rLoop Revolectrix Cell Model – release 1

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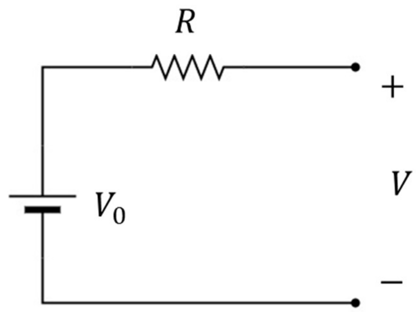
This model will simulate the electrochemical performance and thermal response of a single Revolectrix YS5000 1S RL cell attached to a one phase change material (PCM) unit. The model outputs cell voltage, cell current, and cell temperature. Model has been validated with testing data acquired during 2016 Q4. The model is written in Matlab and is fully compatible with GNU Octave.

The cell is modeled as a voltage source in series with a resistor; and as a simple lump mass with a thermal path to a heat sink. The PCM is modeled as a simple lump mass with a variable heat capacity. The cell's voltage will change as a function of SOC (State-of-Charge) and the resistor's value changes as a function of cell temperature.

Contents

Governing Equations

The cell is modeled with a very simple equivalent circuit model



Cell voltage is:

$$V = V_0 + IR$$

Equation 1

Here, V_0 is the open circuit voltage, I is the current through the cell, R is the cell resistance, and V is the cell terminal voltage. In a constant power (P) situation, the equation becomes:

$$V = V_0 + \frac{P}{V}R$$

We solve for cell terminal voltage using the quadratic equation, giving us:

$$V = \frac{1}{2}\left(V_0 + \sqrt{V_0^2 - 4PR}\right)$$

Equation 2

In a constant load resistance (R_L) situation,

$$V = IR_L$$

$$V = \left(\frac{V_0}{R + R_L}\right)R_L$$

$$V = \left(\frac{R_L}{R + R_L}\right)V_0$$

Equation 3

The integral of current gives us the depth of discharge Q, which is used for calculating open circuit voltage and entropy change coefficient.

$$Q = \int Id$$

Equation 4

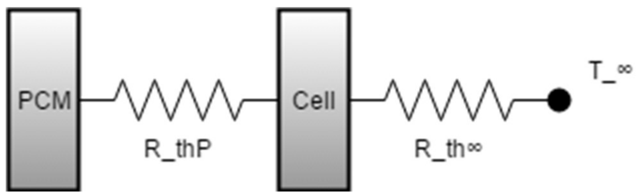
The cell's resistance value changes with temperature, and the value is expected to grow over life. We assign a double exponential fit to the resistance/temperature function and assign an aging factor.

$$R = f\left(k_1 e^{-\frac{T}{k_2}} + k_3 e^{-\frac{T}{k_4}}\right)$$

Equation 5

Here, f is the aging factor, and k_N are four fit factors to the resistance/temperature data.

The cell is treated as a lump mass with an internal heat generation term and two transfer terms: to ambient and to PCM.



$$mC\frac{dT}{dt} = I^2R + \frac{dV}{dT}TI - \frac{1}{R_{thP}}(T - T_P) - \frac{1}{R_{th}}(T - T_\infty)$$

Equation 6

Here, m is the mass of the cell, C is the specific heat capacity of the cell, T is the temperature of the cell, T_∞ is the temperature of the ambient (or heat sink), T_P is the temperature of the PCM, $R_{th\infty}$ is the thermal resistance to the environment, R_{thP} is the thermal resistance to the phase change material, dV/dT is the entropy change coefficient of the cell's chemistry. The entropy change coefficient is solely a function of SOC. The PCM thermal balance equation is

$$m_P C_P \frac{dT_P}{dt} = \frac{1}{R_{thP}}(T - T_P)$$

Equation 7

Here, m_P is the mass of the PCM, C_P is the specific heat capacity of the PCM. To model the phase change behavior, the PCM's specific heat capacity is variable with a constant baseline value and a large peak in the melting point. This simulates an increase in the thermal inertia of the PCM mass when passing through the melting temperatures, creating a near isothermal condition. The equation chosen is a Gaussian distribution, thus

$$C_P = C_{P0} + L\left(\frac{1}{\sqrt{\pi\Delta T^2}} e^{-\frac{(T_{melt} - T_P)^2}{\Delta T^2}}\right)$$

Equation 8

Here, C_{P0} is the specific heat capacity of the PCM, L is the latent heat capacity of the PCM, T_{melt} is the melting point of the PCM, ΔT is the melting temperature range.

The equations above describe a cell lump mass that heats up instantly evenly throughout the cell and that the sensing of cell temperature is infinitely fast. We see from comparing this model with the data obtained that it is unrealistic, especially in the very fast discharge scenarios. There must be some lag between the cell heat making its way from the interior of the cell towards the temperature sensor, so we define a first order lag to the sensor. The temperature sensor value is then governed by the following equation

$$\frac{dT_M}{dt} = \frac{1}{\tau}(T - T_M)$$

Equation 9

Here, T_M is the measured temperature of the cell, and τ is the sensor time constant

Equations 1 through 9 define the system's governing equations. The system has four states, the state of charge of the cell and the three temperatures (cell, PCM, and sensor).

Cell Data Analysis

The open circuit voltage is variable and depends on the depth of discharge of the cell. The cell's open circuit voltage was determined from three sources, which will be explained below:

- Revolectrix Data Sheet Analysis
- 2A Discharge Data from cell S/N 0394
- Kumerasan et al "Thermal Model for a Li-Ion Cell", 2008

The resulting three OCV curves are plotted on top of each other below to show that there is a good level of agreement. The data used in the model for OCV comes directly from the rLoop Test.

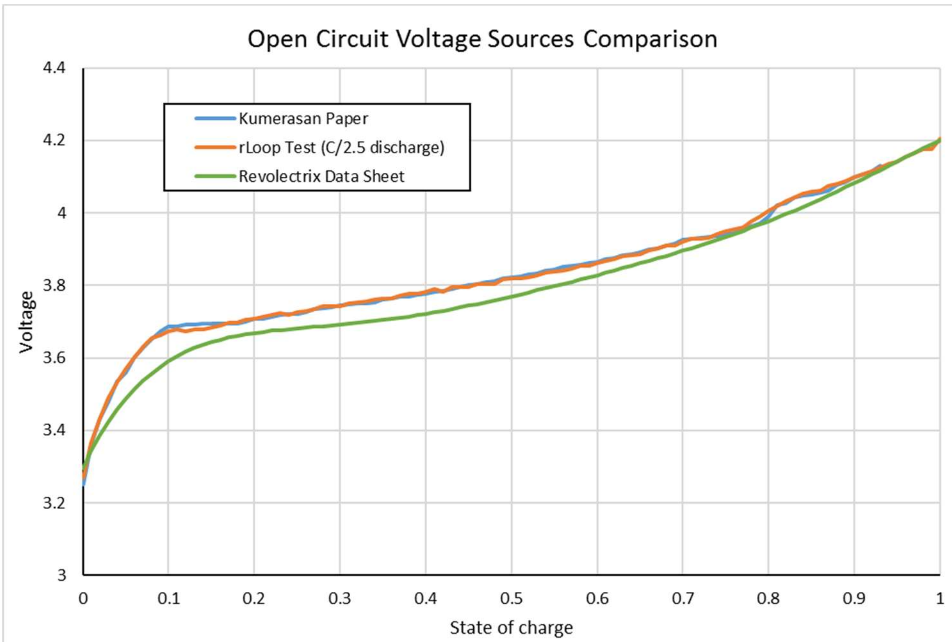


Figure 1. Cell OCV Curves from various sources

Cell discharge data from Revolectrix was used to calculate an expected OCV curve by comparing the discharge curves at two rates. This allows the calculation of both OCV and resistance at each point in the discharge. Although this OCV curve was not used in the model, the resultant resistance calculations were used. The curve below shows the raw data at 125A and 175A, the calculated OCV, and the calculated resistance. The fit is clamped at 0% DOD to 4.2V (the charge voltage), and the first five percent of the discharge is ignored to allow the dynamic response effects to eliminate out. The resistance curve shows a decreasing trend throughout the discharge which is expected as the cell heats up. An average between 5% and 80% is used for the resistance of the cell. This results in the assumed beginning of life resistance value of the cell R, about 1.2mΩ.

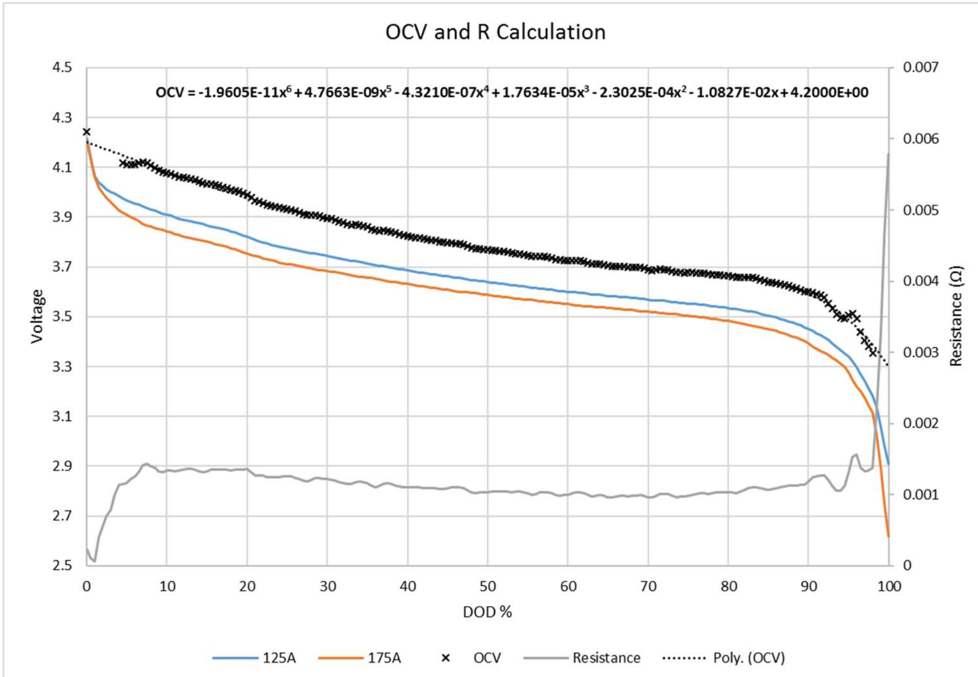


Figure 2. Cell OCV calculation from Revolectrix data

Additional data provided by the supplier gives information about the changes we should expect to resistance from temperature. Since we know the resistance of the cell at ambient, we can see the amount of voltage difference at the different temperatures, which must be attributed to changes in resistance. This gives us five data points which we can use to derive the constants for Equation 5. The Revolectrix provided data then gives us a beginning of life resistance value, an expected OCV curve, and the temperature sensitivity of resistance.

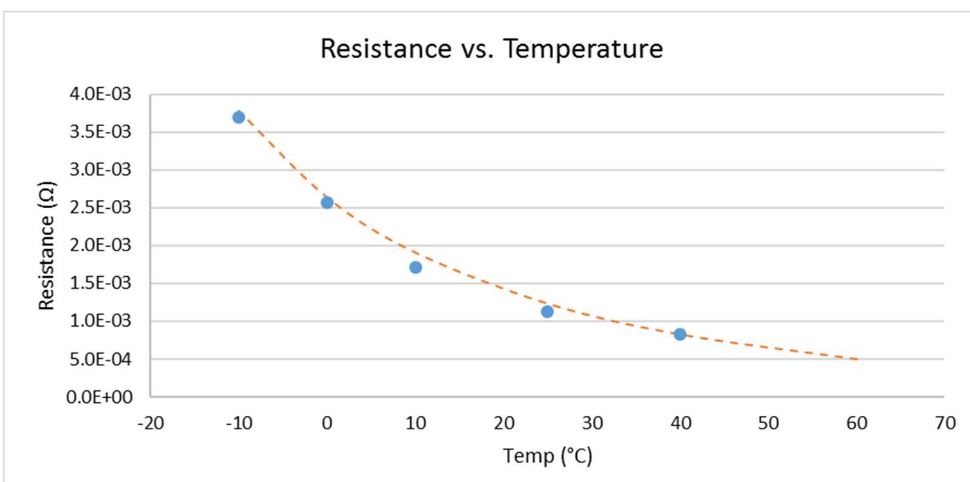


Figure 3. Resistance vs. Temperature Relationship

An actual 2A discharge curve has been used as the source for the OCV curve put into the model. The 2A curve is appropriate because it is a relatively slow discharge compared to the actual current capabilities of the cell (cell is rated for 300A continuous discharge). There is a small drop in voltage upon starting the 2A discharge, about 10 mV, which will be assumed to be negligible.

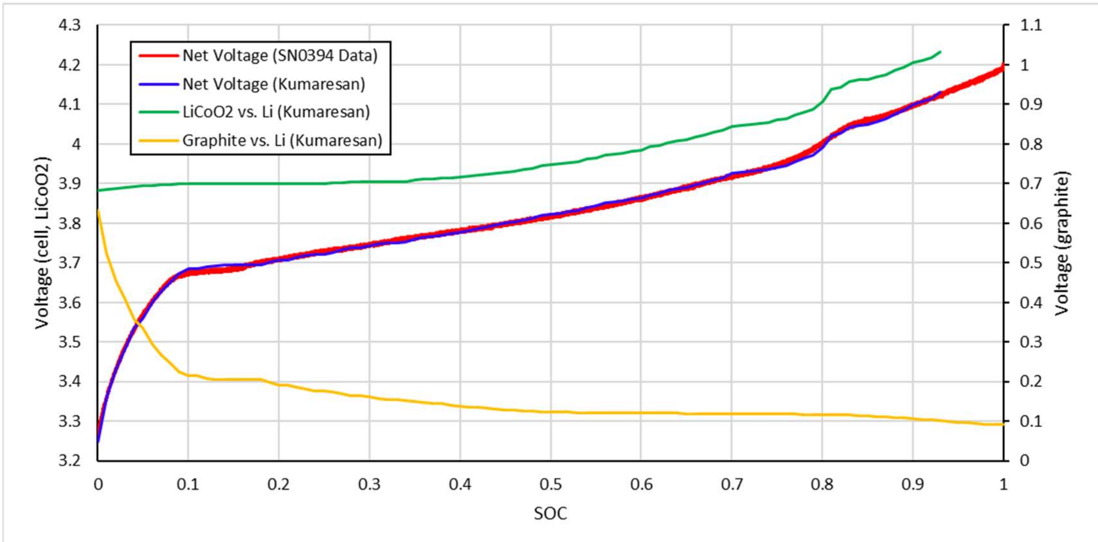


Figure 4. OCV Curve: actual low rate discharge vs literature curve

The shape of this curve is very similar to that of a LiCoO2/Graphite system, so a paper by Kumerasan et al was used to verify the cell chemistry. The curves in the Kumerasan paper were extracted and used to determine the lithium fraction in either electrode such that the resulting OCV curve from Kumerasan would match the SN0394 discharge. The resulting fit is excellent. Knowing the electrode chemistry and the lithium fraction in each electrode, we can extract the entropy change curve dV/dT, an important component to the internal cell heat generation. The cell's capacity was determined directly from the measured capacity out of the cell during the discharge.

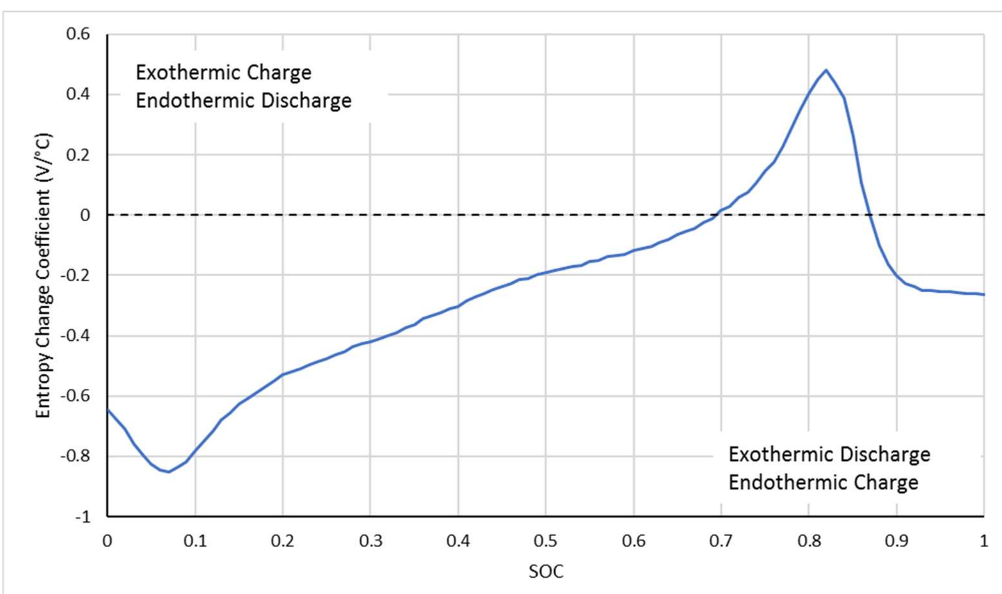


Figure 5. Entropy change coefficient curve

The cell's mass was measured on a single cell, and the heat capacity was approximated as 1 J/g/K, from a cursory literature search. A 1999 paper by Maleki et al cites heat capacity as 1.04 +/- 0.02 J/g/K at mid SOC for a cell of similar chemistry.

Parameter	Value	Units
Resistance at 0°C	2.6	mΩ
Resistance at 25°C	1.2	mΩ
Resistance at 40°C	0.8	mΩ
Cell capacity	4.8	Ah
Mass of cell	138	g
Specific heat capacity	1	J/g/K

Sources:

- **Revolectrix data sheet:** FB-8645152XT-5000 (Cell Curve).pdf
  https://drive.google.com/drive/folders/0B8eWgH3l5E2LZWlVVnZFaTdPc0k
- **Kumerasan et al**: 2008 thermal model for a li-ion cell kumaresan sikha whi te.pdf
  https://drive.google.com/drive/folders/0B8eWgH3l5E2LZWlVVnZFaTdPc0k
- **OCV and entropy curve analysis:** Revolectrix Cell Characterization.xlsx
  https://drive.google.com/drive/folders/0Bz9CbhgsXuIVM2lCZ3kxNXpoVnc
- **Raw SN0394 file, cycle 1, 10/4/2016:** SN0394C01D.csv
  https://drive.google.com/drive/folders/0Bz9CbhgsXuIVSGRCajE0R2syQnc
- **Specific Heat Capacity:** Maleki et al
  http://jes.ecsdl.org/content/146/3/947.abstract

Phase Change Material Characterization

There are some important unknown variables for the PCM system: the thermal resistance from the cell to the PCM and the mass of the PCM. Although the PCM bags can easily be weighted, it is not known the exact amount of material that successfully participates in the phase change reaction. For these issues, a test was devised that would allow the extraction of the parameters.

A PCM bag was heated in an oven to 60°C, then transferred to a room temperature cell, while both temperatures of the cell and the PCM were tracked. Upon transferring the PCM to the cell, the test article is wrapped in insulation to minimize losses to ambient. The cell immediately warms up and the PCM cools down. The cell/PCM combo eventually equalize in temperature and the whole article cools down to ambient. The cell temperature data can be fit to the model with the mass and thermal resistance as parameters to be fit. Equations 5, 6 and 7 are used. The resulting fit is very good for the cell temperature data, giving confidence in the model's ability to capture the thermal dynamics of the system.

Two of these tests were conducted, one with and one without thermal grease between the PCM and the cell. The grease greatly improves thermal resistance (we want lower to more efficiently transfer heat). Thermal grease was used in the construction of the battery pack, so we can expect the actual thermal resistance to be close to 1 K/W in the optimistic case, and 8 K/W in the worst case.

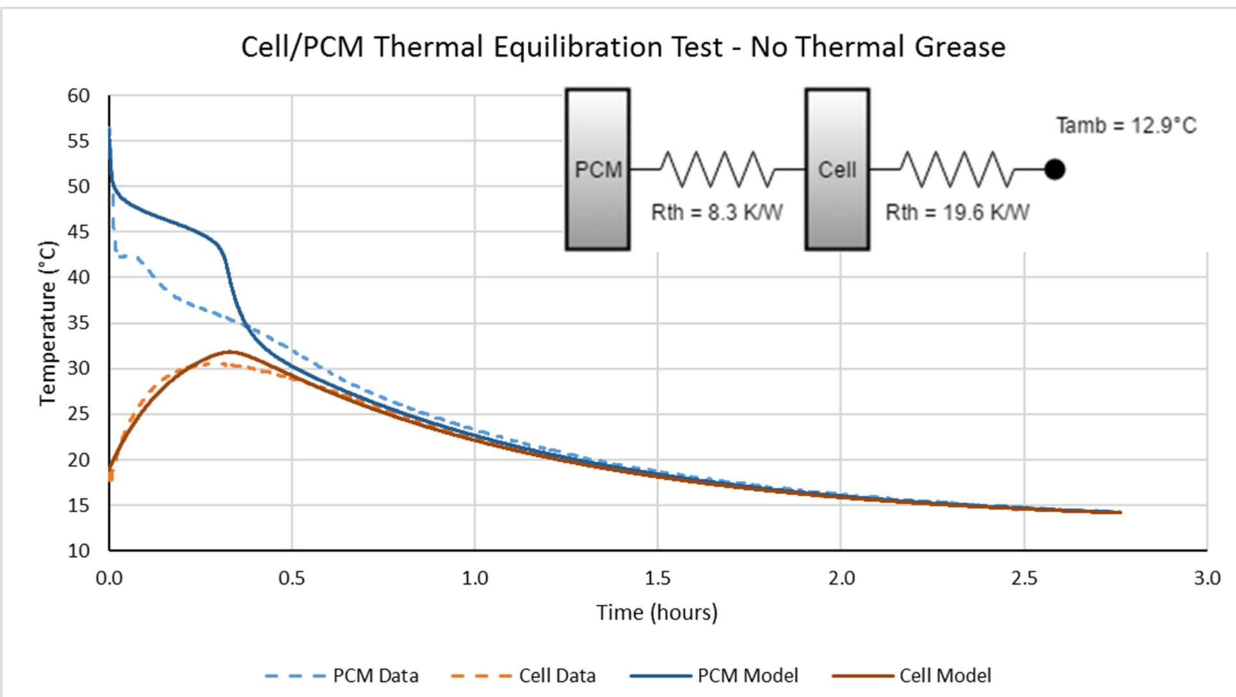


Figure 6. PCM Equilibration test without thermal grease

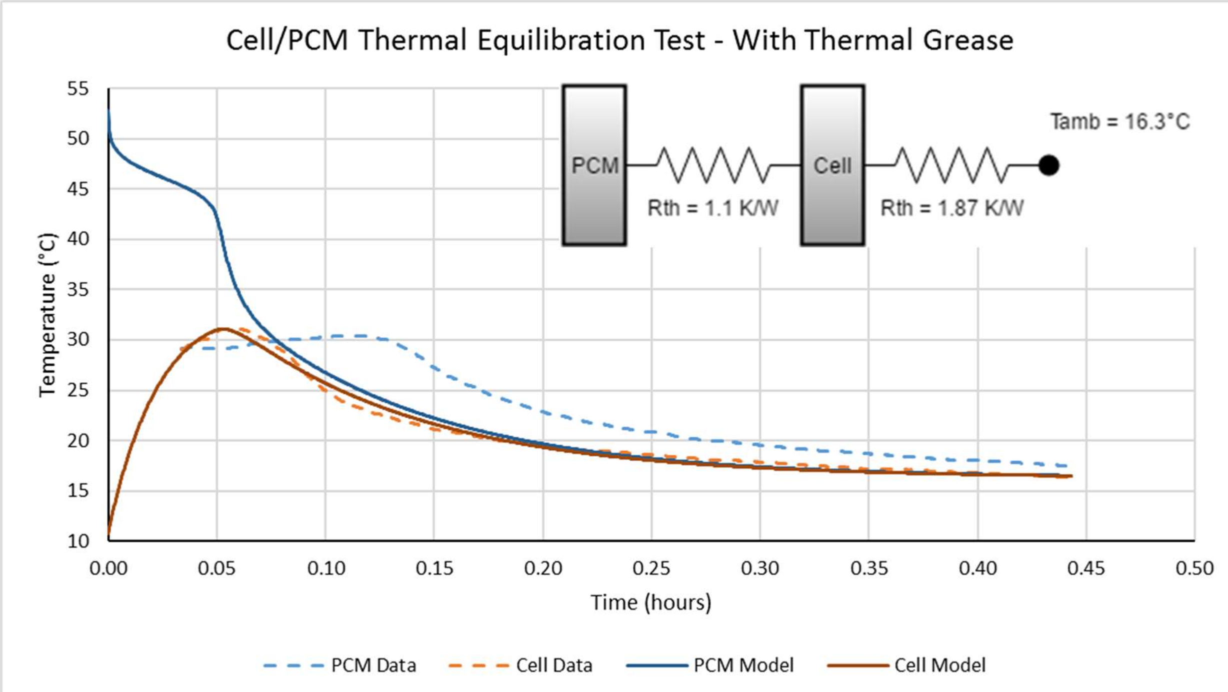


Figure 7. PCM Equilibration test with thermal grease

Some parameter values are obtained by supplier data; the material chosen is PlusICE A44.

Parameter	**Value**	**Units**
Specific Heat Capacity	2.1	J/g/°C
Latent Heat Capacity	242	J/g
Temperature Range (est)	2.5	°C
Melting Temperature	46.7	°C
Thermal Resistance (w grease)	1	K/W
Thermal Resistance (w/o grease)	8	K/W
PCM Mass	12	g

Sources:

- **Specific Heat Capacity and Latent Heat Capacity:** PCM Product Data sheet http://www.pcmproducts.net/files/PlusICE%20Range-2013.pdf
- **Temp Range and Melting Temperature:** A44 1609010 DSC.pdf https://drive.google.com/drive/folders/0B8eWgH3l5E2LZWlVVnZFaTdPc0k
- **Thermal Equilibration Test Analysis:** PCM Thermal Equilibration https://drive.google.com/drive/folders/0Bz9CbhgsXuIVM2lCZ3kxNXpoVnc

Test Validation

At this point, all variables have been explained except for the cell's aging factor, sensor time constant and thermal resistance to environment.

We start with a discharge simulation at 0.05Ω, using an aging factor of 1. We simply compare the resulting voltage curve to the real cell, and recognize that using an aging factor of 1 is likely incorrect due to the near constant offset error in voltage. An aging factor of 1.5 works much better and it was found to work in all tested cells, so we set aging factor to 1.5. It is expected that battery resistance will increase consistently from manufacture.

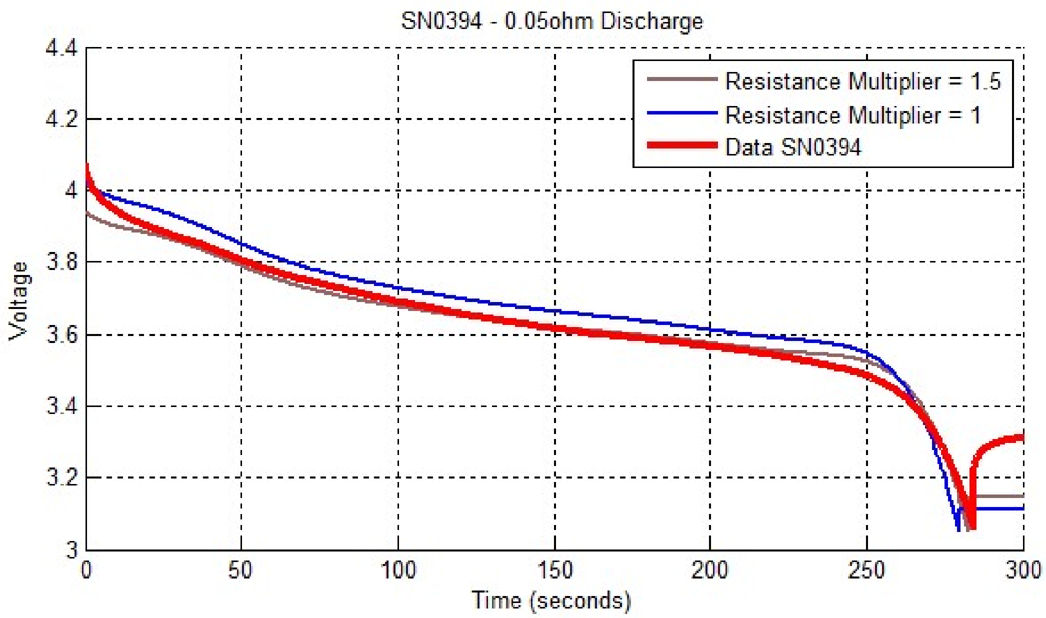


Figure 8. Determination of aging factor

For the thermal resistance to the environment, we run a 2A discharge simulation with infinite thermal resistance to environment. We can then compare the temperature data between model and measured. The real thermal behavior of the cell shows miniscule temperature growth, but the simulation shows a large increase, this is because there is no heat loss to the environment. The thermal resistance to environment was set to 3 K/W which worked well in all simulations and matches the cooldown rate post discharge.

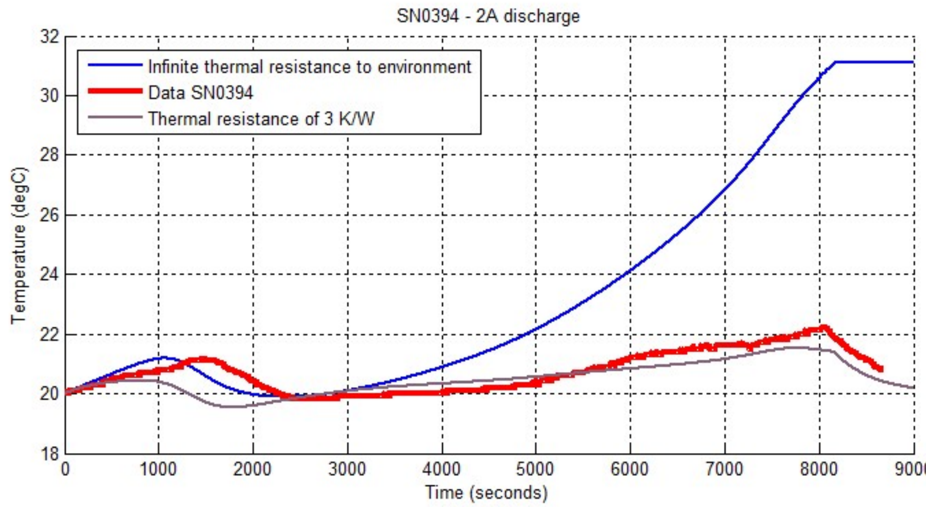


Figure 9. Determination of thermal resistance to ambient

Finally, the sensor time constant comes into play only in very fast discharges such as the 0.05Ω test. The parameters stated above do a great job explaining the temperature rise in all discharges except 0.05Ω. The model overestimates heat rise in the 0.05Ω case, which is attributed to a sensor delay. Here, the sensor delay time constant was set to 50 seconds.

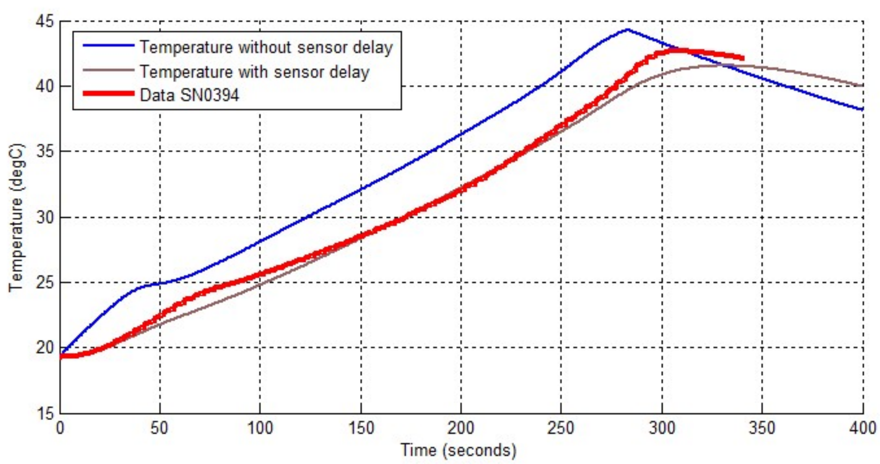


Figure 10. Determination of sensor time constant

More simulation results are available here:
https://docs.google.com/presentation/d/1bSJ4OxiEgkDRgei6fAR8L4aMIbpwTWnb_z2Rq9GSsbE/edit?usp=sharing

Parameter	**Value**	**Units**
Aging factor	1.5	Unitless
Thermal resistance to ambient	3	K/W
Sensor Time Constant	50	seconds

Use Case Simulation

The primary motivation behind this modeling activity was to predict cell performance in an environment that cannot be easily tested with available equipment. We seek to avoid thermal limits while providing sufficient power to pod for the required amount of time. The most aggressive test performed is a 0.05Ω discharge for a single cell in an open ambient air environment, however this is limited due to:

- Discharge condition in pod usage will be constant power, not constant resistance. This will have the effect of increasing current as the discharge progresses, unlike in the resistor discharge test. This will mean lower run time and more heating.
- The thermal environment in the pod will not be the same as the thermal environment in the test area. The worst case situation is a cell in the middle of the center module, which will have less heat sinking capabilities than the test condition. This will mean more heating.

Here we will run two simulations side by side, comparing the test condition and the pod run condition. We will assume a single pack and a 28kW constant power load. This is equivalent to 260W load on a single cell.

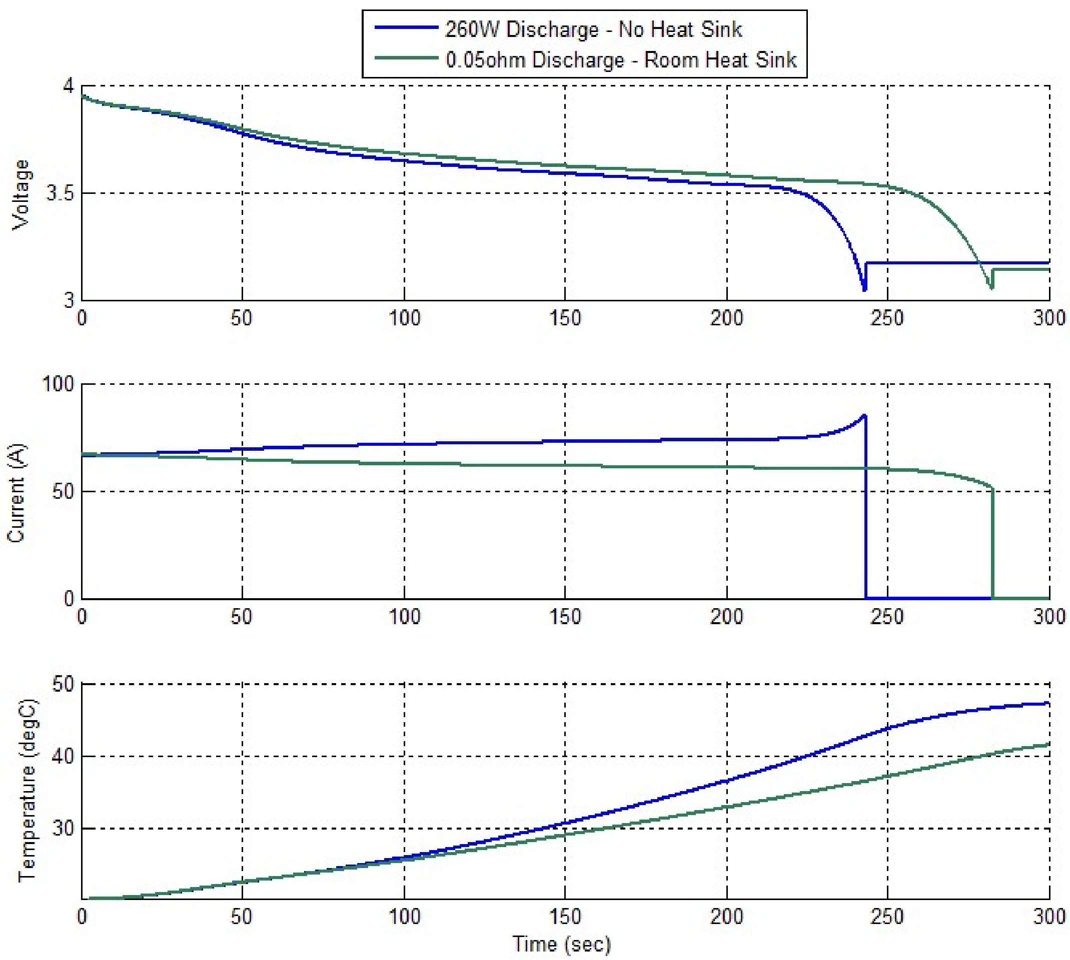


Figure 11. Comparison between a cell level high rate test and an actual pod use case

Although the test and pod run conditions start at practically the same current level, we clearly see divergence between test and pod run condition. The actual use case is much more aggressive than the test that was performed. We get 240 seconds of run time vs. 280 seconds, and a temperature rise that is 6°C higher. So, although the tests were extremely valuable in terms of demonstrating capability and in terms of model development, the model should be used for any pod level calculations.

A secondary question is related to the highest starting temperature in which we can safely start the pod without reaching thermal limits. We assume infinite thermal resistance to environment (adiabatic worst case), a best case PCM thermal connection, and a 260W load. We start the pod discharge between 15°C and 50°C and plot the sensor time series. We can see that the PCM successfully hinders temperature growth for all scenarios below the PCM melting temperature. At 50°C starting temperature, the PCM is melted and thus does not help mitigate temperature rise.

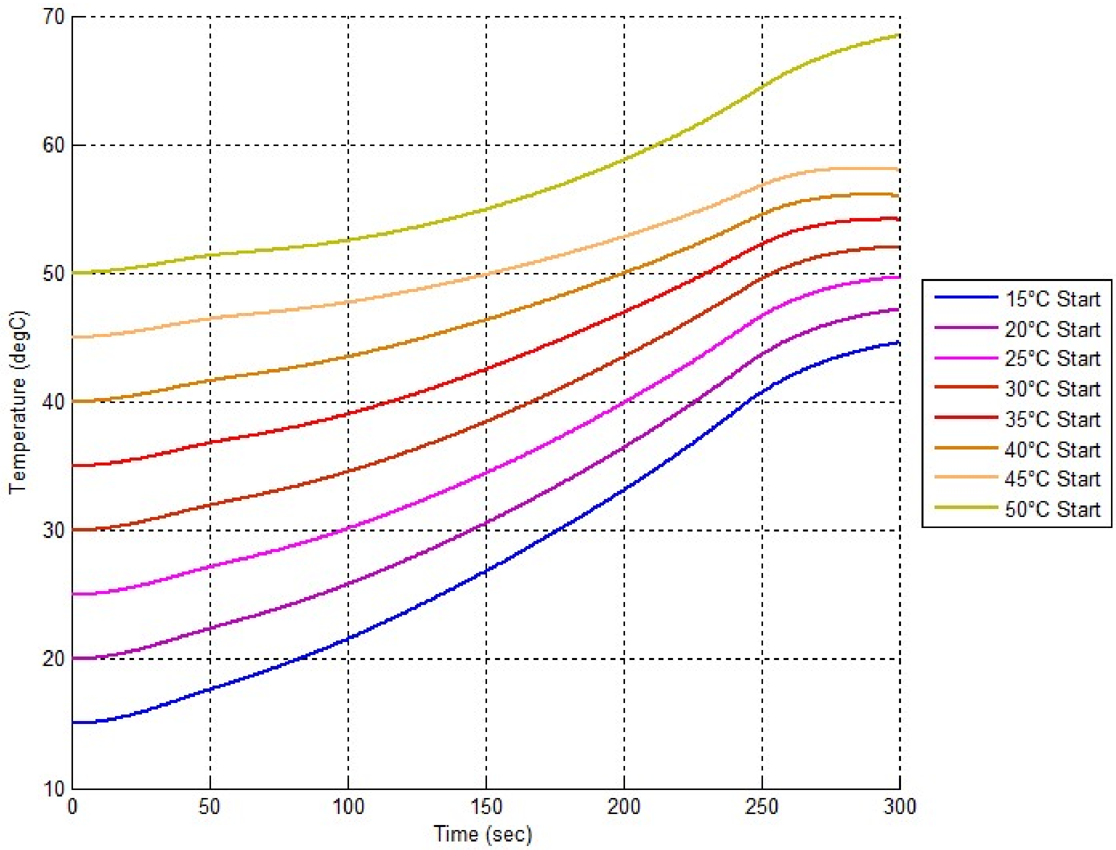


Figure 12. Family of simulation results with varying starting temperatures for pod use case

Battery maximum run time as a function of starting temperature can be plotted, by simulating all starting temperatures between 15°C and 50°C and extracting max run time based on voltage (3.2V limit) and temperature sensor (55°C limit). We can clearly see that below 40°C, the battery is limited by the amount of charge; above 40°C, the battery limited by temperature. It is also worthwhile simulating without the PCM, which shows us the improvement achieved by adding PCM.

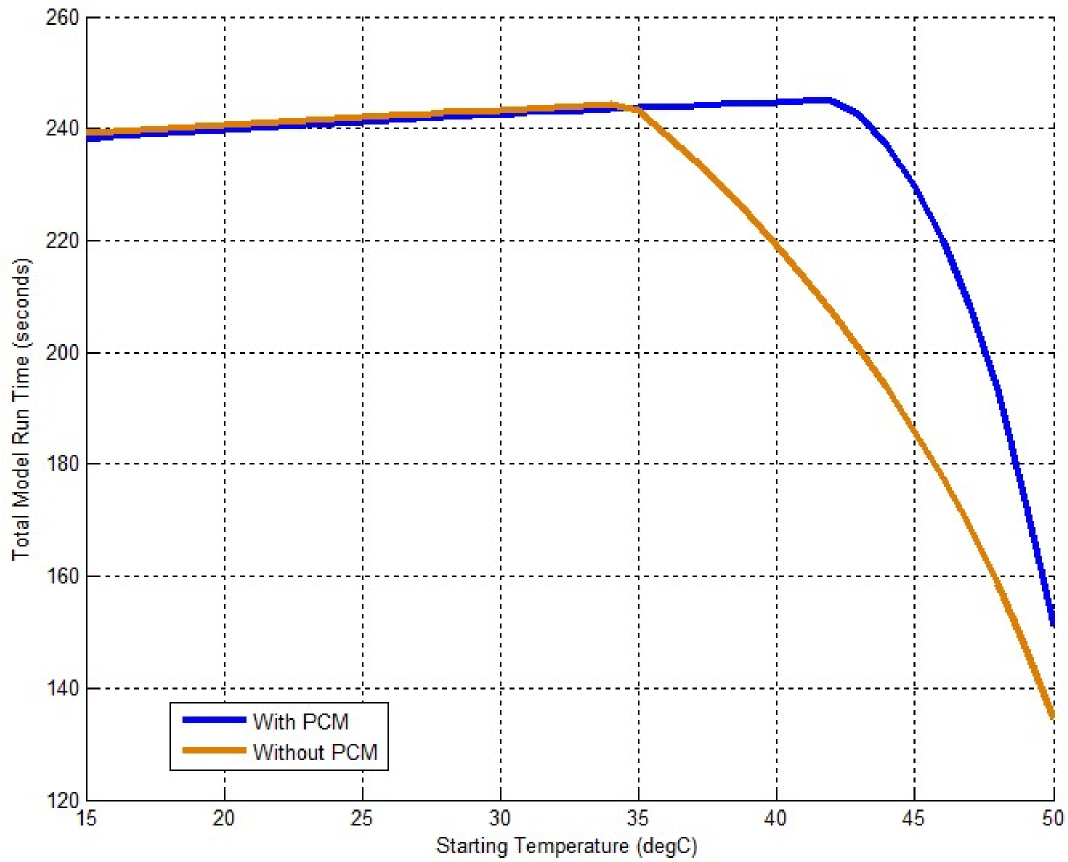


Figure 13. Total battery run time based on voltage and temperature limits

Many more questions can be answered with this model, but there are limitations:

- Transient voltage dynamics is not captured in the model. This is evident when looking at the first 10% of a discharge.
- There seem to be consistent errors in voltage curvature at low SOC, lower than 20%. This could be due to diffusion limits and these are very difficult to simulate. Additionally, cell aging will cause lower capacities over time. For power budget/run time calculations, always apply a margin of 10%-20% (for example, if run time in model is 240 seconds, it would be smart to plan a mission profile that uses 192 seconds instead).
- Over time, the cell will age, and the model will understate voltage drop and heat generation. Always calibrate model and real data whenever possible.
- Within the scenarios analyzed so far, there seems to be a maximum temperature error of +/- 5°C. For thermal calculations, apply a 5°C margin (if simulation outputs a maximum temperature of 50°C, expect up to a 55°C temperature in reality). This will be made worse with aging.

As always, models are not a substitute for testing. Stay skeptical of model results and always use in conjunction with recent validation data.

MATLAB/Octave usage guide

Ensure you have downloaded all files in the model folder on the Google Drive into a local folder. The model can be run using *"cell_sim_model_r1"*. No inputs are required. The model will default into a pod run condition (260W discharge, adiabatic condition, good PCM contact).

The output plots will show voltage, current, and temperatures. The voltage plot shows both actual cell voltage and OCV. The temperature plot shows cell temperature, sensor temperature, and PCM temperature.

To make any changes to conditions, simply change them in the command line and rerun model. For instance, if you want to turn off PCM, set the thermal resistance for the PCM to infinity. This will overwrite the default settings.

```
>>resistThPCM = Inf;
>>cell_sim_model_r1;
```

The model will look for discharge conditions in *loadPower, loadCurrent, loadResist*. Set any one of them to the desired value, but ensure all others are zero to avoid confusion.

The model refers to a parameter set matrix that is loaded from *"parameterSet.mat"*. The first row is the default run condition, and if you would like to run other conditions, change *paramChoice* to the appropriate row. Currently the other parameter sets will load real test data to compare model outputs with. You can use "*ModelAllParam*" to run through all the simulations in the parameter set.

Below is a partial list of simulation parameters to explore:

Variable Name	Symbol	Equation #	Default value	Notes
`loadPower`	P	2	260 W	Constant power condition
`loadCurrent`	I	1	0	Constant current condition
`loadResist`	R_L	3	0	Constant resistance condition
`resistMultiplier`	f	5	1.5	Increase in case of cell aging
`cellCap`	Q (max)	4	17280 C (4.8 Ah)	Lower in case of cell aging
`resistThAmb`	$R_{th\infty}$	6	Inf	Set to 3 K/W for open ambient air condition
`resistThPCM`	R_{thP}	7	1 K/W	Set to 8 K/W for worst case, set to Inf to turn off PCM
`tempAmb`	T_∞	6	20°C	Ambient temperature
`tempCellInit`	T	6	20°C	Starting cell temperature
`tempPCMInit`	T_P	7	20°C	Starting PCM temperature
`DODInit`	Q (at t=0)	4	0 (full charge)	Can be set for any state of charge
`timeTot`				Increase for more simulation time