The P2D model for Lithium-Ion Battery Electrodes: When Is It Really Needed?

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PolyU, October, 2021

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:

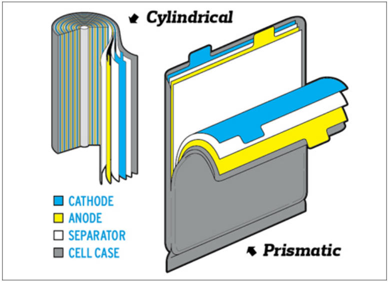
- medical devices
- mobile electronics
- cars
- power storage

Advantages:

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

Battery Geometry

Cylindrical and Prismatic Cells



Panasonic NCR18650B, rated 3.2Ah:

Larger Scale Power

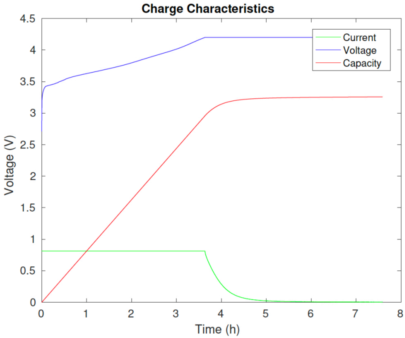
Cell → Brick → Pack

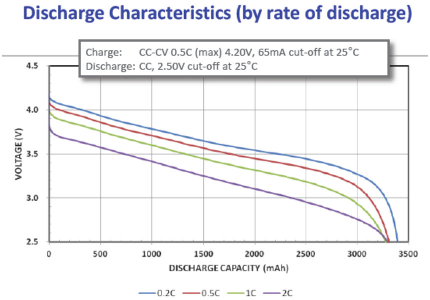
Original Tesla car batteries were built of 7,104 type 18650 cells:

- 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





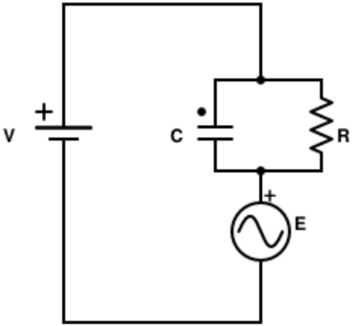
Simple SOC estimation from discharge curves

Equivalent Circuit Model

Simplest Case

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

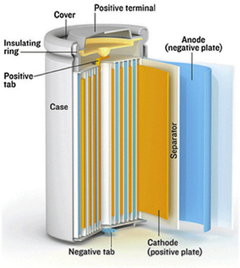
- V – battery voltage
- E – Battery equilibrium potential [fitted]
- θ – depth of discharge
- I – battery current
- R, C [fitted]
- E, R, C fits possibly (θ, history, SOH, T)
- Extend to RRCRC circuit

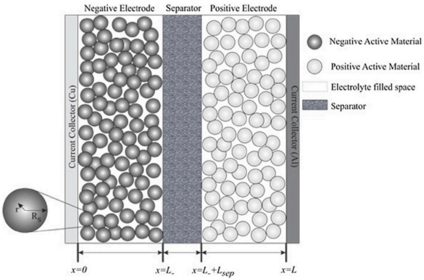


No electrochemistry needed

Lithium Ion Batteries

Open up the Battery

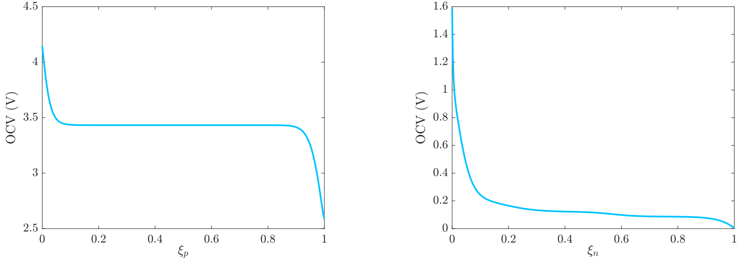




- Negative Electrode: Graphite
- Positive Electrode: Lithium Cobalt Oxide or Lithium Iron Phosphate
- Intercalation: Energetically favourable in the positive electrode
- Electrolyte: Lithium salt in an organic solvent

Lithium Ion Batteries

Electrode Potentials

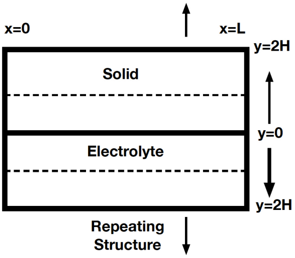


(a) Positive Electrode. (b) Negative Electrode.

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

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

Consider current density I for battery operation

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 the discharge time $Lc_{\max}F/(2I)$
- Scale j by $2IH/(LF)$
- $\epsilon = H/L \ll 1$ One ingredient for P2D model structure

P2D Model

Scaling

- Intercalated flux $-D_c c_y$.
- Dilute electrolyte flux $-D_u u_x \pm \frac{FD_u}{RT} u\phi_x$.
- 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:
    - $I/I_1 := \mathcal{I}$
    - $I/I_2 := \mathcal{I}_*$

P2D Model

Scaled Asymptotic Equations

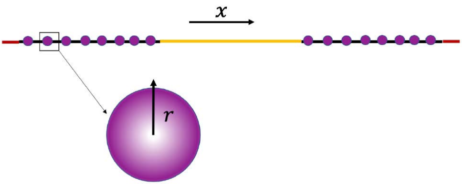
$$\mathcal{I} = 2H^2 I/(FLD_c c_{max})$$
$$\mathcal{I}_* = 2IL/(FD_u u_{\text{eq}})$$

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

- If $\mathcal{I}_*, \mathcal{I} \ll 1$ then equivalent circuit model Moyles.
- If $\mathcal{I}_*$ small, then single particle model.
- If $\mathcal{I}$ small, electrolyte only model.
- If both $\mathcal{I}_*, \mathcal{I}$ are $O(1)$, the P2D model is appropriate.

P2D Model

Spherical Particles



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

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

to

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

D_u should include tortuousity effects.

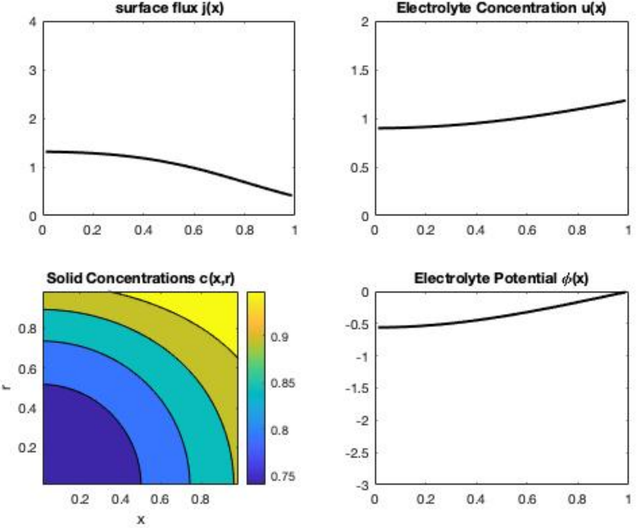
Computations

Implemented the P2D model in MATLAB:

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

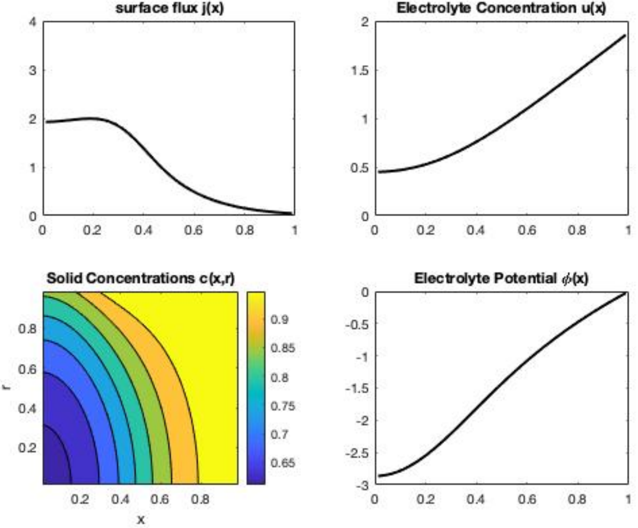
Computations

$\mathcal{I} = 1$ and $\mathcal{I}_* = 1$



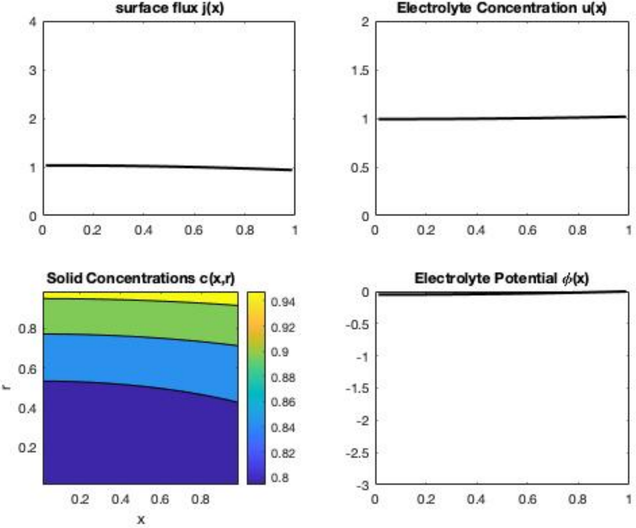
Computations

$\mathcal{I} = 1$ and $\mathcal{I}_* = 4$



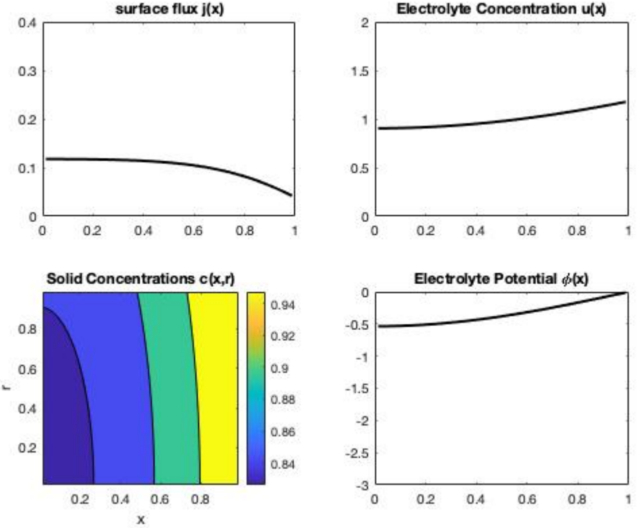
Computations

$\mathcal{I} = 1$ and $\mathcal{I}_* = 1/10$) near SPD



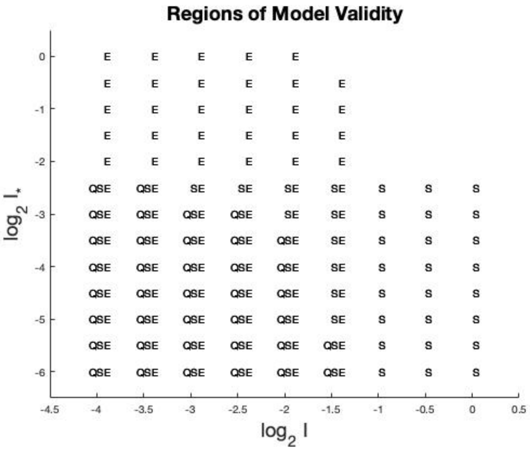
Computations

$\mathcal{I} = 1/10$ and $\mathcal{I}_* = 1$ near ELM



Criteria for model selection

Using a computational accuracy criteria, the regions where the reduced models give sufficient accuracy are shown below.



Additional Computational Work

Current implementations (e.g. COMSOL Multiphysics, Oxford's PyBaMM) of the P2D model are too slow for real time estimation and control in battery management systems.

with McKay and Gopaluni

- Machine Learned battery models based on SPD simulation.
- Incorporate data to correct SOC and adjust for SOH.

with Han and Macdonald

- Fast Solver using traditional numerical linear algebra ideas.
- Pre-elimination of the tridiagonal problems for concentrations in each particle.
- A banded system with only electrolyte variables results.

Summary

- Rechargeable Lithium Ion Battery basics
- Scaling that leads to the P2D model
- Computational results
- Quantitative reduced model selection criteria