56th Battery Conference Japan, Nagoya, Japan, 11-13th, November, 2015

Analytical Modelling of Planar Potential and Current Distributions in Electrodes of Lithium-Ion Batteries

D. Adair[1*], T. Hara[2], Y. Massalin[1,] K. Ismailov[1] and Z. Bakenov[1,2]

[1] Nazarbayev University, Astana, 010000, Kazakhstan
[2] Institute of Batteries, Astana, 010000, Kazakhstan

NAZARBAYEV UNIVERSITY

Institute of Batteries

*Corresponding author: dadair@nu.edu.kz

Introduction

- Mathematical modelling can play an important role in the design of a lithium-ion cell in that many design iterations can be performed at relatively little cost.

- Electrochemical models are useful for cell design and optimization but can be typically high-order and complex and hence computationally expensive, and, are therefore not suitable for real-time applications.

- Much reduced order electrochemical models for lithium-ion cells have been developed, with these type of models more suitable for use with real-time on-board electronic control units.

- However, a difficulty with these methods is that the current-voltage behavior for different operating conditions cannot be predicted.

Present Work

- In the present work, a two-dimensional model for a lithium-ion battery is developed.

- Calculations of the potential and current density distributions during discharge on the electrodes of a lithium-ion battery using a procedure similar to Kwon *et al.*[1].

- A simple concentration-independent polarization expression is used to describe the collective behavior of complex processes in the electrolyte solution between the electrodes.

[1]K. H. Kwon, C. B. Shin, T. H. Kang, C.-S. Kim, J. Power Sources 163 (2006) 151-157.

Experimental Battery to be Simulated

- The cell considered here is a Zn/ $LiFePO_4$ aqueous pouch cell.
- Dimensions of the battery layers and position of tabs are given in Table 1.
- Thickness and electrical conductivity of battery components listed in Table 2.

Table 1: Dimensions of electrode domains in *x*-*y* plane

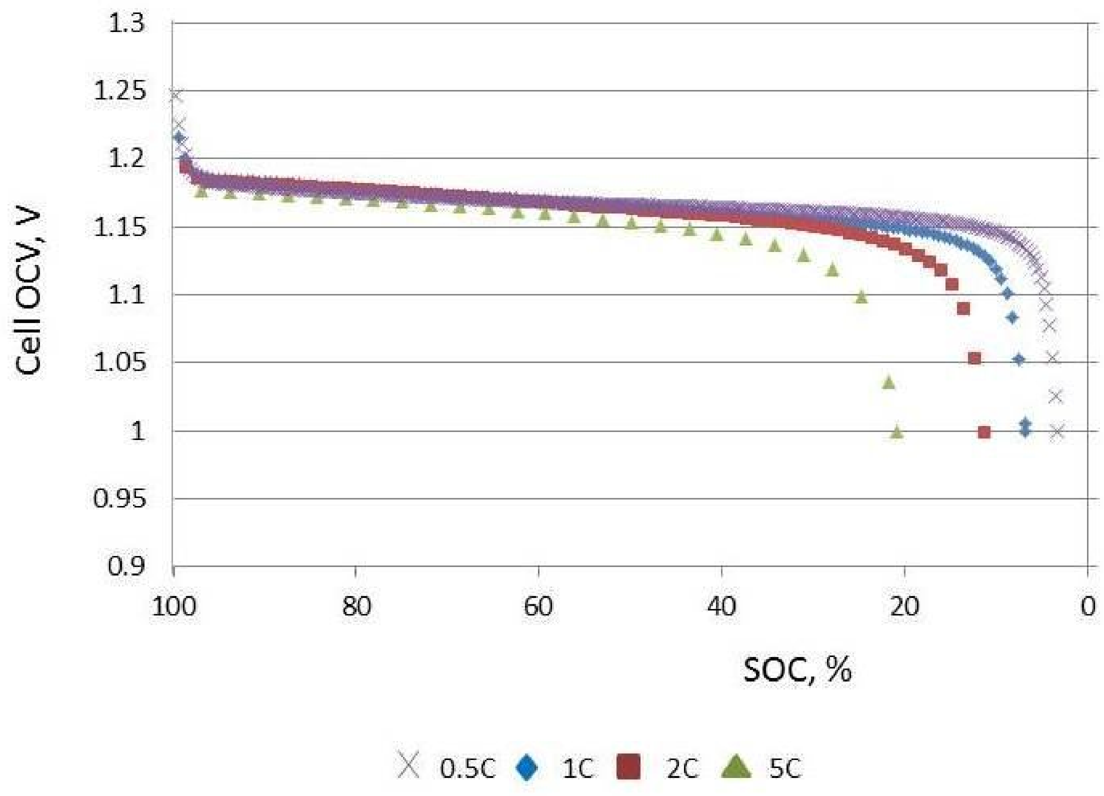
Electrode	w (m)	h (m)	t (m)	l_i (m)
Positive	19.5×10^{-3}	30.0×10^{-3}	2.00×10^{-4}	4.25×10^{-3}
Negative	19.5×10^{-3}	3.00×10^{-3}	2.00×10^{-4}	14.0×10^{-3}

Table 2: Thickness and electrical conductivity of components in cell

Material/layer	Thickness, δ (m)	Electrical conductivity (S m^{-1})
Graphite Paper/Positive electrode	380×10^{-6}	$2.12 \text{ x}10^{3}$
Zinc/Negative electrode	100×10^{-6}	16.6×10^{6}
Separator sheet	650×10^{-6}	–

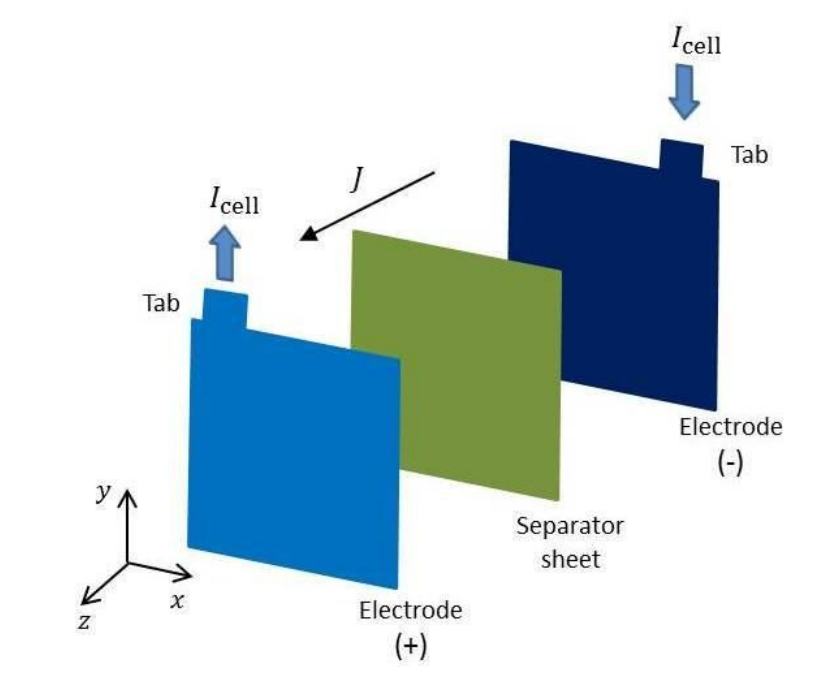
Experimental Battery to be Simulated

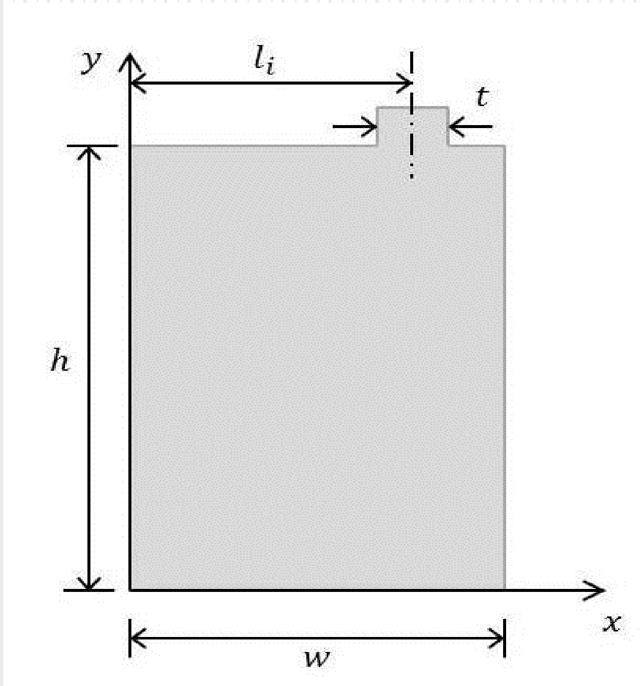
Voltage response of the experimental battery at various C-rates (0.5C, 1C, 2C and 5C) at a temperature of 25°C are shown below for experimental battery to be simulated.



Formulation of the Problem

- Each cell assembly includes a negative electrode, a positive electrode with a separator sheet in between.





Formulation of the Problem

- By considering continuity of current the governing differential equation for the charge balance for each electrode is

$$\frac{1}{r_j}\left(\nabla^2 V_j\right) = -\frac{\mathbf{J}\cdot\mathbf{n}_j}{\delta_j} \qquad (j = p, n), \qquad V_j = V_j(x, y)$$

- The reaction current density vector on the electrodes is $\mathbf{J} = \{J_x, J_y, J\}$ with $J_x \to 0$ and $J_y \to 0$

- Boundary conditions for positive electrode (negative b.c.s are similar)

$$-\frac{1}{r_p}\frac{\partial V_p}{\partial x} = 0 \quad \text{at} \quad x = 0$$

$$-\frac{1}{r_p}\frac{\partial V_p}{\partial x} = 0 \quad \text{at} \quad x = w$$

$$-\frac{1}{r_p}\frac{\partial V_p}{\partial y} = 0 \quad \text{at} \quad y = 0$$

$$-\frac{1}{r_p}\frac{\partial V_p}{\partial y} = i_{tab,p} \text{ at } l_p - \frac{t}{2} < x < l_p + \frac{t}{2}, y = h$$

$$-\frac{1}{r_p}\frac{\partial V_p}{\partial y} = 0 \text{ at } l_p + \frac{t}{2} < x < l_p - \frac{t}{2}, y = h$$

Polarization Expression

- Distribution of the reaction current J is dictated by the local rate of electrochemical reactions in the electrodes.

- A linear polarization expression can be assumed as

$$J(x, y) = Y\left[V_p(x, y) - V_n(x, y) - V_{oc}\right]$$

- The current of cell assembly I_{cell} and the current of battery I_{batt} are related to J via

$$I_{cell} = \int_0^w \int_0^h J(x, y)dy\, dx \quad \text{and} \quad I_{batt} = I_{cell}N$$

where N is the number of cell assemblies inside the battery core.

Polarization Expression

- In the mathematical model both Y and V_{oc} are considered to solely depend on DOD with their dependency expressed in polynomial form

$$Y = \sum_{l=0}^{L} \mathcal{C}_l (\text{DOD})^l \qquad V_{oc} = \sum_{m=0}^{M} \mathcal{D} (\text{DOD})^m$$

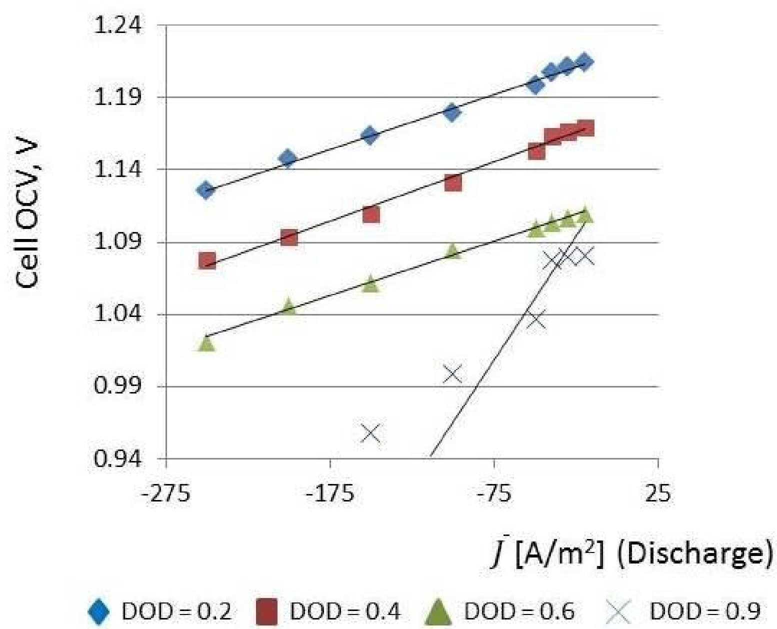
where $\mathcal{C}_l$ and $\mathcal{D}_m$ are the constants determined from experiments during constant-current discharge.

- In this work, DOD is defined as

$$\text{DOD}(t) = \text{DOD}(0) + \frac{1}{3600 Q_{cell}} \int_0^t |I_{cell}(t)| \, \text{d}t$$

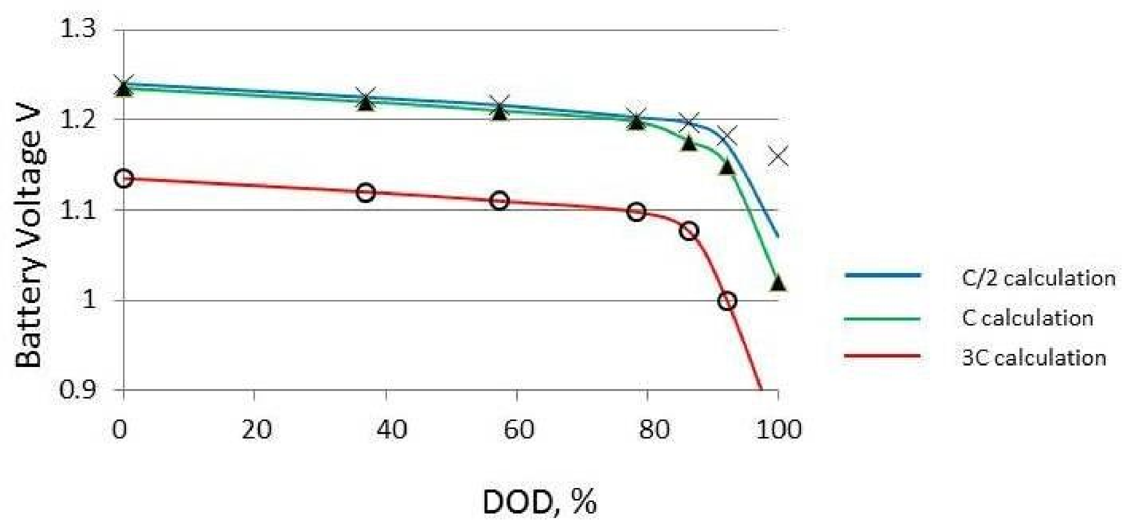
Polarization Expression

- To find $\mathcal{C}_l$ and $\mathcal{D}_m$ experimental data of the type used on the figure below was used



- In effect variations of the battery voltage versus reaction current density shown above by symbols can be represented by linear lines and Y is the inverse of the slope of the line and V_{oc} is the intercept.

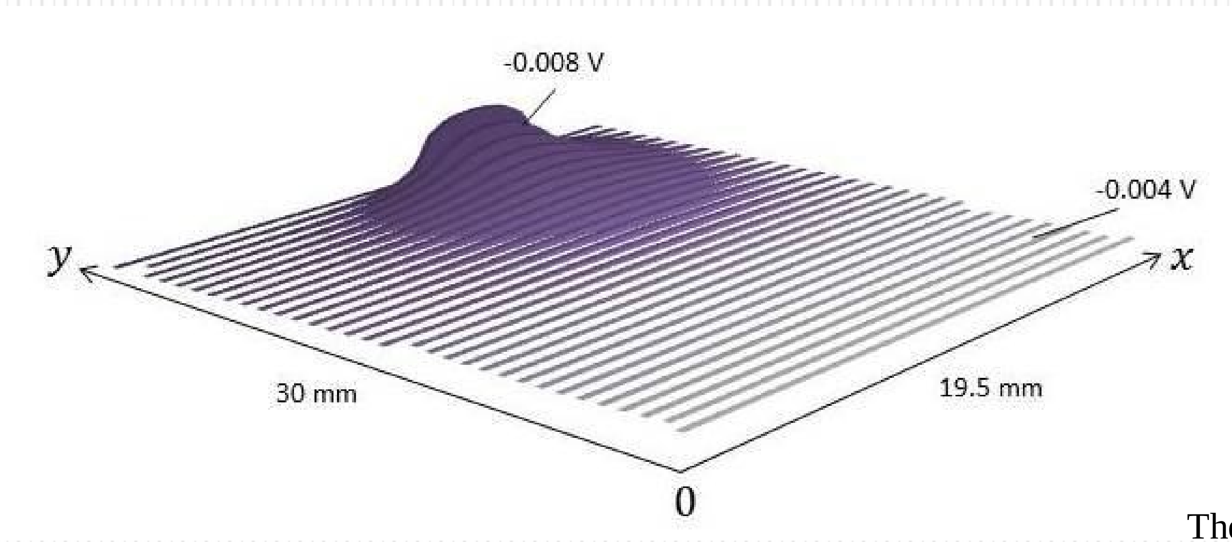
Some Results



- The figure above shows voltage response of battery at some different discharge rates.
- The lines are the calculations and the symbols are experimental measurements.
- Generally the results are in good agreement except for extreme discharge rates.
- Disagreement started to occur for 0.5 > C > 5 and much disgreement for C > 10 rates

Some Results - negative electrode

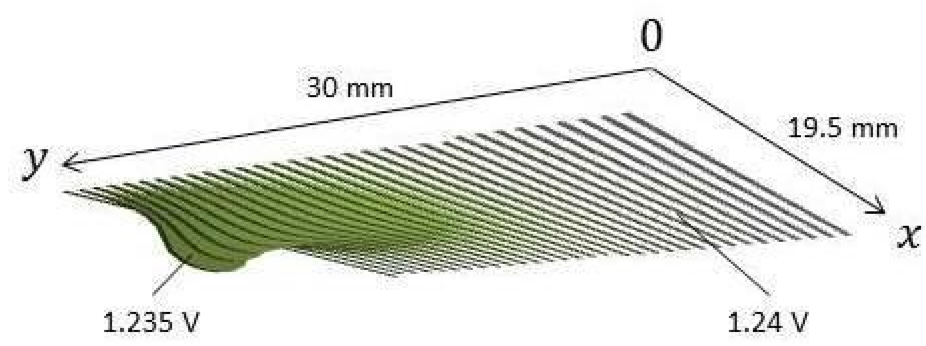
- Potential distribution on the negative electrode (DOD = 10%, 1 C - rate discharge).



The variation of potential was found to be of the order of millivolt.

Some Results - positive electrode

- Potential distribution on the positive electrode (DOD = 10%, 1 C - rate discharge).



The variation of potential was found to be of the order of millivolt.

- Numerical calculations have been carried out to solve the above equations together with appropriate boundary conditions. It should be noted the above Poisson equations for positive and negative domains are non-homogeneous and strongly coupled via their source terms.

Thank you