The Lithium-Ion Cell: Model, State Of Charge Estimation and Battery Management System

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Outline

✓ Cell Generalities

✓ Principle of Functioning
  - Electrochemical Model
  - Reduced Order Model
  - Parameter Identification

✓ State of Charge Estimation
  - Extended Kalman Filter
  - Critical SOC Definition

✓ Cell SOC Equalization
  - Battery Management System

❖ Neutron Scattering Analysis
  - Custom Designed Case
  - Preliminary Results
Lithium-ion battery: Why choose it?

- Lithium Ion
- Lead Acid
- Ni-Zn
- Ni-Cd, NiMH
- Zn/MnO₂

(WH/kg)

Lead acid, NiCd, NiMH, Manganese Li-ion, Phosphate Li-ion, Cobalt Li-ion.

WattHours / Kilogram

- Lithium Polymer
- Lithium Phosphate
- Lithium Ion
- Nickel Cadmium
- Nickel Metal Hydride
- Lead Acid

WattHours / Litre

Grace
Lithium-ion battery: Cell build

- Anode terminal
- Anode
- Separator + Electrolyte
- Insulating packing
- Cathode (oxide)
- Cathode terminal

- Cover
- Positive terminal
- Insulating ring
- Positive tab
- Case
- Anode (negative plate)
- Negative tab
- Cathode (positive plate)
Lithium-ion battery: Cell behavior

Cell Types Compared:

Energy Release (W/kg)

Capacity versus current at 20°C

Typical discharge profiles (1.4 A - C/5 rate)

SAFT, “MP176065” Datasheet
Lithium-ion battery: Cell degradation profiles

S. Choi and H. S. Lim, "Factors that affect cycle-life and possible degradation mechanisms of a Li-ion cell based on LiCoO2", Journal of Power Sources
Lithium ions and $e^-$ are produced in the anode. The $e^-$ produce current in the external circuit, while lithium ions travel via diffusion through the solution to the cathode, where the external circuit $e^-$ are adsorbed.

At anode, the solid active material diffuses through the spherical particles toward surface (electrolyte-solid interface) where it reacts due to the over-potential, transferring lithium-ions into the solution and $e^-$ to collector. At the cathode lithium ions and $e^-$ react and insert into metal solid particles.
Lithium-ion battery: Cathodic Intercalation

Lithium-ion battery: Anodic intercalation

Basal Surface Plan

A

B

0.3354 nm

Voltage [V]

Lithium concentration x in Li$_x$C$_6$

0.14 nm

Grace
\[
\frac{di_s}{dx} = j^{Li} \\
\sigma \varepsilon_s \frac{d\phi_s}{dx} = -i_s \\
\int_0^\delta j^{Li}(x) dx = \frac{I}{A} \\
\frac{di_e}{dx} = 0 \\
k \varepsilon_e \frac{d\phi_e}{dx} = -i_e
\]

\[
\frac{\partial c_s}{\partial t} = D_{sn} \left( \frac{\partial^2 c_s}{\partial r^2} + \frac{2}{r} \frac{\partial c_s}{\partial r} \right)
\]

\[
j^{Li} = a_{sn} j_0 \left[ \exp\left( \frac{\alpha_a F}{RT} \eta \right) - \exp\left( - \frac{\alpha_c F}{RT} \eta \right) \right]
\]

\[
\eta = \phi_s - \phi_e - U(c_{se})
\]

\[
j_0 = j_0(c_{se})
\]

--- Charge Conservation, Solid Phase
--- Solid Diffusion Equation
--- Charge Conservation, Electrolyte Phase
--- Butler-Volmer Equation
Lithium-ion battery: Cell reduced order model

PDEs based systems are not useful for control applications and cannot be used for real time simulations.

A model reduction is necessary in order to derive a set of classical ODE based system. Typically this is accomplished by introducing some approximations.

Electrolyte concentration $c_e$ constant.

Average solution of micro-current density $j^{Li}$.

$$\frac{\partial j}{\partial x} = 0 \Rightarrow \int_0^\delta j^{Li}(x)dx = \frac{I}{A} = j^{Li} \delta$$

$$V = (\eta_p - \eta_n) + (\phi_p - \phi_n) + (U_p - U_n) - \frac{R_f}{A} I$$

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

$$\dot{c}_s = Ac_s + Bu \quad u = \bar{j}^{Li}$$

$$y = Cs + Du \quad y = c_{se}$$

D. Di Domenico, A. Stefanopoulou, and G. Fiengo., Reduced Order Lithium-ion Battery Electrochemical Model And Extended Kalman Filter State Of Charge Estimation. ASME JDSMC, 2008
Lithium-ion battery: Critical SOC definition

By defining solid surface concentration stoichiometry (also indicated as normalized concentration) as:

\[ \theta = \frac{c_s}{c_{s,\text{max}}} \]

the battery critical SOC can be conveniently defined as follows:

\[ SOC = \frac{\theta_p - \theta_{0\%}}{\theta_{100\%} - \theta_{0\%}} \quad \theta_p = \frac{C_{se,p}}{C_{se,p/\text{max}}} \]

Where \( \theta_{100\%} \) and \( \theta_{0\%} \) are respectively the positive solid surface concentration stoichiometry of a full charged and a full discharged battery.

The SOC can be defined equivalently on the positive or negative solid concentration, but is defined on the positive because of its greater range of variation during battery charge and discharge operations.
Lithium-ion battery: OCP identification

The negative electrode is composed of graphite (LiC₆), so it is possible to utilize the empirical relationship between the solid concentration and OCP from Doyle et al. The positive electrode instead, is composed of a mixture of Lithium metal oxides, so the correlation function \( U_p \) needs to be identified as well.
Lithium-ion battery: OCP identification

The identification of the $U_p$ function is part of the global identification procedure and it is obtained through a series of iterative refinements as shown below:
Lithium-ion battery: Validation results

Validation test results – Increasing amplitude HPPC profiles
Lithium-ion battery: Extended Kalman Filter

The system has a poor observability because the output is the difference of two sub-systems!

A further reduction:
The single electrode model.

The negative electrode quantities are estimated through inversion of the positive SOC calculation.

Lithium-ion battery: EKF results

HPPC profiles, with increasing reference current charge and discharge.
Lithium-ion battery: Cell balancing

Fully charged and balanced cells

Half charged and unbalanced cells

Lithium-ion battery: Cell balancing

Charge Shunting

Switched Transformer

Charge Shuttling

Multiple Transformer

Lithium-ion battery: Cell balancing

The charge equalization circuit is a modified version of the charge shuttling method.

A switched capacitor drains energy from the battery pack and releases energy on the weaker cell, raising its SOC to equalize the battery.

The BMS algorithm utilizes the EKF estimation to select the weaker cell in the pack.
BMS – Cell equalization algorithm

✓ Each cell is polled by the EKF for 10 s. The gain of the filter have been chosen in order to ensure the estimation convergence in less than 5 s.

✓ The SOC of the cells that are not polled by the EKF are tracked by simple coulomb counting integrator models:

\[ SOC(i) = \frac{1}{C} \int I(t) dt + SOC(i)_0 \]

The cell equalization procedure is the following:

1. Identify the lowest charged cell while charging the capacitor up to a fixed threshold \( HV \);
2. Discharge the capacitor over the selected cell until its voltage goes under a fixed threshold \( LV \);
3. Check SOC difference for all the cell;
4. Repeat step 1, 2 and 3 until maximum difference in SOC becomes lower than 2%. 

\[ \text{SOC} \]
Lithium-ion battery: BMS results

- Cells start with a strong unbalance.
- Cell 1 is the first to be selected.
- When cell 1 and cell 3 have the same SOC they start to be alternatively selected.
- The equalization process ends at 8000 s.
- High initial voltage difference because cell 1 and 3 are almost totally discharged.
- When a cell is selected by the BMS, it receives a charge injection, raising its SOC.
- Final voltage difference is less than 0.02V. Final SOC difference is less than 1%.
Lithium-ion battery: BMS results

- Current spikes correspond to an energy extraction from the capacitor. Valleys instead correspond to energy injection from the capacitor.

- Cell 1 receives all the injections until its SOC becomes equal to cell 3 SOC, at 2400 s.

- Cell 2 is never selected for injection because its higher SOC respect to cell 1 and 3.

- Red line is the Kalman Filter polling.

- Solid blue line is cell 1 SOC.

- The green dot line is the cell 1 simple coulomb counting model. The initial value of the integral is updated only when the cell is not selected for charge injection.
Lithium-ion battery: BMS results

Bi-directional current input

![Graphs showing current and voltage over time for different cells](image)

- **Current (A) vs. Time [s]**: Graphs for Cell 1, Cell 2, and Cell 3 showing bi-directional current input.
- **Voltage [V]**: Graphs for Cell 1 and Cell 2 showing voltage over time.
- **State of Charge (SOC) [%]**: Graphs for Cell 1 and Cell 2 showing SOC over time.
Neutron scattering analysis

Rubber + EC:DMC solvent
Neutron scattering analysis
Neutron scattering analysis
Conclusions

**International publications**

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**In submission**

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<tr>
<td>C. Speltino, A. Stefanopoulou and G. Fiengo</td>
<td><strong>Identification and Validation a Lithium Battery Reduced Model Based Extended Kalman Filter for State Of Charge Estimation</strong>, IEEE Transactions on System Control Technology.</td>
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**Current activities**

- Experimental research on Power Split Control aimed to validate the previous results obtained in simulation;
- On-line parameter identification for cell aging and deterioration estimation;
- Multi-cell BMS control strategy.