Asymptotic Analysis of Lithium-Ion Battery Models

Brian Wetton Iain Moyles Tim Myers
Matt Hennessey

IRISH RESEARCH COUNCIL
An Chomhairle um Thaighde in Éirinn

Mathematics Department
University of British Columbia
www.math.ubc.ca/~wetton

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Overview

- Basic Battery Operation
- Models: Simple and Complex
- Pseudo 2D Scaling Fuller, Doyle, and Newman (1994)
- Computational Results

Goal: identify when P2D models are needed to describe battery operation.

Rechargeable Lithium Ion Batteries

Used in:

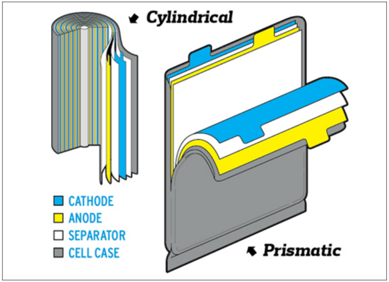
- medical devices
- mobile electronics
- cars
- power storage

Advantages:

- long lifetime
- high energy density
- low self-discharge rates

Battery Geometry

Cylindrical and Prismatic Cells



Panasonic NCR18650B, rated 3.2Ah:

Larger Scale Power

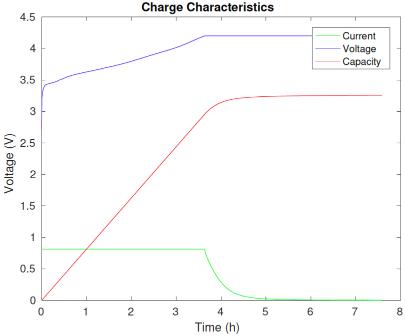
Cell $\rightarrow$ Brick $\rightarrow$ Pack

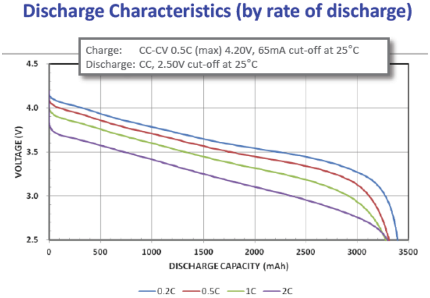
Original Tesla car batteries were built of 7,104 type 18650 cells:

- 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.

Experimental Results

Charging and Discharging





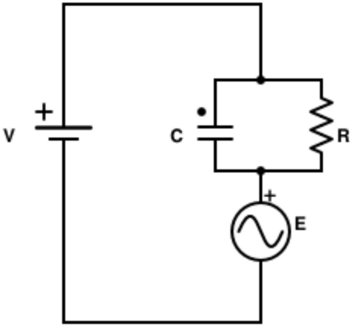
Simple SOC estimation from discharge curves

Equivalent Circuit Model

Simplest Case

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

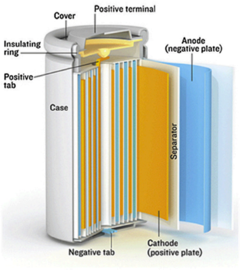
- V – battery voltage
- E – Battery equilibrium potential [fitted]
- θ – depth of discharge
- I – battery current
- R, C [fitted]
- E, R, C fits possibly (θ, history, SOH, T)
- Extend to RRCRC circuit

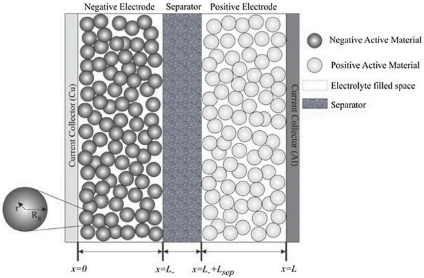


No electrochemistry needed

Lithium Ion Batteries

Open up the Battery

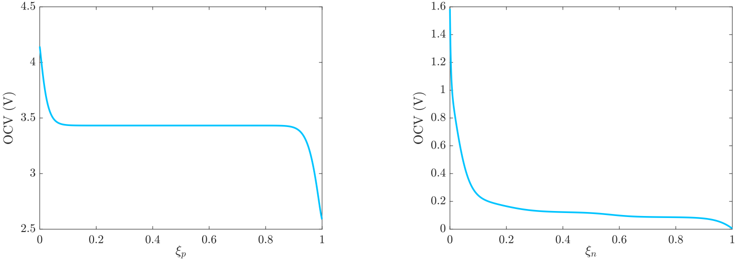




- Negative Electrode: Graphite
- Positive Electrode: Lithium Cobalt Oxide or Lithium Iron Phosphate
- Intercalation: Energetically favourable in the positive electrode
- Electrolyte: Lithium salt in an organic solvent

Lithium Ion Batteries

Electrode Potentials



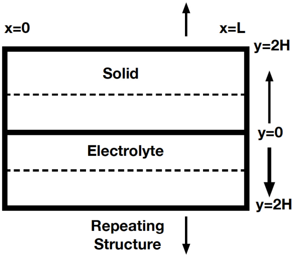
(a) Positive Electrode.

(b) Negative Electrode.

$$E(\theta) = V_{\text{left}}(\theta) - V_{\text{right}}(1-\theta)$$

Pseudo Two Dimensional (P2D) Model

Single Electrode Domain



Solid: intercalated Lithium $c(y, t; x)$ P2D,
potential $\psi(t)$ high solid conductivity
Electrolyte: ionic concentration $u(x, t)$,
potential $\phi(x, t)$
Interface: Flux $j(x, t)$ of Li^+ ions into solid

P2D Model

Ingredients and Scaling

- Intercalated flux $-D_c c_y$.
- Dilute electrolyte flux $-D_u u_x \pm \frac{FD_u}{RT} u\phi_x$.

Scaling:

- Scale x by L, y by H
- Scale ψ and ϕ by RT/F $(RT/F \approx 0.01)$
- Scale c by $c_{\max}$, u by u_{eq}
- Scale t by H^2/D_c, j by $D_c c_{\max}/H$
- $\epsilon = H/L \ll 1$ One ingredient for P2D model structure

P2D Model

Scaling

- Consider current density I for battery operation !
- Diffusive flux in the solid $-D_c c_y$ (unscaled) gives a current limit of order
$$I_1 = \frac{FLD_c c_{\max}}{2H^2}$$
- Diffusive flux in the electrolyte gives a current limit of order
$$I_2 = \frac{FD_u u_{eq}}{2L}$$
- Current not limited by surface flux or electrolyte resistance
- P2D scaling: I, I_1 and I_2 have roughly the same magnitude
- Dimensionless parameters:
    - $I_2/I_1 = \epsilon^2 \frac{D_u u_{\mathrm{eq}}}{D_c c_{\max}} := \mathcal{D}$
    - $I/I_1 := \mathcal{I}$

P2D Model

Scaled Asymptotic Equations

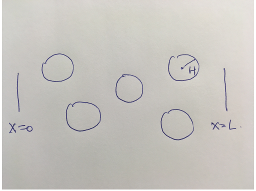
$$I_1 = \frac{FLD_c c_{\max}}{2H^2}, \quad I_2 = \frac{FD_u u_{eq}}{2L}$$
$$I_2/I_1 := \mathcal{D}, \quad I/I_1 := \mathcal{I}$$

$$\begin{aligned}
c_t &= c_{yy} \text{ with } c_y\,|_{y=1} = 0, \quad c_y\,|_{y=0} = j \\
\mathcal{D}u_{xx} &= j/2 \text{ with } \int_0^1 u(x)dx = 1, u_x\,|_{x=0} = 0 \quad ! \\
\mathcal{D}(u\phi_x)_x &= j/2 \text{ with } \phi_x\,|_{x=0} = 0, \quad \phi\,|_{x=1} = 0 \\
j &= R\sqrt{uc(1-c)} \ \exp\{-\psi + \phi\} \text{ with } \int_0^1 j(x)dx = \mathcal{I}
\end{aligned}$$

- If $I \ll \min\{I_1, I_2\}$ then equivalent circuit model (preprint).
- If $\mathcal{D}$ large, then single particle model.
- If $\mathcal{D}$ small, electrolyte only model.
- Otherwise, P2D model is appropriate.

P2D Model

Spherical Particles



Considering spherical particles of radius H with 50% volume fraction, change

$$c_t = c_{yy} \text{ with } c_y\,|_{y=1} = 0, \quad c_y\,|_{y=0} = j$$

to

$$c_t = \frac{1}{r^2}(r^2 c_r)_r \text{ with } c_r\,|_{r=0} = 0, \quad c_r\,|_{r=1} = j/3.$$

D_u should include tortuousity effects.

Computations

Implemented the P2D model in MATLAB:

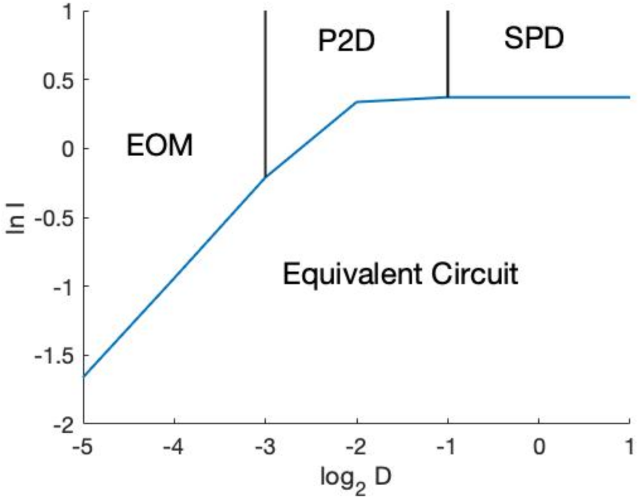
- Cell centred finite difference method in x and y or r
- Implicit time stepping (Backward Euler)
- Newton iterations for the resulting nonlinear problems

Movies:

1. Full P2D scaling, solid phase diffusion limiting
2. Full P2D scaling, electrolyte diffusion limiting
3. Large electrolyte diffusivity $I_1 \ll I_2$ (large $\mathcal{D}$, SPD)
4. Large solid diffusivity $I_2 \ll I_1$ (small $\mathcal{D}$, EOM)
5. Small current $I \ll \min\{I_1, I_2\}$ (equivalent circuit)

Criteria for model selection

For each $\mathcal{D}$, identify the scaled current $\mathcal{I}$ such that there is a 10% capacity loss from the model.



Summary

- Rechargeable Lithium Ion Battery basics
- Scaling that leads to the P2D model
- Computational results
- Future Work:
  - Fast solver for P2D model $\rightarrow$ real time control
  - Identify features on voltage discharge curves that give signatures of P2D regime dynamics