Modelling Lithium Ion Batteries

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Overview

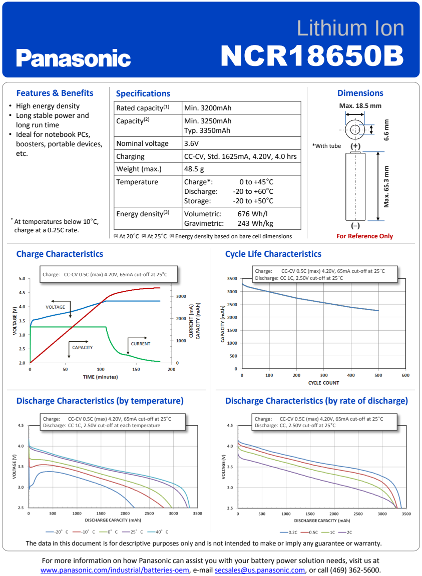
- Basic Battery Operation [PIMS MMIW 2016 project]
- State of Health Modelling [JTT Electronics]
- Pseudo 2D Scaling [The Irish Connection]
- Cartoon Model [Computational Framework]

Get a Battery

Panasonic NCR18650B

Panasonic NCR18650B

Manufacturer’s Specification Sheet



Panasonic

Lithium Ion

NCR18650B

Features & Benefits

- High energy density
- Long stable power and long run time
- Ideal for notebook PCs, boosters, portable devices, etc.

* At temperatures below 10°C, charge at a 0.25C rate.

Specifications

Rated capacity[1]	Min. 3200mAh
Capacity[2]	Min. 3250mAh Typ. 3350mAh
Nominal voltage	3.6V
Charging	CC-CV, Std. 1625mA, 4.20V, 4.0 hrs
Weight (max.)	48.5 g
Temperature	Charge*: 0 to +45°C Discharge: -20 to +60°C Storage: -20 to +50°C
Energy density[3]	Volumetric: 676 Wh/l Gravimetric: 243 Wh/kg

[1] At 20°C [2] At 25°C [3] Energy density based on bare cell dimensions

Dimensions

For Reference Only

Charge Characteristics

Charge: CC-CV 0.5C (max) 4.20V, 65mA cut-off at 25°C

Cycle Life Characteristics

Charge: CC-CV 0.5C (max) 4.20V, 65mA cut-off at 25°C
Discharge: CC 1C, 2.50V cut-off at 25°C

Discharge Characteristics (by temperature)

Charge: CC-CV 0.5C (max) 4.20V, 65mA cut-off at 25°C
Discharge: CC 1C, 2.50V cut-off at each temperature

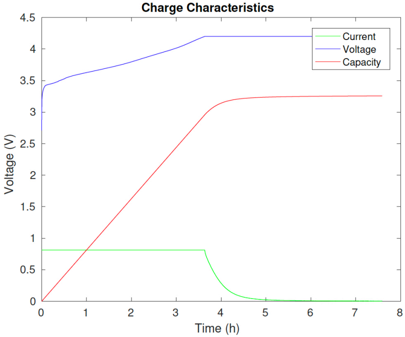
Discharge Characteristics (by rate of discharge)

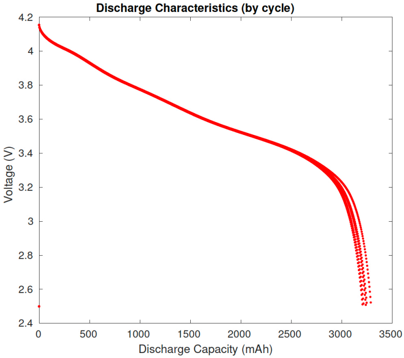
Charge: CC-CV 0.5C (max) 4.20V, 65mA cut-off at 25°C
Discharge: CC, 2.50V cut-off at 25°C

For more information on how Panasonic can assist you with your battery power solution needs, visit us at www.panasonic.com/industrial/batteries-oem, e-mail secsales@us.panasonic.com, or call (469) 362-5600.

Experimental Results

Charging and Discharging

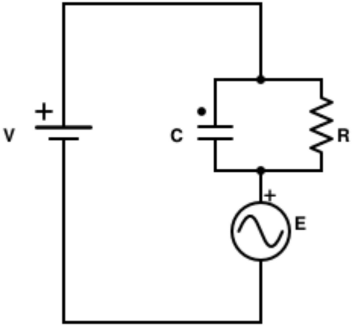




Equivalent Circuit Model

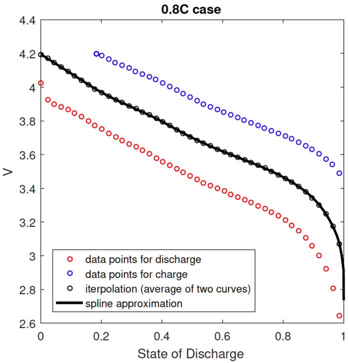
$$RC\frac{dV}{dt} + V(t) = E(\theta) + RC\frac{dE}{dt} - RI$$

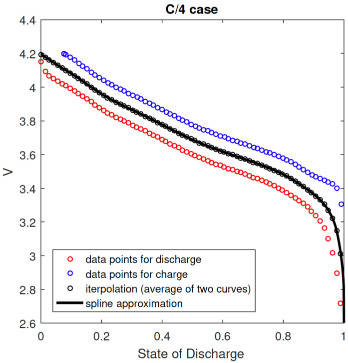
- V – battery voltage
- E – Battery equilibrium potential [fitted]
- θ – depth of discharge
- I – battery current
- R, C [fitted]



Equivalent Circuit Model

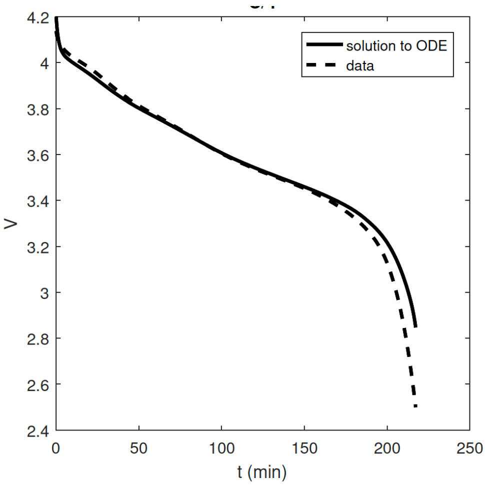
Fitting R and $E(\theta)$





Equivalent Circuit Model

Validation: Constant Resistance Discharge



Battery Packs

Cell → Brick → Pack

Tesla car batteries were built of 7,104 type 18650 cells:

- 16 battery packs connected in series.
- Each pack had 444 type 18650 cells in 6 bricks in series.
- Each brick had 74 cells connected in parallel.
- 74 times the current, $16 \times 6 = 96$ times the voltage.

Equivalent Circuit Modelling of Parallel and Series Connections

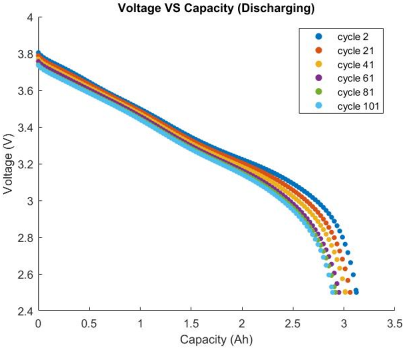
- The previous ODE model extends to a system of DAEs describing a battery bricks in series with cells connected in parallel.
- Two configurations compared:
  - Configuration 1: 12 bricks, with 6 cells in each brick
  - Configuration 2: 6 bricks, with 12 cells in each brick
- Cells were given a 5% standard deviation Gaussian distribution of capacity.

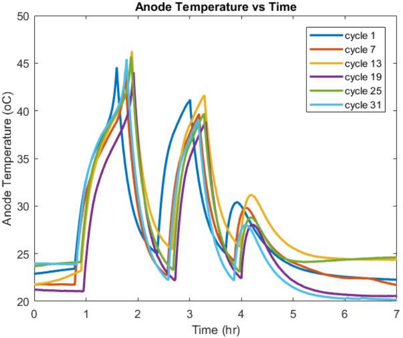
Configuration	Discharge Time	Output Energy
12 bricks × 6 cells	1.933	839.6
6 bricks × 12 cells	1.960	849.5

State of Health Modelling

Capacity

- Engage grant with JTT Electronics
- 100+ 1C charge and discharge cycles.
- Voltage/Current, Temperature and Impedance measurements





State of Health Modelling

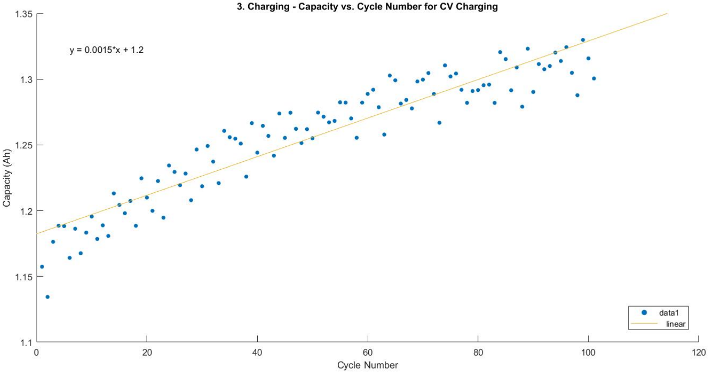
Model

- Consider the 1C cycle number γ as a proxy for SoH.
- Let θ be the cumulative discharge in Ah from the fully charged cell.
- We have experimental measurements of $V(\theta, \gamma)$ that can be fitted empirically, including an effective resistance to account for different current operation.
- From measured $V(\theta)$ we can deduce γ. This could be done in a BMS with only the history of one operating cycle.
- Interesting if the SoH loss other in operational conditions follows $V(\theta, \gamma)$, although γ will no longer correspond to cycle number.

State of Health Modelling

Capacity from CV charging

Capacity from CV charging may be a diagnostic for SoH that can be implemented effectively in a BMS.



State of Health Modelling

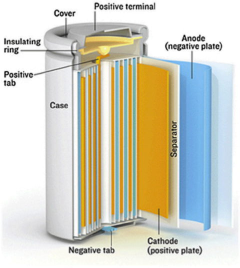
Ongoing Experiments

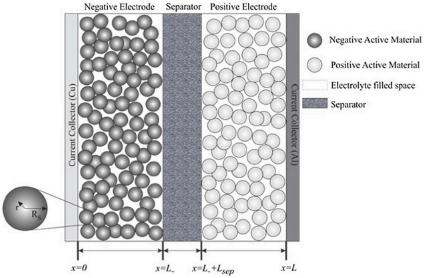
Additional cycling experiments to determine SoH under different conditions:

- 2C cycling
- No current (shelf life degradation)
- Thermal cycling with no current. The results would disambiguate SoH loss to 1C cycling versus just the thermal effects of the cycling.

Lithium Ion Batteries

Open the Hood





- Negative Electrode: Graphite
- Positive Electrode: Lithium Cobalt Oxide, Lithium Iron Phosphate
- Intercalation: energetically favourable in the positive electrode
- Electrolyte: Lithium salt in an organic solvent

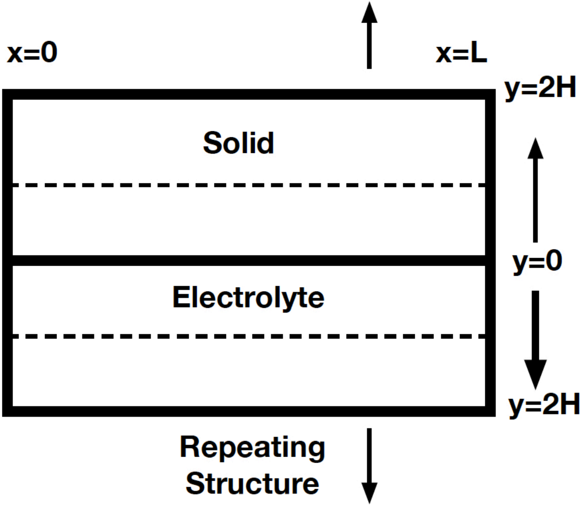
P2D Model (Diffusion Only)

Scaling

- Consider particles of size $2H$, $H \sim 0.025\mu - 2.5\mu$.
- Electrodes of width $L \sim 50\mu$.
- Diffusion of intercalated Li in particles $D_1 \sim 5 \times 10^{-14} m^2/s$
- Diffusion of Li$^+$ ions in electrolyte $D_2 \sim 3 \times 10^{-10} m^2/s$
- Dimensionless parameters:
    - $\epsilon = H/L \sim 0.0005 - 0.05$
    - $D = D_1/(\epsilon^2 D_2) \sim 0.07 - 700$

P2D Model (Diffusion Only)

Domain



P2D Model (Diffusion Only)

Scaled, Asymptotic Equations

- Intercalated Li concentration $c(y,t;x)$:

$$c_t = Dc_{yy}$$

  with $c_y(1,t;x) = 0$

- Electrolyte concentration of Li^+, $K(x,t)$:

$$K_t = K_{xx} + Dc_y(0,t;x)$$

  with $K_x(0,t) = 0$ and $K_x(1,t) = -I$ (I given).

- Continuity condition $c(0,t;x) = K(x,t)$.

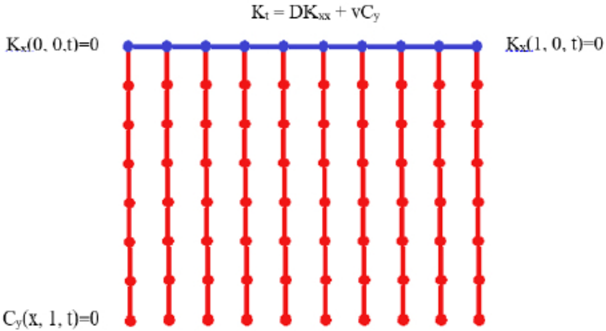
Note the Pseudo-2D structure

Doyle, Fuller, and Newman (1993)

Most P2D models take the solid particles as spherical.

P2D Model

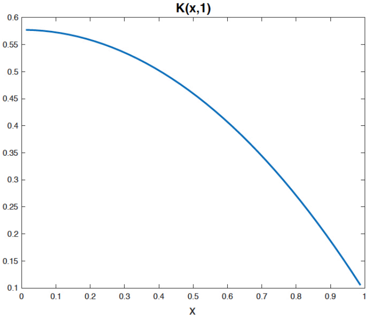
Graphic

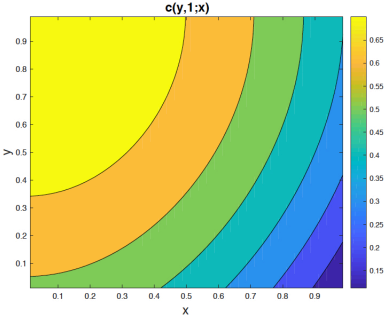


Sparse implicit solver will be fast

P2D Model

Computational Results





P2D Model

large D (small particles) part I

$$\begin{aligned} c_t &= Dc_{yy} \\ K_t &= K_{xx} + Dc_y(0,t;x) \end{aligned}$$

Large D asymptotics, $c \sim c^{(0)} + \frac{1}{D}c^{(1)} + \cdots$

$$\begin{aligned} c^{(0)} &\equiv K(x) \\ c^{(1)}(y) &= \frac{K_t}{2}(y^2 - 2y) \\ Dc_y(0,t;x) &= -K_t \text{ to highest order} \end{aligned}$$

$$K_t = \frac{1}{2}K_{xx}$$

Corresponds to volume averaging

P2D Model

large D (small particles) part II

$$K_t = \frac{1}{2} K_{xx}$$

Next order approximation

$$K_t = K_{xx} - K_t + \frac{1}{3D} K_{tt}$$

Same asymptotic order obtained by introducing $a(x,t)$, the average of $c(y,t;x)$ over y, and $j(x,t)$, the flux from solid to electrolyte:

$$\begin{aligned} \frac{da}{dt} &= -j \\ K_t &= K_{xx} + j \\ j(x,t) &= 3D(a - K) \end{aligned}$$

More obviously conservative, not higher order in time

Typical linear transfer factor $3D$

Like a crude discretization in y, many variants in the literature.

P2D Model

small D (large particles)

$$\begin{aligned} c_t &= D c_{yy} \\ K_t &= K_{xx} + D c_y(0, t; x) \end{aligned}$$

Small D asymptotics with $I = O(D)$, time scale change to D_1.

$$\begin{aligned} c(y, t) &: \quad c_t = c_{yy} \\ K(t) &: \quad \frac{dK}{dt} = -I + c_y(0, t) \end{aligned}$$

Single particle dynamics

Cartoon Electrode Model

Cartoon Philosophy

- Quantities $a(x,t)$, $c(x,t)$, $j(x,t)$ as before
- Electrolyte potential $\phi(x,t)$.
- Assume the solid phase potential is constant.

Now $c(x,t)$ is the concentration of both the Li^+ ions and the X^- counter ions (electroneutrality):

$$\begin{aligned} c_t &= c_{xx} + (c\phi_x)_x + j \quad (\mathrm{Li}^+) \\ c_t &= Ec_{xx} - E(c\phi_x)_x \quad (\mathrm{X}^-) \end{aligned}$$

Which can be rewritten:

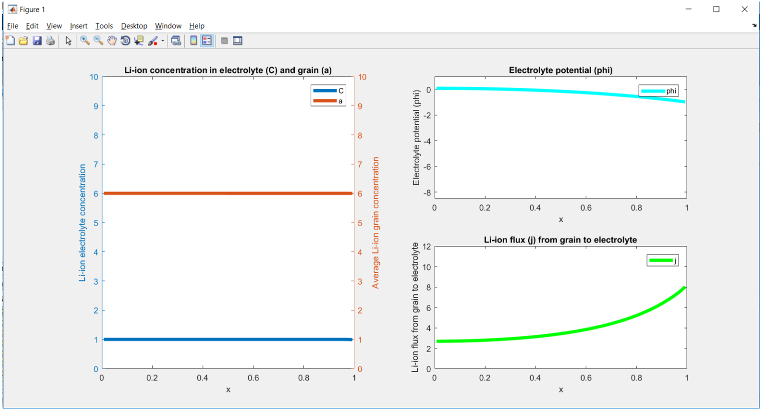
$$\begin{aligned} c_t &= \frac{2E}{E+1}c_{xx} + \frac{E}{E+1}j \\ 0 &= (1-E)c_{xx} + (1+E)(c\phi_x)_x + j \end{aligned}$$

We add cartoon "electrochemistry"

$$j = \sinh(-\phi + \ln a - \ln c)$$

Cartoon Electrode Model

Computational Implementation [David Kong]



Movie

Summary

1. Model future SoH experimental results.
2. Fast Solver for full P2D model [David] → Real time control [Bhushan]
3. Update solver to well-scaled model including temperature effects [Iain]