ENERGY 294 Homework 3

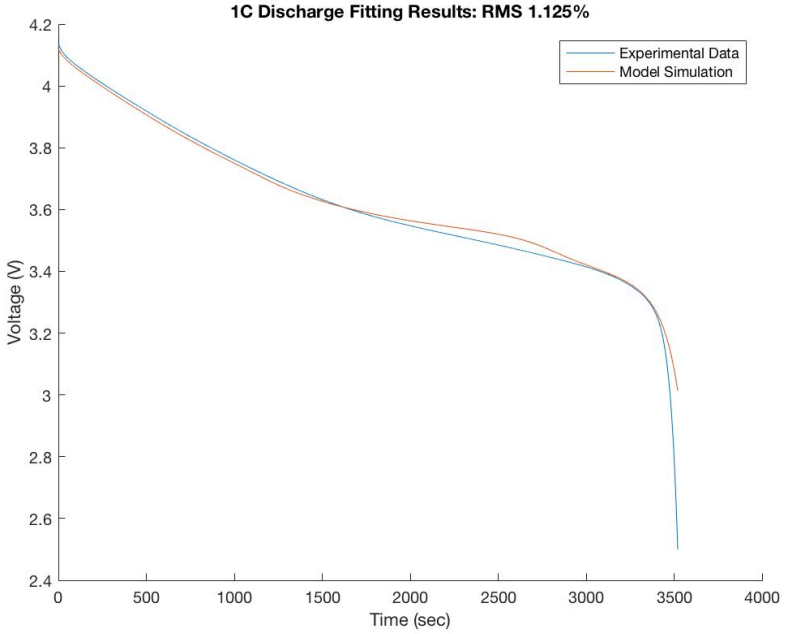
Sam Kramer

May 26, 2018

1 Problem 1: Parameter Identification

The upper and lower bounds used for the parameters and the final results can be seen in the table below. The overall RMS error achieved was 1.125%. Figure 1 shows the fit of these optimal parameters in comparison with the experimental data.

Parameter	Units	Lower Bound	Upper Bound	Result
L_n	m	4.50E-05	8.00E-05	6.42E-05
L_p	m	2.00E-05	4.50E-05	4.05E-05
R_n	m	1.00E-06	9.00E-06	8.92E-06
R_p	m	1.00E-06	9.00E-06	7.99E-06
A_{cell}	m^2	0.08	0.125	9.79E-02
$x_{100\%,n}$	-	0.6	0.95	7.58E-01
$y_{100\%,p}$	-	0.15	0.55	3.39E-01
$y_{0,p}$	-	0.8	1	9.41E-01
$C_{s,max,n}$	$mol\ m^{-3}$	22000	37000	2.91E+04
$C_{s,max,p}$	$mol\ m^{-3}$	43000	56000	4.47E+04
$\epsilon_{s,n}$	-	0.4	0.7	5.96E-01
$\epsilon_{s,p}$	-	0.4	0.7	6.86E-01
$i_{0,n}$	$A\ m^{-2}$	14	56	1.40E+01
$i_{0,p}$	$A\ m^{-2}$	10	40	3.99E+01
$D_{s,n}$	$m^2\ s^{-1}$	1.40E-15	1.40E-13	2.36E-14
$D_{s,p}$	$m^2\ s^{-1}$	2.00E-15	2.00E-13	4.99E-14
R_c	Ω	6.00E-05	5.00E-02	4.45E-02

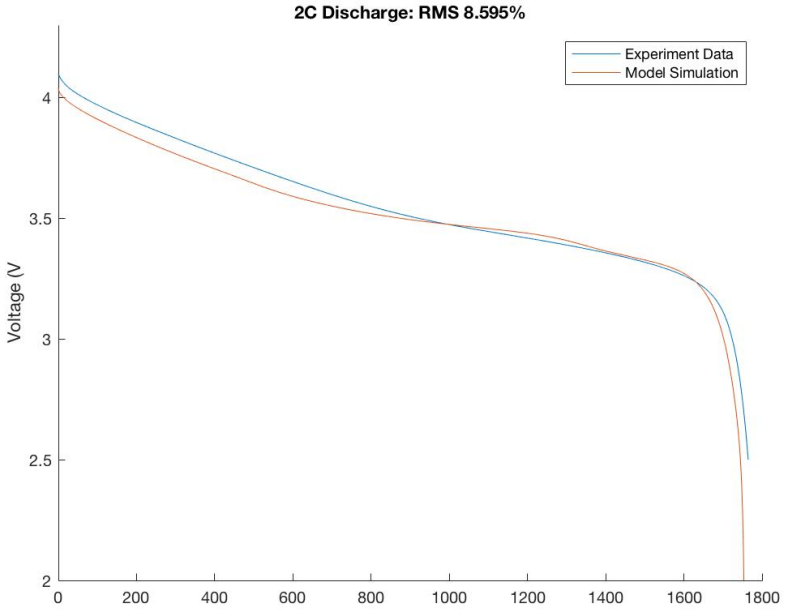


2 Problem 2: Model Validation

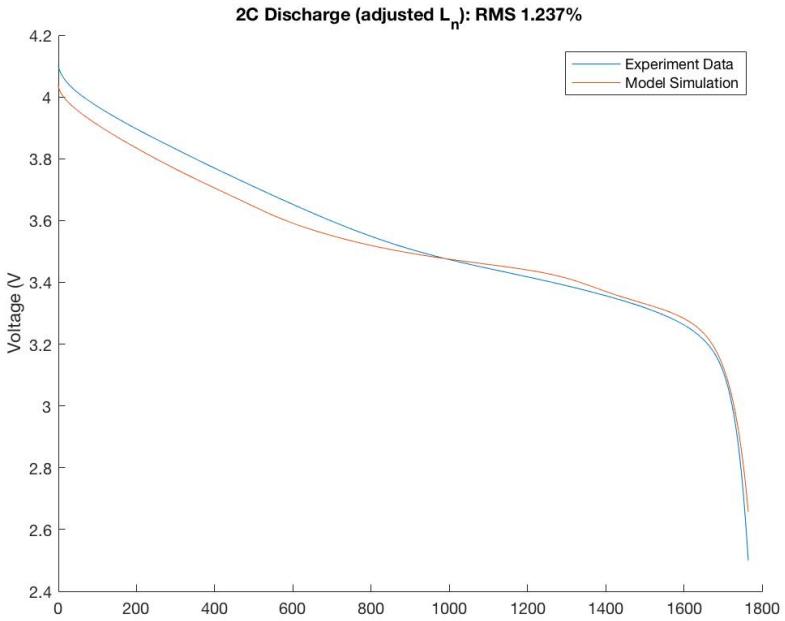
The RMS for each validation can be seen in the title of the accompanying plot.

2.1 2a) 2C Capacity Test

In this validation, the voltage of the cell fell quickly to a negative value at the end of the discharge cycle. This is because the optimized parameters do not allow for sufficient charge to be extracted from the battery under a 2C discharge current, so the concentration in the anode becomes negative.

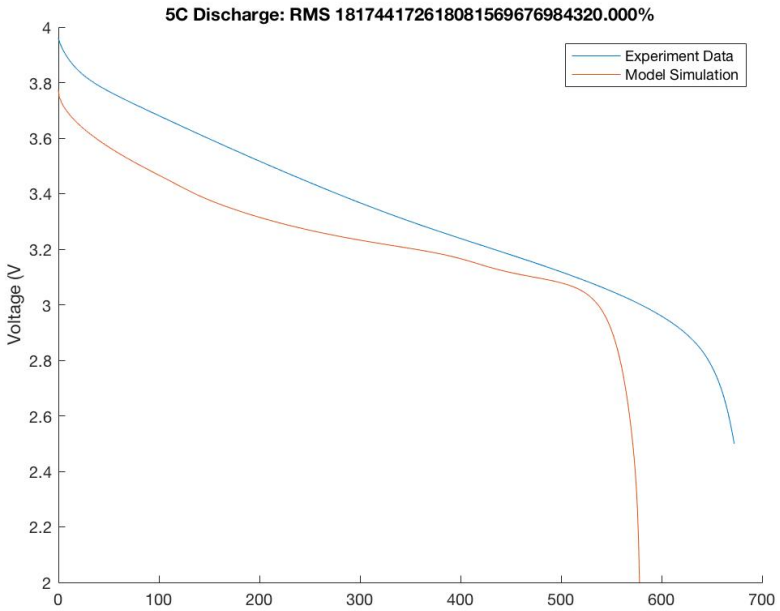


The parameter L_n was increased by 1.5% in order to give the battery enough capacity to model the 2C discharge profile. A plot of this fit is shown below.

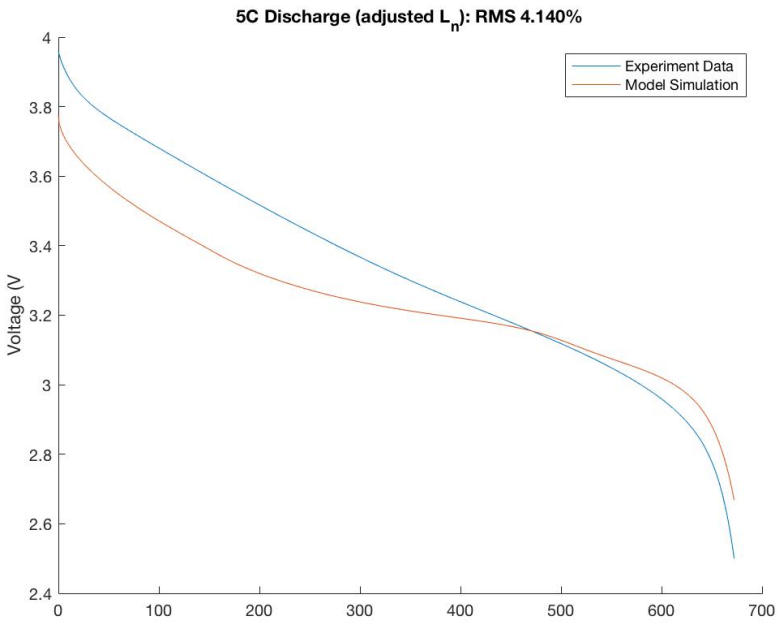


2.2 2b) 5C Capacity Test

Similarly to the 2C capacity test case, there is not enough capacity in the battery with these model parameters to allow for discharge without reaching negative voltage. This model falls rapidly to a negative voltage of large magnitude.



Again, the L_n parameter was increased, this time by 15%. This model was run again and the fit can be seen below.



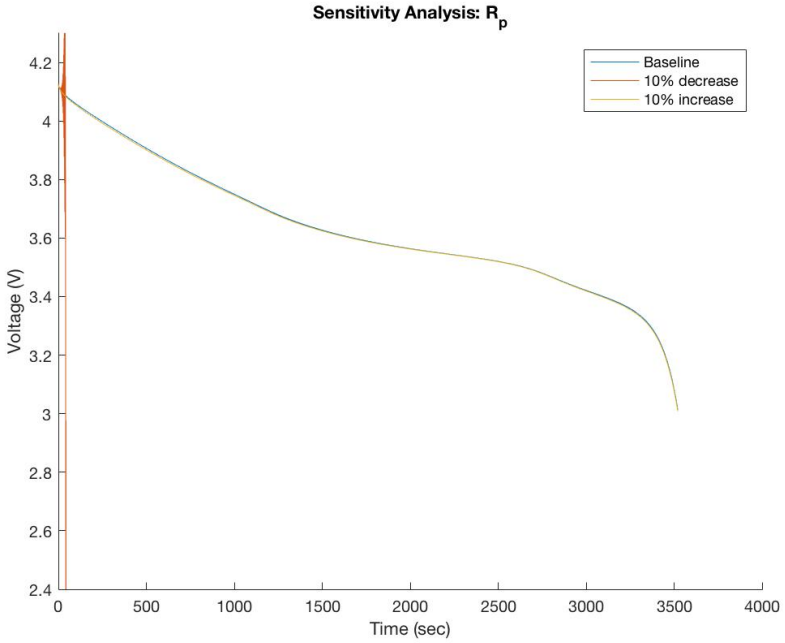
3 Problem 3: Sensitivity Analysis

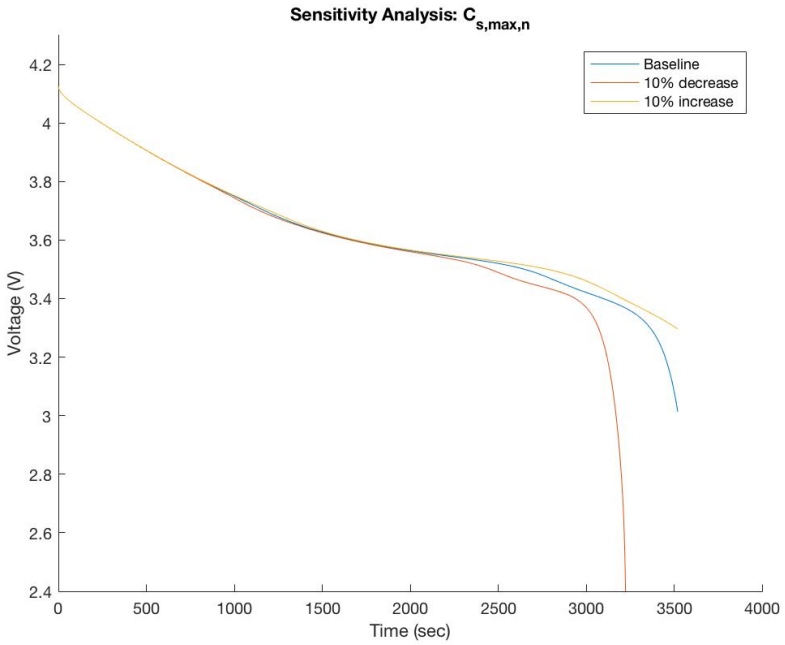
3.1 3a) Tabulation of Parameters

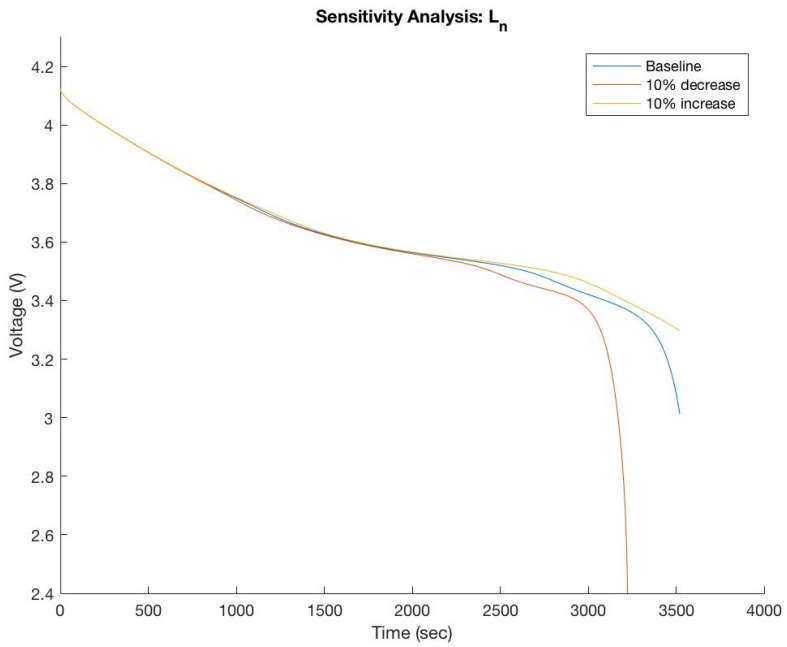
Parameter	10% Decrease	10% Increase
R_p	NaN	8.58E+00
L_n	1.26E+19	1.51E+01
A_{cell}	1.26E+19	1.85E+01
$C_{s,max,n}$	1.26E+19	1.51E+01
$\epsilon_{s,n}$	1.26E+19	1.51E+01
$x_{100\%,n}$	1.81E+17	1.54E+01
$y_{100\%,p}$	1.18E+01	9.69E+00
$C_{s,max,p}$	8.72E+00	1.17E+01
L_p	8.71E+00	1.17E+01
$\epsilon_{s,p}$	8.71E+00	1.17E+01
R_n	1.09E+01	5.12E+00
$D_{s,n}$	6.89E+00	9.87E+00
R_c	9.15E+00	8.42E+00
$D_{s,p}$	8.61E+00	8.72E+00
$i_{0,n}$	8.66E+00	8.68E+00
$i_{0,p}$	8.68E+00	8.66E+00
$y_{0,p}$	8.67E+00	8.67E+00

3.2 3b) Sensitivity Plots

Several of the parameters had similar levels of sensitivity, so only 3 were used for plotting.







3.3 3c) Commentary

The model seems quite sensitive to some parameters, while much less sensitive to others. It is most sensitive to the anode parameters which affect the calculated capacity of the anode. This is intuitive because the genetic must meet this constraint and a slight perturbation will drastically affect the model. A slight decrease in any of these parameters will result in a model of the battery which does not have an appropriate storage capacity in the anode, so the model will calculate negative capacities at the anode and the model will go to extremely unphysical values. Increasing these parameters, however, does not change the model much since there is simply slightly more capacity than necessary, which is why the voltage does not drop as steeply as it should at the end of the profile. I think that this model finds a reasonably good approximation of the system parameters, but it is by no means perfect. These parameter estimates should be taken with a grain of salt and more complexity may be needed in the model to successfully identify the parameters.