Machine Learning of Electrochemistry Battery Models

Maricela Best McKay, Bhushan Gopaluni, Brian Wetton

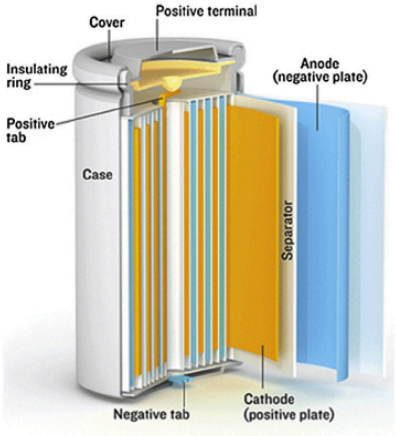
Mathematics Department
University of British Columbia
wetton@math.ubc.ca
www.math.ubc.ca\~wetton

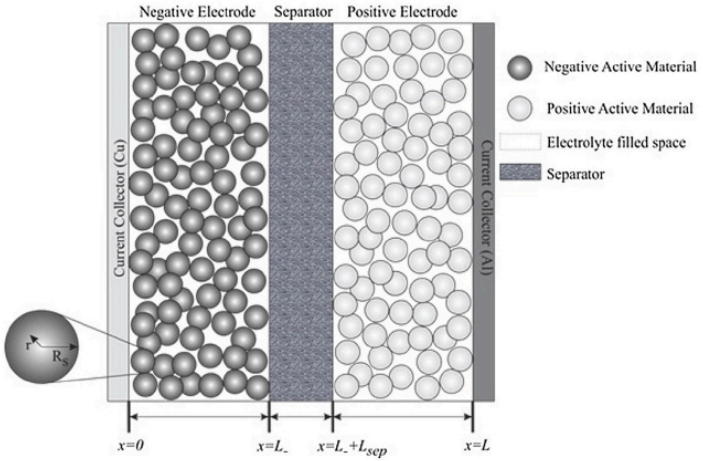
UBC Institute of Applied Mathematics

- Faculty participation from many departments.
- Interdisciplinary graduate program.

Lithium Ion Batteries

Open up the Battery

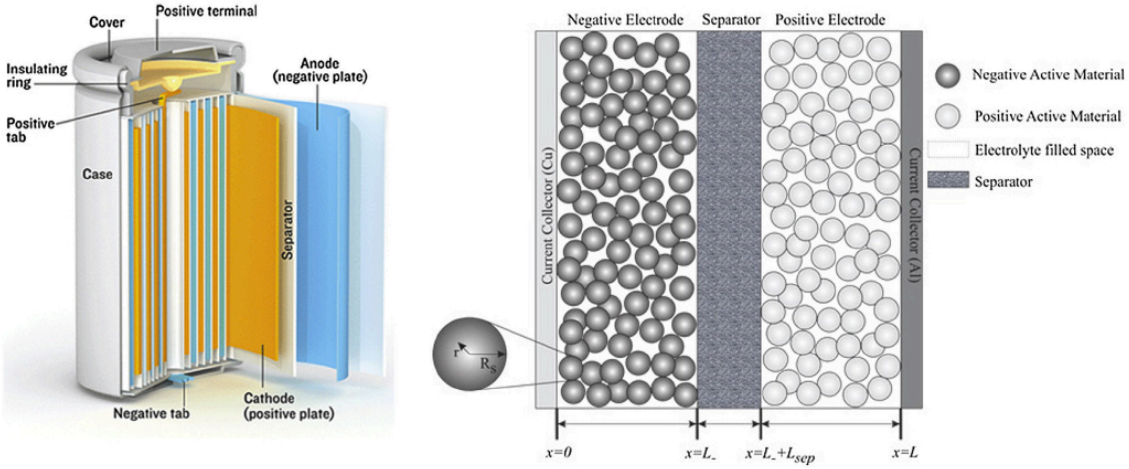




- Negative Electrode: Graphite
- Positive Electrode: Lithium Cobalt Oxide
- Electrolyte: Lithium salt in an organic solvent
- Intercalation: Energetically favourable in the positive electrode
- Lithium moves from negative to positive in discharge.

Pseudo Two Dimensional (P2D) Model

Single Electrode Domain



Solid: intercalated Lithium $c(r, t; x)$ 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

Scaled Asymptotic Equations

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

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

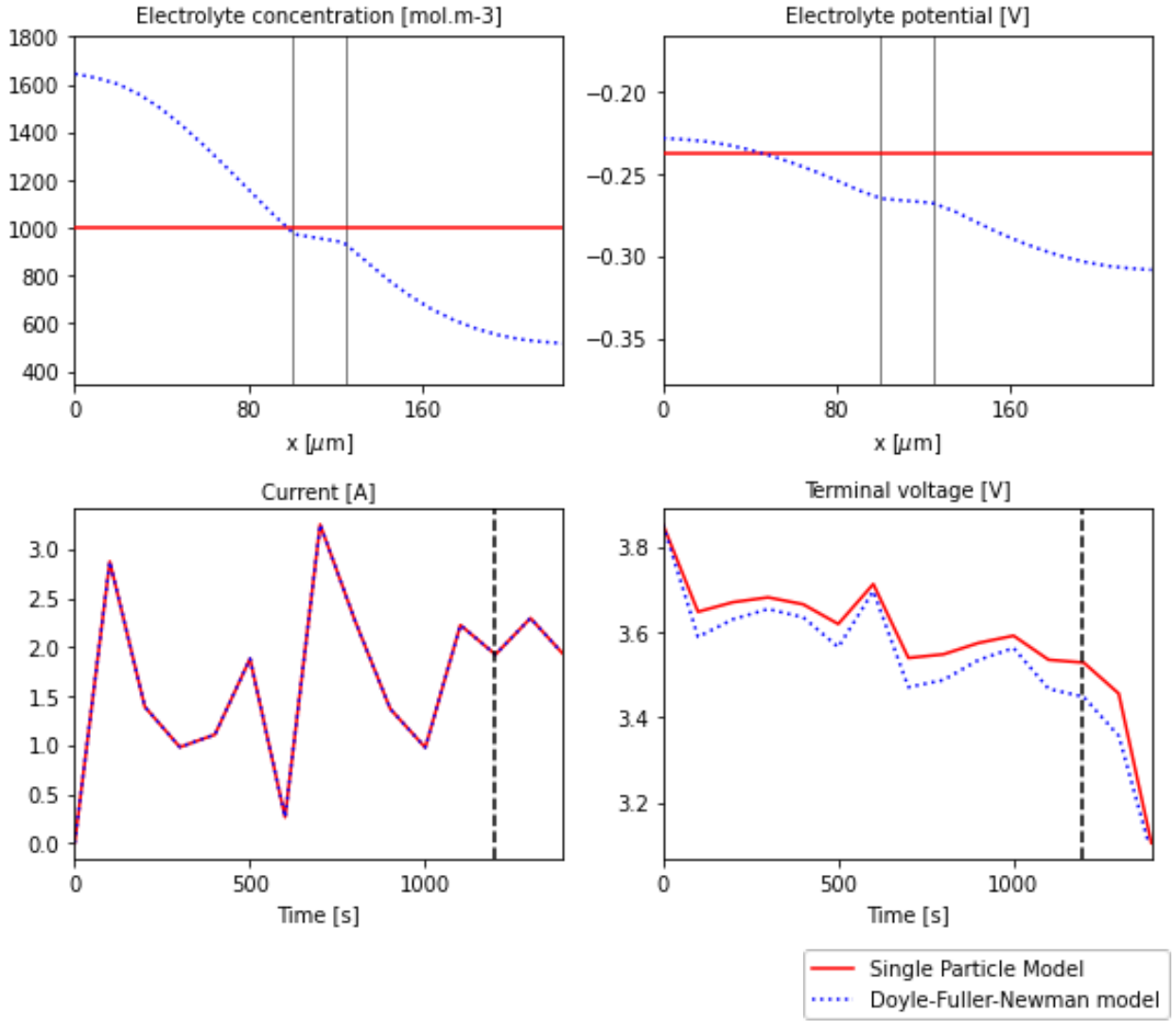
- If $\mathcal{I}_*, \mathcal{I} \ll 1$ then equivalent circuit model Moyles.
- If $\mathcal{I}_*$ small, then single particle model.
- If $\mathcal{I}$ small, electrolyte only model.
- If both $\mathcal{I}_*, \mathcal{I}$ are $O(1)$, the P2D model is appropriate.

Machine Learned P2D

- P2D model computationally intensive to compute.
- Replace surrogate computations of the P2D (in PyBaMM) with a deep neural network.
- Simulate a driving cycle with random currents, starting at full charge. Predict:
  - voltages every 100 seconds.
  - "hidden" particle concentrations.
  - battery failure.

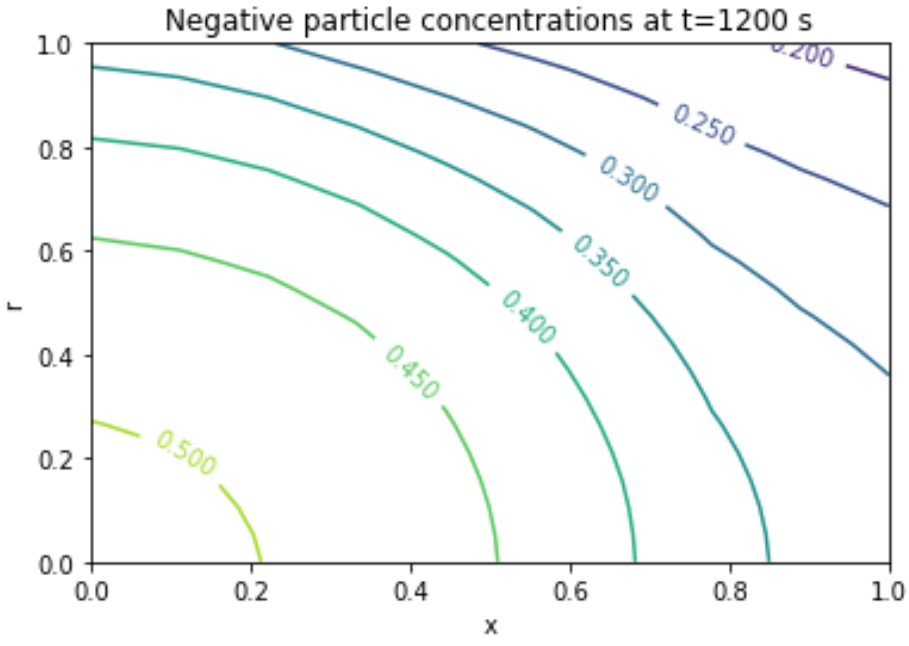
Machine Learned P2D

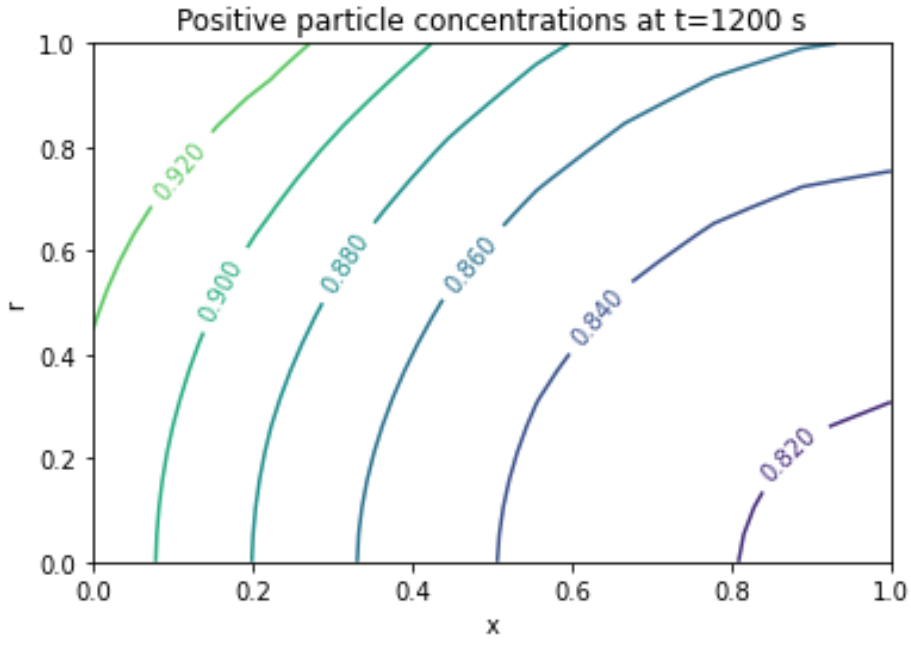
Driving Cycle



Machine Learned P2D

Particle Concentrations

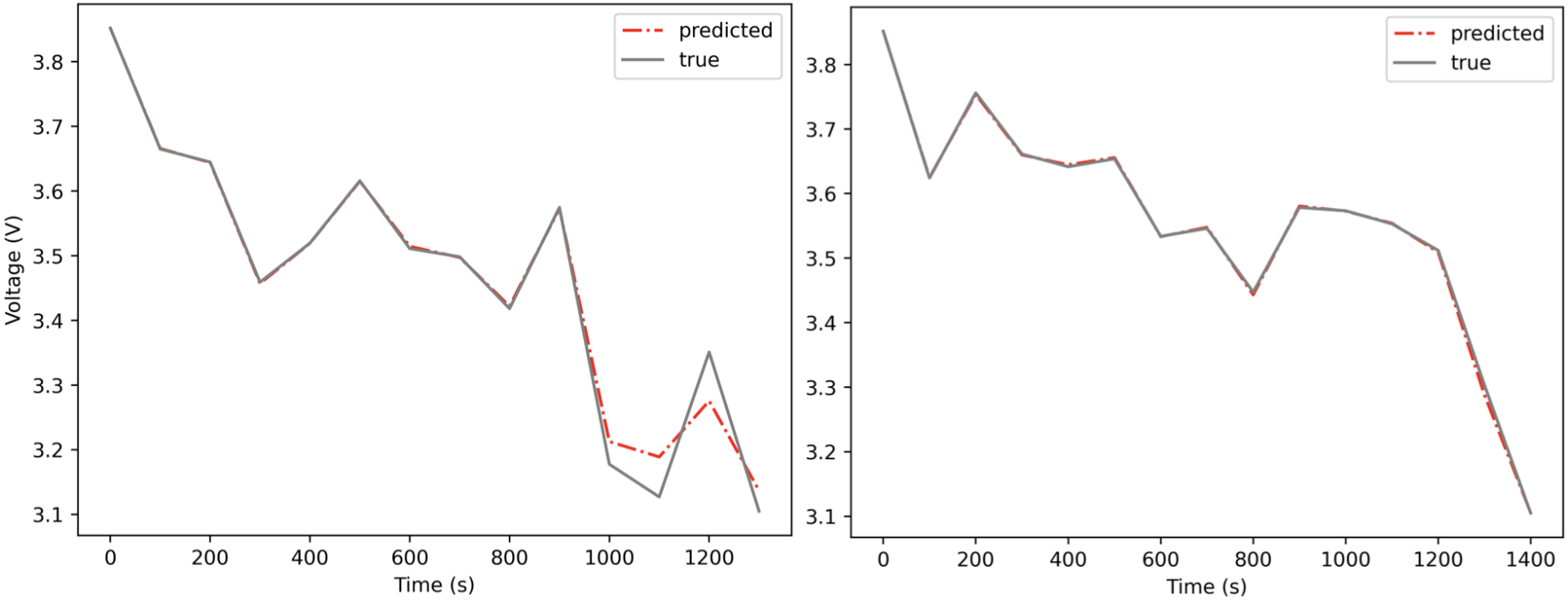




Computational resolution 20×20

Machine Learned P2D

K-Step Voltage Prediction



"Worst" case result (left), average case (right).

1.5% average maximum error in Voltage, 6% in Concentrations

Machine Learned P2D

NN Architecture

- Inputs: I_0, I_1, V_0, $C_{0,n}$, $C_{0,p}$
- Outputs: V_1, $C_{1,n}$, $C_{1,p}$, P_{failure}
- Three ReLU-activated convolutional layers each followed by a Max-Pooling layer ($C_{0,n}$ and $C_{0,p}$ considered as images).
- Two fully connected layers, I_0, I_1, V_0 added.
- Two separate final layers: one for V_1, $C_{1,n}$, $C_{1,p}$ (flattened) and one for failure probability (logistic regression).

Training:

- 15,000 simulations for training, 3,000 testing
- Stochastic optimization using ADAM optimizer
- Scaled mean squared error loss function

More Results

Failure Prediction

Threshold %	False Negative %	False Positive %
10	0	1.72
20	0.08	1.2

False Negatives are unpredicted failures

More Results

Predicting SOH

- SOH parameter $\gamma \in (0, 1]$. Currents $I \to I/\gamma$ in the model, combines effects:
  - Reduced capacity (uniform loss of active catalyst)
  - Increased electrolyte resistance
- Post-processing voltage curves (grid search) gives 2-3 digit accuracy for γ after 5 cycles.

Summary

- Computationally intensive electrochemical models for batteries can be replaced by computationally cheap ML surrogate models for given driving cycles.
  - PyBaMM run 23 seconds; ML 65 milliseconds
- Voltages and failure accurately predicted.
- Hidden variables (concentrations) also accurately predicted.
- SOH parameters can be identified.
- (future work) Real data can be incorporated into the surrogate model.