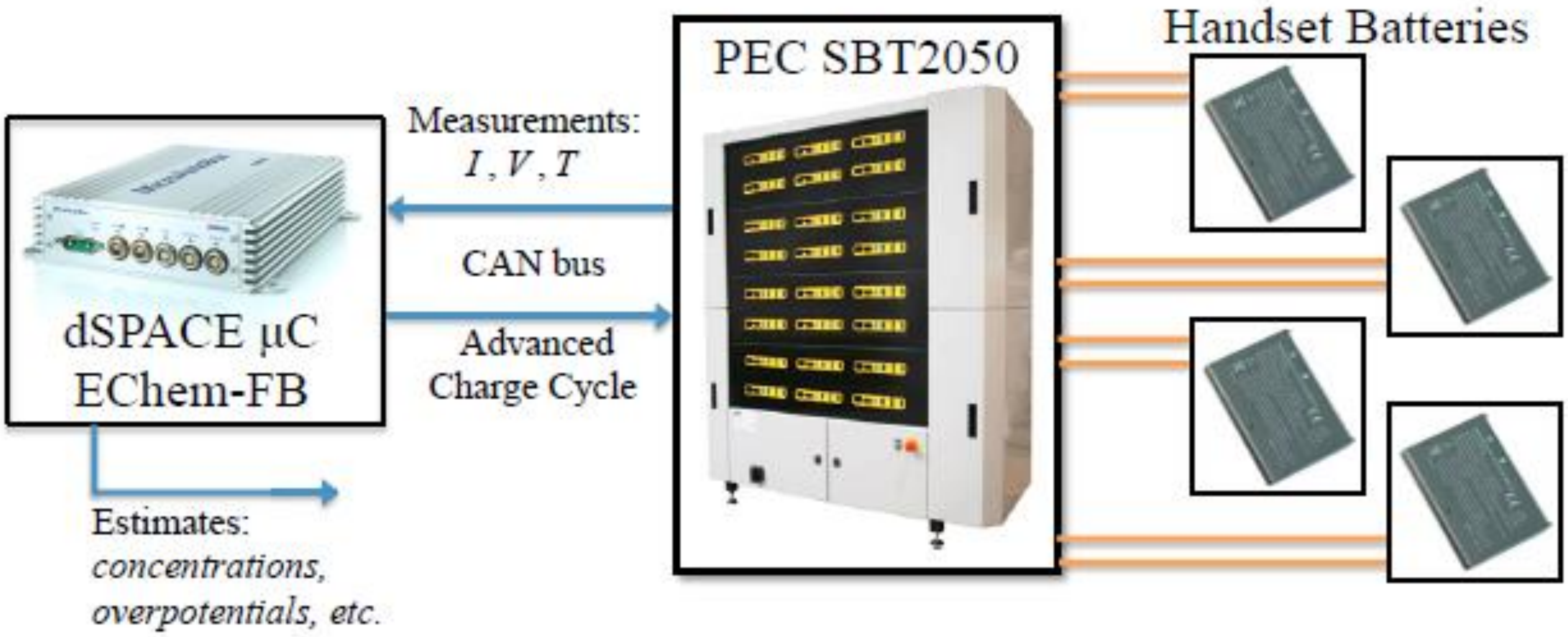
[13] M. Krstic and A. Smyshlyaev, Boundary Control of PDEs: A Course on Backstepping Designs. Philadelphia, PA: Society for Industrial and Applied Mathematics, 2008.

[14] S. Santhanagopalan and R. E. White, “Online estimation of the state of charge of a lithium ion cell,” Journal of Power Sources, vol. 161, no. 2, pp. 1346 – 1355, 2006.

[15] S. J. Moura, N. Chaturvedi, and M. Krstic, “PDE Estimation Techniques for Advanced Battery Management Systems - Part I: SOC Estimation,” in Proceedings of the 2012 American Control Conference, Montreal, Canada, June 2012.

[16] S. Moura, J. Stein, and H. Fathy, “Battery-Health Conscious Power Management in Plug-In Hybrid Electric Vehicles via Electrochemical Modeling and Stochastic Control,” Control Systems Technology, IEEE Transactions on, vol. 21, no. 3, pp. 679–694, 2013.

Questions?



PEC SBT2050
Handset Batteries
Measurements:
I, V, T
CAN bus
Advanced
Charge Cycle
dSPACE μC
EChem-FB
Estimates:
concentrations,
overpotentials, etc.

Numerical Implementation

Finite Central Difference Method

Recall Sensitivity PDE:

$$S_{1_t}(r,t) = \varepsilon_0 S_{1_{rr}}(r,t;\theta_0) + \hat{c}_{rr}(r,t;\theta_0) - p_1(r) S_1(1,t;\theta_0)$$

Initial Condition and Boundary Conditions:

$$S_1(r,t_0) = S_1(0,t) = 0$$

$$S_{1_r}(1,t) - S_1(1,t) = -p_{10} S_1(1,t)$$

Let:

$$S_{1_i} = S_1(i\Delta r, t; \theta_0), \quad i = 0, 1, \ldots, N$$

First and Second Order Partial Derivative in Space:

$$S_{1_{r_i}} \approx \frac{S_{1_{i+1}} - S_{1_i}}{\Delta r} \qquad S_{1_{rr_i}} \approx \frac{\frac{S_{1_{i+1}} - S_{1_i}}{\Delta r} - \frac{S_{1_i} - S_{1_{i-1}}}{\Delta r}}{\Delta r} = \frac{S_{1_{i+1}} - 2S_{1_i} + S_{1_{i-1}}}{\Delta r^2}$$

Let First Order Partial Derivative in Time be:

$$S_{1_{t_i}} = \dot{S}_{1_i}$$

Numerical Implementation

Turn PDE into set of ODEs:

$$\dot{S}_{1_i} = \varepsilon_0 \left(\frac{S_{1_{i+1}} - 2S_{1_i} + S_{1_{i-1}}}{\Delta r^2} \right) + \hat{c}_{rr}(i\Delta r, t; \theta_0) - p_1(i\Delta r) S_{1N}$$

Let:

$$\alpha_1 = \frac{\varepsilon_0}{\Delta r^2} \qquad \hat{c}_{rr}(i\Delta r, t) = \hat{c}_{rr}(i\Delta r, t; \theta_0)$$

ODE is now:

$$\dot{S}_{1_i} = \alpha_1 (S_{1_{i+1}} - 2S_{1_i} + S_{1_{i-1}}) + \hat{c}_{rr}(i\Delta r, t) - p_1(i\Delta r) S_{1N}$$

Note, this set of ODEs is defined for $i = 1, \ldots, N-1$

The IC is defined as an AE:

$$S_{1_0} = 0$$

The BC is defined as an AE:

$$\frac{S_{1_N} - S_{1_{N-1}}}{\Delta r} - S_{1_N} = -p_{10} S_{1_N}$$

Which turns into:

$$(1 - \Delta r + \Delta r p_{10}) S_{1_N} - S_{1_{N-1}} = 0$$

Numerical Implementation

Rearranging the ODEs and AEs:

$$\dot{S}_1 = M_{1_1} S_1 + M_{1_2} S_{1_z} + B_{1_1} \hat{c}_{rr},$$

$$N_{1_3} = N_{1_1} S_1 + N_{1_2} S_{1_z}$$

Where:

$$\dot{S}_1 = \begin{bmatrix} \dot{S}_{1_1} \\ \dot{S}_{1_2} \\ \vdots \\ \dot{S}_{1_{N-1}} \end{bmatrix} \quad S_1 = \begin{bmatrix} S_{1_1} \\ S_{1_2} \\ \vdots \\ S_{1_{N-1}} \end{bmatrix} \quad S_{1_z} = \begin{bmatrix} S_{1_0} \\ S_{1_N} \end{bmatrix} \quad \hat{c}_{rr} = \begin{bmatrix} \hat{c}_{rr}(\Delta r, t) \\ \hat{c}_{rr}(2\Delta r, t) \\ \vdots \\ \hat{c}_{rr}((N-1)\Delta r, t) \end{bmatrix} \quad B_{1_1} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & 1 \end{bmatrix}$$

$$M_{1_1} = \begin{bmatrix} -2\alpha_1 & \alpha_1 & 0 & \dots & \dots & 0 \\ \alpha_1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \alpha_1 \\ 0 & \dots & \dots & 0 & \alpha_1 & -2\alpha_1 \end{bmatrix} \quad M_{1_2} = \begin{bmatrix} \alpha_1 & -p_1(\Delta r) \\ 0 & -p_1(2\Delta r) \\ \vdots & \vdots \\ \vdots & -p_1((N-2)\Delta r) \\ 0 & (\alpha_1 - p_1((N-1)\Delta r)) \end{bmatrix}$$

$$N_{1_2} = \begin{bmatrix} 1 & 0 \\ 0 & (1 - \Delta r + \Delta r p_{10}) \end{bmatrix} \quad N_{1_3} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Numerical Implementation

For the set of AEs, we can solve for:

$$S_{1_z} = N_{1_2}^{-1} N_{1_3} - N_{1_2}^{-1} N_{1_1} S_1 = -N_{1_2}^{-1} N_{1_1} S_1$$

Plug that into the set of ODEs:

$$\dot{S}_1 = M_{1_1} S_1 + M_{1_2}(-N_{1_2}^{-1} N_{1_1} S_1) + B_{1_1} \hat{c}_{rr}$$

Which simplifies to:

$$\dot{S}_1 = (M_{1_1} - M_{1_2} N_{1_2}^{-1} N_{1_1}) S_1 + B_{1_1} \hat{c}_{rr}$$

We define this as a SS system:

$$\dot{S}_1 = A_1 S_1 + B_1 \hat{c}_{rr}$$

Where:

$$A_1 = (M_{1_1} - M_{1_2} N_{1_2}^{-1} N_{1_1})$$

$$B_1 = B_{1_1}$$

Numerical Implementation

The output to this system is:

$$S_{1_{0\to N}} = M_{1_{1out}} S_1 + M_{1_{2out}} S_{1_z}$$

Where:

$$M_{1_{1out}} = \begin{bmatrix} 0 & \cdots & \cdots & 0 \\ 1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 \\ 0 & \cdots & \cdots & 0 \end{bmatrix} \quad M_{1_{2out}} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \\ 0 & 1 \end{bmatrix} \quad S_{1_{0\to N}} = \begin{bmatrix} S_{1_0} \\ S_{1_1} \\ \vdots \\ S_{1_N} \end{bmatrix}$$

The output becomes:

$$S_{1_{0\to N}} = M_{1_{1out}} S_1 + M_{1_{2out}} \left(-N_{1_2}^{-1} N_{1_1} S_1\right)$$

$$S_{1_{0\to N}} = \left(M_{1_{1out}} - M_{1_{2out}} N_{1_2}^{-1} N_{1_1}\right) S_1$$

The output is then:

$$S_{1_{0\to N}} = C_1 S_1$$

$$C_1 = \left(M_{1_{1out}} - M_{1_{2out}} N_{1_2}^{-1} N_{1_1}\right)$$