Stanford | SCHOOL OF EARTH, ENERGY & ENVIRONMENTAL SCIENCES

Homework 4 (120 points)

ENERGY 294 - Electrochemical Energy Storage Systems: Modeling and Estimation

Spring Quarter 2018

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Due May 25, 2018 at 12:01 PM (Electronic pdf copy in CANVAS and hard-copy to the TA)

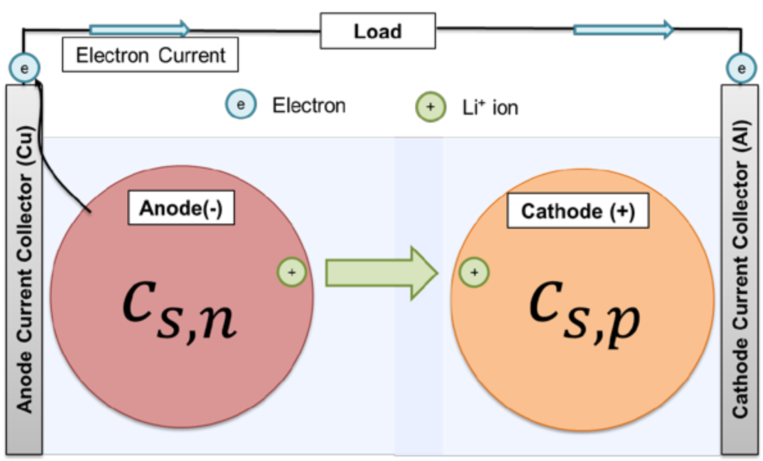
The objective of this homework is to learn how to 1) implement the single particle model (SPM) in Matlab/Simulink, and 2) perform parameter identification and model validation using data from experiments conducted on the US18650VTC4 lithium-ion cell H1 and 3) carry out a sensitivity study to understand which parameters most influence the model-predicted output voltage. The data sets provided to you are summarized below:

Data Set	Temperature	Utilization
1 C-rate capacity test in discharge	23°C	Problems 1 and 3
2 C-rate capacity test in discharge	23°C	Problem 2 a)
5 C-rate capacity test in discharge	23°C	Problem 2 b)
Urban Dynamometer Driving Schedule (UDDS) test	23°C	Problem 2 c)
US06 test	23°C	Problem 2 d)
0.025 C-rate capacity test in discharge	23°C	Problem 2 d)

use for Voc-SOC relationship

Problem 1: Parameter Identification (60 points)

The schematic of a single particle model is shown in the figure below. This model predicts battery terminal voltage by resolving concentration dynamics in the electrodes during charge/discharge through the mass transport equation.



Implement the SPM in MATLAB/Simulink and identify the parameters of this model, defined by the vector θ:

$$\theta = \left[L_n\ L_p\ R_{s,n}\ R_{s,p}\ A_{cell}\ x_{100\%,n}\ x_{0\%,n}\ y_{100\%,p}\ y_{0\%,p}\ c_{s,max,n}\ c_{s,max,p}\ \varepsilon_{s,n}\ \varepsilon_{s,p}\ i_{0,n}\ i_{0,p}\ D_{s,n}\ D_{s,p}\ R_c\right]^T$$

Use the *ga* algorithm for parameter identification. A root mean square (RMS) error of less than 5% is expected to be achieved. The percentage RMS error must be calculated using the expression

$$RMS = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(V_{exp}(i) - V_{SPM}(\theta; i)\right)^2} \cdot \frac{100 \cdot N}{\sum_{i=1}^{N} V_{exp}(i)},$$

where V_{exp} is the experimentally measured voltage response, V_{SPM} is the model-predicted voltage response that is a function of θ, N is the total number of data samples, and i is the time index.

During identification, the following constraints **must** be satisfied:

a) The thickness of the anode must be greater than the thickness of the cathode.

b) The maximum lithium storage concentration of the cathode is greater than the maximum lithium storage concentration of the anode.

c) The cathode is the limiting electrode.

d) The N/P ratio (ratio of capacity of the anode and the capacity of the cathode) must be equal to 1.10 [1]. The authors of [1] report that an N/P ratio of 1.10 can be effective in suppressing the lithium plating battery degradation mechanism.

The initial guess for the elements of the vector θ can be obtained by reviewing the reference paper [2]. Tabulate the results of the identification study. Report the overall achieved % RMS error, and provide a plot comparing the experimental and the model-predicted voltage response.

Problem 2: Model Validation (30 points)

The identified SPM based on the *ga* approach must be validated against the:

a) 2 C-rate capacity test in discharge data set.

b) 5 C-rate capacity test in discharge data set.

c) The UDDS driving cycle profile. Consider only the dynamic charge/discharge portion.

d) The US06 driving cycle profile. Use the 0.025 C-rate capacity test in discharge data set to obtain the open circuit voltage (OCV) vs. state-of-charge (SoC) plot. Then determine the cell SoC at the beginning of the US06 test. Using the definition of the anode and cathode bulk SoC from the Lecture 8 slides, calculate the initial electrode concentration values.

For each of the four validation data sets, report the % RMS error obtained from model validation, and provide a plot comparing the experimental and the model-predicted voltage response.

Problem 3: Sensitivity Analysis (30 points)

Using the input current profile that was used for the SPM identification, perform the following tasks:

a) Analyze the sensitivity of the model-predicted voltage using the identified values from the *ga* algorithm between the voltage range of 4.20 V and 2.50 V. This analysis must be conducted by varying only one element of the vector θ at a time. If we denote the parameter being varied as θ_i, then the sensitivity analysis must be carried out for the following scenarios:

   i. A 10% decrease in θ_i while keeping all the remaining parameters fixed.

   ii. A 10% increase in θ_i while keeping all the remaining parameters fixed.

   For each scenario, tabulate the value of the sensitivity of the model. The sensitivity can be defined as follows:

   Let f be a function that describes the relationship between the output of a model y, the states of the model x, the input u, and the model parameters θ, i.e. $y = f(x, u, \theta)$.

   For a given set of values of the parameters θ_0, we have an output $y_0 = f(x, u, \theta_0)$. The sensitivity of the output to the model parameters can then be defined as:

$$\frac{\partial y}{\partial \theta} = \frac{\|\Delta y / y_0\|}{\|\Delta \theta / \theta_0\|},$$

   where $\|\cdot\|$ represents the Euclidean norm. The Euclidean norm of a vector $\boldsymbol{x} = (x_1, x_2, \cdots, x_n)$ is given by:

$$\|\boldsymbol{X}\|_2 = \sqrt{x_1^2 + x_2^2 + \cdots x_n^2}.$$

   Based on the results, tabulate the parameters of the models in decreasing order of sensitivity, i.e. the parameter for which the model output is most sensitive, to the parameter for which the model output is least sensitive.

b) From the table generated, select the top three parameters. Illustrate the voltage response for the baseline (original identified values), the 10% decrease, and the 10% increase, on the same plot for each of these 3 parameters. A total of three plots must be provided.

c) Comment on the results observed from the sensitivity studies. What can you infer about the identifiability of the SPM parameters based on this study?

Note:

1) Submit all the Matlab files pertaining to this homework in a zipped folder. Report all calculations in your submitted pdf.

2) All the experiments are conducted using an Arbin BT-2000 tester, for which the current convention is positive during charge and negative during discharge. As mentioned in the slides, the general current convention is the opposite for charge and discharge.

References:

1. C-S. Kim, K. M. Jeong, K. Kim, and C-W. Yi, "Effects of Capacity Ratios between Anode and Cathode on Electrochemical Properties for Lithium Polymer Batteries", *Electrochimica Acta*, vol. 155, pp. 431-436, (2015). DOI: https://doi.org/10.1016/j.electacta.2014.12.005

2. T. R. Tanim, C. D. Rahn, and C-Y. Wang, "State of charge estimation of a lithium ion cell based on a temperature dependent and electrolyte enhanced single particle model", *Energy*, vol. 80, pp. 731-739, (2015). DOI: https://doi.org/10.1016/j.energy.2014.12.031